Full wwPDB EM Validation Report (i)

Jul 13, 2024 – 01:04 PM EDT

PDB ID	:	8TOW
EMDB ID	:	EMD-41460
Title	:	Structure of a mutated photosystem II complex reveals perturbation of the oxygen-evolving complex
Authors	:	Flesher, D.A.; Liu, J.; Wang, J.; Gisriel, C.J.; Yang, K.R.; Batista, V.S.; Debus, R.J.; Brudvig, G.W.
Deposited on	:	2023-08-04
Resolution	:	2.14 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:

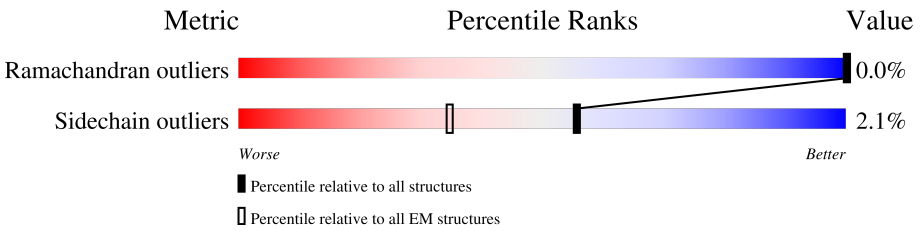
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.14 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	92% • 7%
1	a	360	92% • 7%
2	B	507	98% •
2	b	507	98% •
3	C	460	5% 96% • •
3	c	460	5% 96% • •
4	D	352	96% • •
4	d	352	96% • •
5	E	81	6% 94% • •

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Mol	Chain	Length	Quality of chain
5	e	81	6% 94%
6	F	44	5% 80% 20%
6	f	44	5% 80% 20%
7	H	64	95%
7	h	64	95%
8	I	38	5% 92% 5%
8	i	38	5% 92% 5%
9	J	39	18% 100%
9	j	39	18% 100%
10	K	45	76% 7% 18%
10	k	45	76% 7% 18%
11	L	39	97%
11	l	39	97%
12	M	35	83% 6% 11%
12	m	35	83% 6% 11%
13	O	274	14% 86% 11%
13	o	274	14% 86% 11%
14	Q	149	54% 77% 21%
14	q	149	53% 77% 21%
15	R	39	33% 85% 13%
15	r	39	33% 85% 13%
16	T	31	94%
16	t	31	94%
17	U	131	13% 69% 27%
17	u	131	13% 69% 27%

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Mol	Chain	Length	Quality of chain
18	V	160	6% 80% 16%
18	v	160	6% 80% 16%
19	X	39	5% 95%
19	x	39	5% 95%
20	Y	39	13% 77% 5% 18%
20	y	39	15% 77% 5% 18%
21	Z	62	44% 97%
21	z	62	42% 97%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	A	408	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	C	514	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	a	408	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	513	X	-	-	-
25	CLA	c	514	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 54914 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 II protein D1 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	334	2640	1728	431	466	15	2	0
1	a	334	2640	1728	431	466	15	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	GLU	ASP	conflict	UNP P16033
a	170	GLU	ASP	conflict	UNP P16033

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	506	3958	2584	662	699	13	0	0
2	b	506	3958	2584	662	699	13	0	0

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	450	3493	2293	584	603	13	0	0
3	c	450	3493	2293	584	603	13	0	0

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	341	2726	1807	443	464	12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	341	2726	1807	443	464	12	0	0

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	78	645	419	104	121	1	0	0
5	e	78	645	419	104	121	1	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	35	279	189	46	43	1	0	0
6	f	35	279	189	46	43	1	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	63	494	328	79	85	2	0	0
7	h	63	494	328	79	85	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	37	297	201	46	49	1	0	0
8	i	37	297	201	46	49	1	0	0

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	39	279	188	43	46	2	0	0
9	j	39	279	188	43	46	2	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	K	37	299	210	42	47	0	0
10	k	37	299	210	42	47	0	0

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	39	316	204	54	57	1	0	0
11	l	39	316	204	54	57	1	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	31	245	169	36	39	1	0	0
12	m	31	245	169	36	39	1	0	0

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	243	1873	1186	305	379	3	0	0
13	o	243	1873	1186	305	379	3	0	0

- Molecule 14 is a protein called Sll1638 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Q	118	911	573	163	173	2	0	0
14	q	118	911	573	163	173	2	0	0

- Molecule 15 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	34	Total 258	C 170	N 45	O 43	0	0
15	r	34	Total 258	C 170	N 45	O 43	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total 241	C 163	N 36	O 40	S 2	0	0
16	t	30	Total 241	C 163	N 36	O 40	S 2	0	0

- Molecule 17 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	U	95	Total 740	C 461	N 123	O 156	0	0
17	u	95	Total 740	C 461	N 123	O 156	0	0

- Molecule 18 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	135	Total 1065	C 665	N 179	O 218	S 3	0	0
18	v	135	Total 1065	C 665	N 179	O 218	S 3	0	0

- Molecule 19 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	38	Total 288	C 193	N 46	O 48	S 1	0	0
19	x	38	Total 288	C 193	N 46	O 48	S 1	0	0

- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	32	Total 242	C 165	N 37	O 40	0	0

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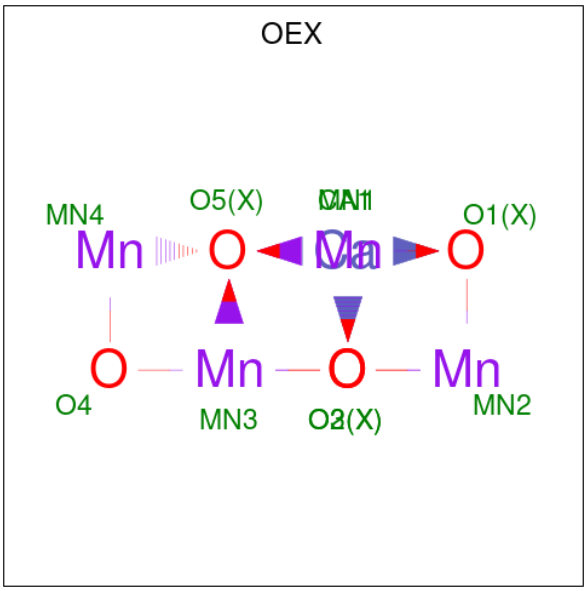
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	y	32	242	165	37	40	0	0

- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Z	60	460	317	70	72	1	0	0
			Total	C	N	O	S		
21	z	60	460	317	70	72	1	0	0

- Molecule 22 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
22	A	1	10	1	4	5	0
			Total	Ca	Mn	O	
22	a	1	10	1	4	5	0

- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
23	A	1	1	1	0

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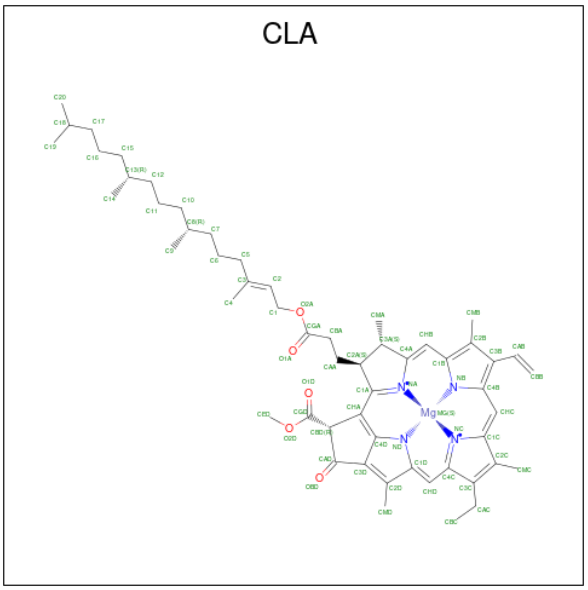
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
23	a	1	1	1	0

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
24	A	2	2	2	0
			Total	Cl	
24	a	2	2	2	0

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
25	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
25	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	B	1	65	55	1	4	5	0

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
25	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	D	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	a	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
25	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms	AltConf
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 65 55 1 4 5	0
25	b	1	Total C Mg N O 60 50 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 55 45 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	c	1	Total C Mg N O 50 40 1 4 5	0
25	c	1	Total C Mg N O 65 55 1 4 5	0
25	d	1	Total C Mg N O 65 55 1 4 5	0
25	d	1	Total C Mg N O 65 55 1 4 5	0

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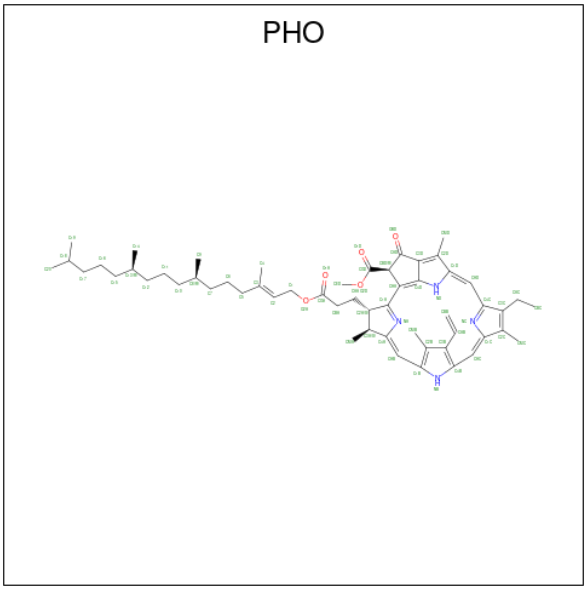
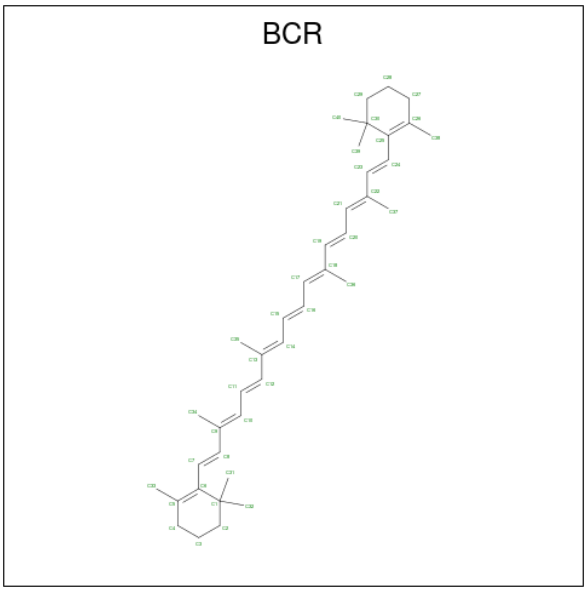
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	d	1	65	55	1	4	5	0

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	A	1	64	55	4	5	0
26	D	1	64	55	4	5	0
26	a	1	64	55	4	5	0
26	d	1	64	55	4	5	0

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
27	A	1	40	40	0
27	B	1	40	40	0
27	B	1	40	40	0
27	B	1	40	40	0
27	C	1	40	40	0
27	F	1	40	40	0
27	K	1	40	40	0
27	K	1	40	40	0
27	Z	1	40	40	0
27	a	1	40	40	0
27	b	1	40	40	0
27	b	1	40	40	0
27	b	1	40	40	0
27	c	1	40	40	0

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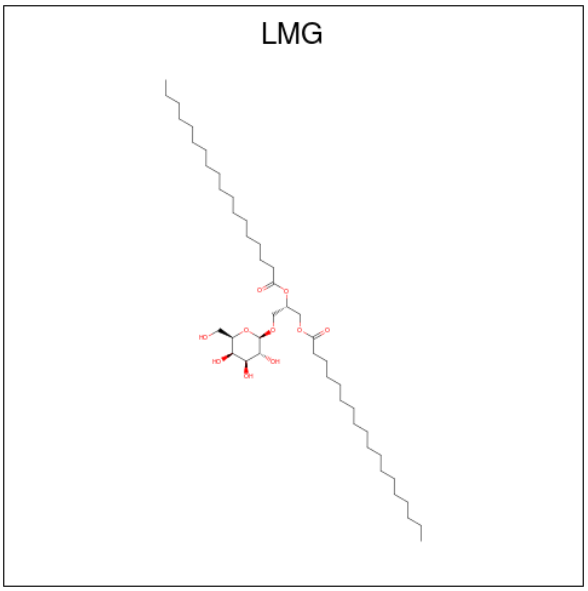
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
27	f	1	40	40	0
			Total	C	
27	k	1	40	40	0
			Total	C	
27	k	1	40	40	0
			Total	C	
27	z	1	40	40	0

- 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	A	1	51	41	10	0
			Total	C	O	
28	A	1	36	26	10	0
			Total	C	O	
28	B	1	51	41	10	0
			Total	C	O	
28	C	1	51	41	10	0
			Total	C	O	
28	C	1	49	39	10	0
			Total	C	O	
28	D	1	44	34	10	0
			Total	C	O	
28	H	1	47	37	10	0

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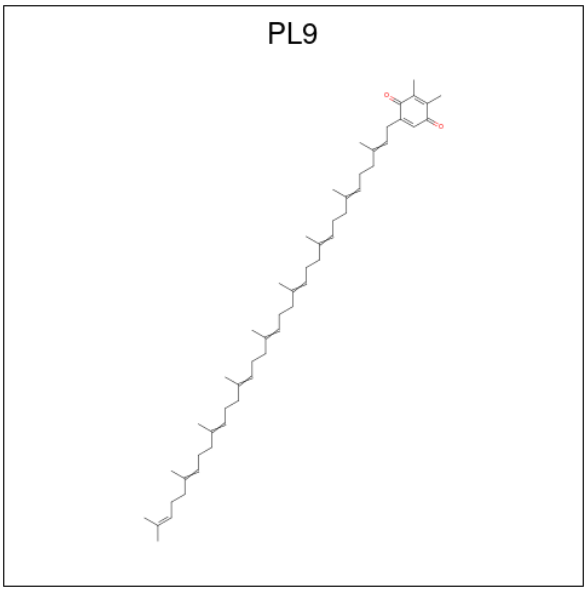
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	a	1	51	41	10	0
28	a	1	36	26	10	0
28	b	1	51	41	10	0
28	c	1	51	41	10	0
28	c	1	49	39	10	0
28	d	1	44	34	10	0
28	h	1	47	37	10	0

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	A	1	55	53	2	0
29	D	1	55	53	2	0
29	a	1	55	53	2	0

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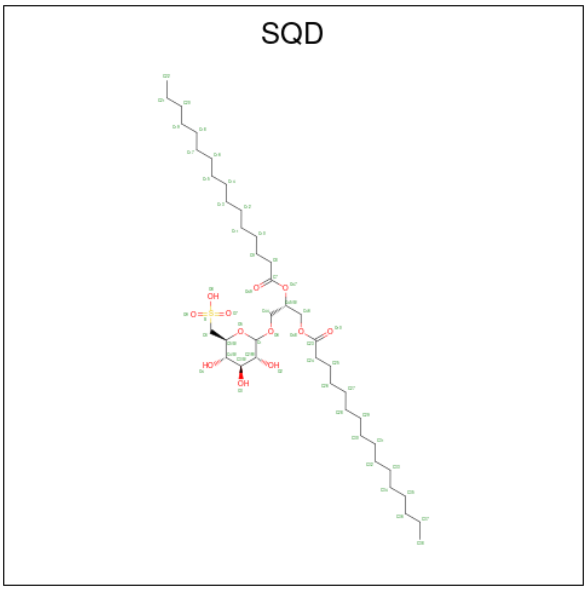
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	d	1	55	53	2	0

- Molecule 30 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	
30	A	1	54	41	12	1	0
			Total	C	O	S	
30	A	1	48	35	12	1	0
			Total	C	O	S	
30	B	1	54	41	12	1	0
			Total	C	O	S	
30	C	1	54	41	12	1	0
			Total	C	O	S	
30	F	1	34	21	12	1	0
			Total	C	O	S	
30	H	1	54	41	12	1	0
			Total	C	O		
30	K	1	41	32	9		0
			Total	C	O	S	
30	a	1	54	41	12	1	0
			Total	C	O	S	
30	a	1	48	35	12	1	0
			Total	C	O	S	
30	b	1	54	41	12	1	0

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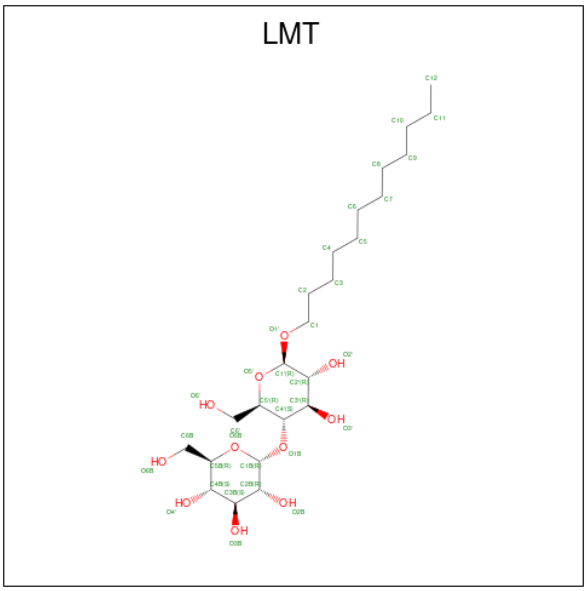
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
30	c	1	54	41	12	1	0
			Total	C	O	S	
30	f	1	34	21	12	1	0
			Total	C	O	S	
30	h	1	54	41	12	1	0
			Total	C	O		
30	k	1	41	32	9		0

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



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	A	1	35	24	11	0
			Total	C	O	
31	A	1	24	18	6	0
			Total	C	O	
31	B	1	35	24	11	0
			Total	C	O	
31	B	1	24	18	6	0
			Total	C	O	
31	B	1	35	24	11	0
			Total	C	O	
31	B	1	24	18	6	0
			Total	C	O	
31	B	1	35	24	11	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	C	1	24	18	6	0
			Total	C	O	
31	C	1	35	24	11	0
			Total	C	O	
31	C	1	21	15	6	0
			Total	C	O	
31	D	1	24	18	6	0
			Total	C	O	
31	D	1	35	24	11	0
			Total	C	O	
31	D	1	35	24	11	0
			Total	C	O	
31	E	1	22	16	6	0
			Total	C	O	
31	E	1	35	24	11	0
			Total	C	O	
31	F	1	35	24	11	0
			Total	C	O	
31	H	1	24	18	6	0
			Total	C	O	
31	I	1	24	18	6	0
			Total	C	O	
31	I	1	24	18	6	0
			Total	C	O	
31	I	1	35	24	11	0
			Total	C	O	
31	I	1	22	16	6	0
			Total	C	O	
31	J	1	24	18	6	0
			Total	C	O	
31	K	1	35	24	11	0
			Total	C	O	
31	M	1	35	24	11	0
			Total	C	O	
31	M	1	24	18	6	0
			Total	C	O	
31	T	1	24	18	6	0
			Total	C	O	
31	X	1	24	18	6	0
			Total	C	O	
31	X	1	22	17	5	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	X	1	22	16	6	0
			Total	C	O	
31	X	1	19	13	6	0
			Total	C	O	
31	X	1	19	13	6	0
			Total	C	O	
31	Y	1	21	15	6	0
			Total	C	O	
31	a	1	35	24	11	0
			Total	C	O	
31	a	1	24	18	6	0
			Total	C	O	
31	b	1	35	24	11	0
			Total	C	O	
31	b	1	24	18	6	0
			Total	C	O	
31	b	1	35	24	11	0
			Total	C	O	
31	b	1	24	18	6	0
			Total	C	O	
31	b	1	35	24	11	0
			Total	C	O	
31	c	1	24	18	6	0
			Total	C	O	
31	c	1	35	24	11	0
			Total	C	O	
31	c	1	21	15	6	0
			Total	C	O	
31	d	1	24	18	6	0
			Total	C	O	
31	d	1	35	24	11	0
			Total	C	O	
31	d	1	35	24	11	0
			Total	C	O	
31	e	1	22	16	6	0
			Total	C	O	
31	e	1	35	24	11	0
			Total	C	O	
31	f	1	35	24	11	0
			Total	C	O	
31	h	1	24	18	6	0

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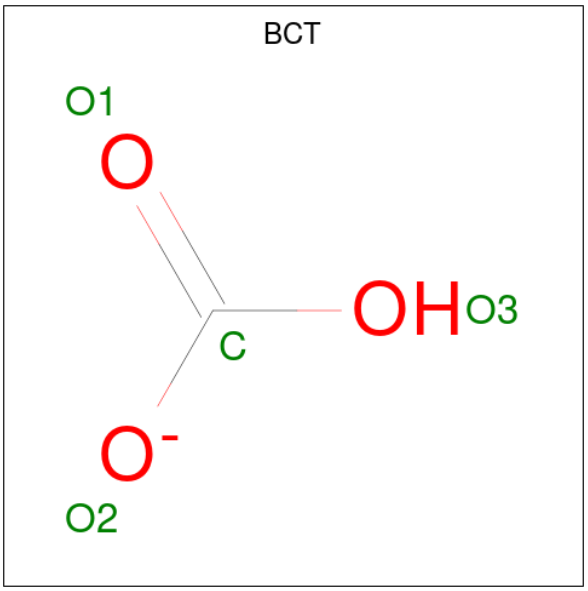
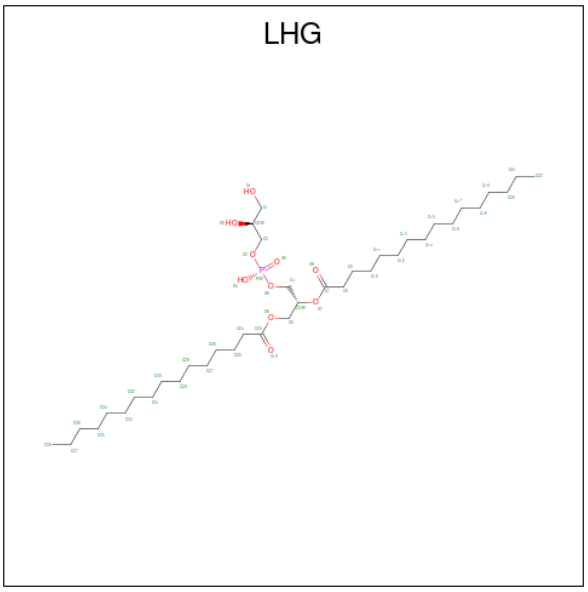
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	i	1	24	18	6	0
			Total	C	O	
31	i	1	24	18	6	0
			Total	C	O	
31	i	1	35	24	11	0
			Total	C	O	
31	i	1	22	16	6	0
			Total	C	O	
31	j	1	24	18	6	0
			Total	C	O	
31	k	1	35	24	11	0
			Total	C	O	
31	m	1	35	24	11	0
			Total	C	O	
31	m	1	24	18	6	0
			Total	C	O	
31	t	1	24	18	6	0
			Total	C	O	
31	x	1	24	18	6	0
			Total	C	O	
31	x	1	22	17	5	0
			Total	C	O	
31	x	1	22	16	6	0
			Total	C	O	
31	x	1	19	13	6	0
			Total	C	O	
31	x	1	19	13	6	0
			Total	C	O	
31	y	1	21	15	6	0

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	A	1	4	1	3	0
			Total	C	O	
32	a	1	4	1	3	0

- Molecule 33 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	
33	B	1	49	38	10	1	0

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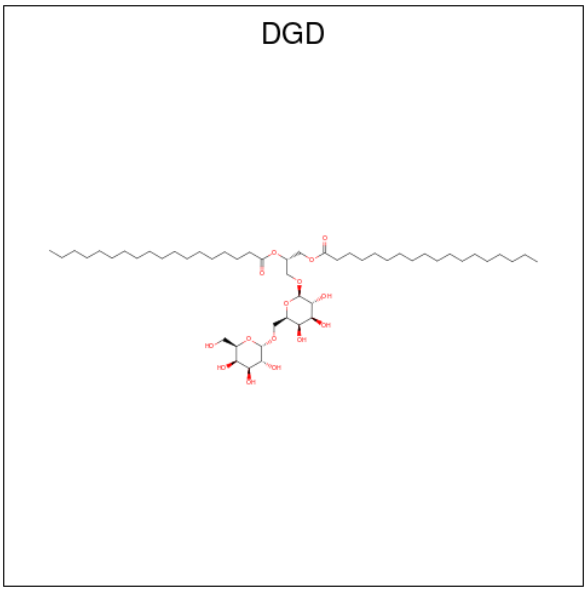
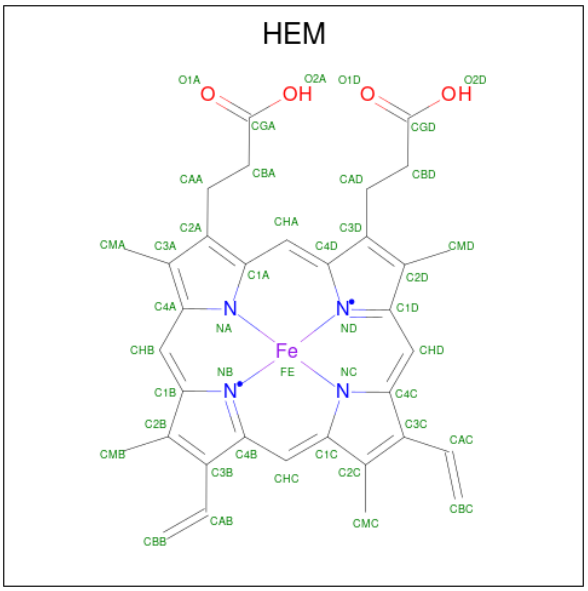
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	B	1	49	38	10	1	0
33	D	1	49	38	10	1	0
33	D	1	49	38	10	1	0
33	D	1	49	38	10	1	0
33	E	1	40	29	10	1	0
33	Z	1	36	27	8	1	0
33	b	1	49	38	10	1	0
33	b	1	49	38	10	1	0
33	d	1	49	38	10	1	0
33	d	1	49	38	10	1	0
33	d	1	49	38	10	1	0
33	e	1	40	29	10	1	0
33	z	1	36	27	8	1	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



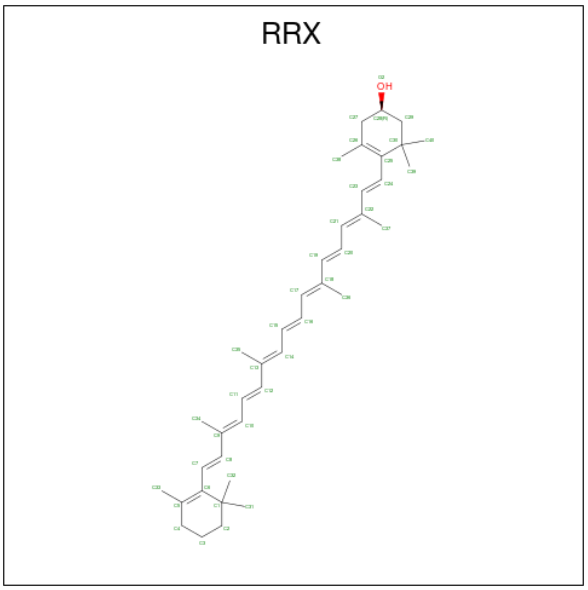
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	C	1	62	47	15	0
			Total	C	O	
34	C	1	62	47	15	0
			Total	C	O	
34	C	1	62	47	15	0
			Total	C	O	
34	H	1	62	47	15	0
			Total	C	O	
34	c	1	62	47	15	0
			Total	C	O	
34	c	1	62	47	15	0
			Total	C	O	
34	c	1	62	47	15	0
			Total	C	O	
34	h	1	62	47	15	0

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
35	E	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
35	V	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
35	e	1	43	34	1	4	4	0
			Total	C	Fe	N	O	
35	v	1	43	34	1	4	4	0

- Molecule 36 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	H	1	41	40	1	0
36	h	1	41	40	1	0

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
37	K	1	1	1	0
37	U	1	1	1	0
37	V	1	1	1	0
37	k	1	1	1	0
37	u	1	1	1	0
37	v	1	1	1	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
38	A	127	127	127	0
38	B	127	127	127	0
38	C	107	107	107	0
38	D	132	132	132	0
38	E	8	8	8	0
38	F	4	4	4	0
38	H	17	17	17	0
38	I	1	1	1	0
38	J	2	2	2	0
38	L	14	14	14	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
38	M	6	6	6	0
38	O	37	37	37	0
38	T	12	12	12	0
38	U	21	21	21	0
38	V	17	17	17	0
38	X	3	3	3	0
38	a	127	127	127	0
38	b	127	127	127	0
38	c	107	107	107	0
38	d	132	132	132	0
38	e	8	8	8	0
38	f	4	4	4	0
38	h	17	17	17	0
38	i	1	1	1	0
38	j	2	2	2	0
38	l	14	14	14	0
38	m	6	6	6	0
38	o	37	37	37	0
38	t	12	12	12	0
38	u	21	21	21	0
38	v	17	17	17	0

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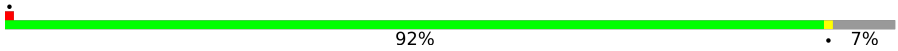
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
38	x	3	3	3	0

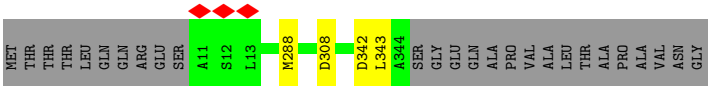
3 Residue-property plots (i)

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 II protein D1 2

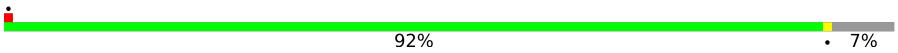
Chain A:

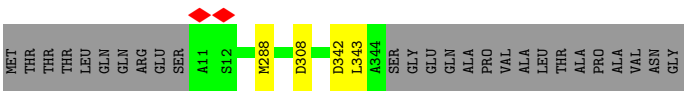




• Molecule 1: Photosystem II protein D1 2

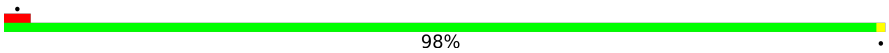
Chain a:

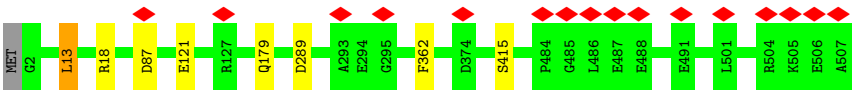




• Molecule 2: Photosystem II CP47 reaction center protein

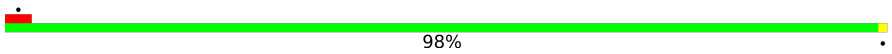
Chain B:

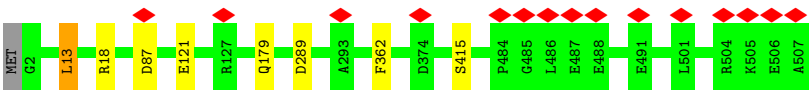




• Molecule 2: Photosystem II CP47 reaction center protein

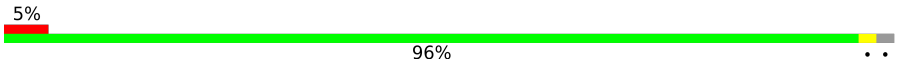
Chain b:

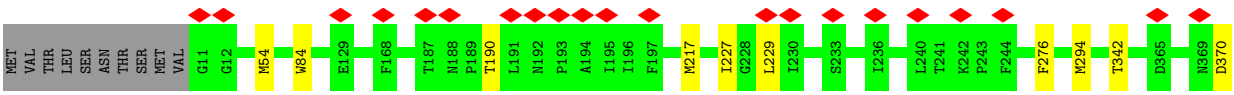




• Molecule 3: Photosystem II CP43 reaction center protein

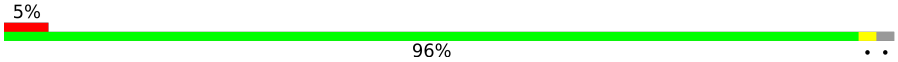
Chain C:

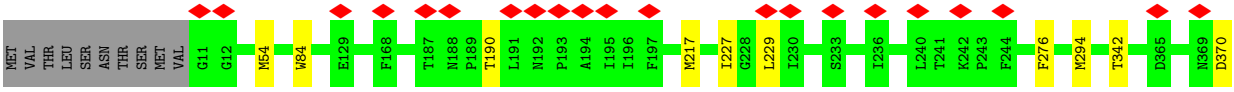




• Molecule 3: Photosystem II CP43 reaction center protein

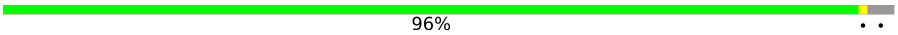
Chain c:

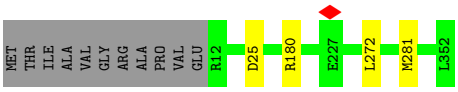




• Molecule 4: Photosystem II D2 protein

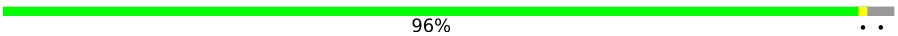
Chain D:

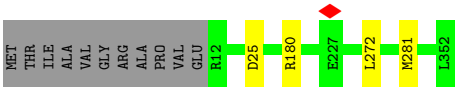




• Molecule 4: Photosystem II D2 protein

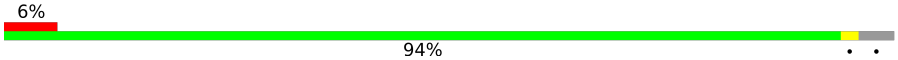
Chain d:

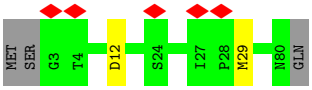




• Molecule 5: Cytochrome b559 subunit alpha

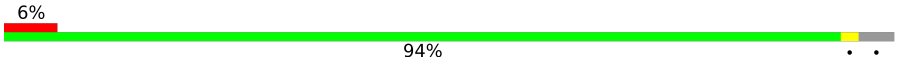
Chain E:

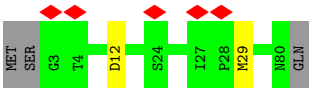




• Molecule 5: Cytochrome b559 subunit alpha

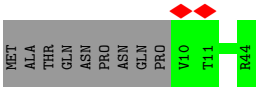
Chain e:





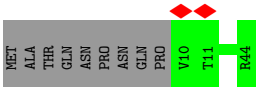
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



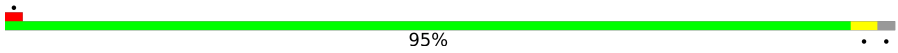
• Molecule 6: Cytochrome b559 subunit beta

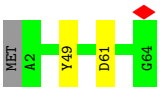
Chain f:



• Molecule 7: Photosystem II reaction center protein H

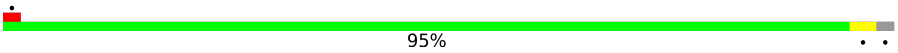
Chain H:





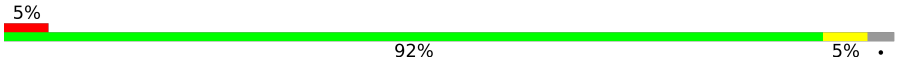
• Molecule 7: Photosystem II reaction center protein H

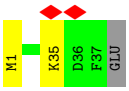
Chain h:



• Molecule 8: Photosystem II reaction center protein I

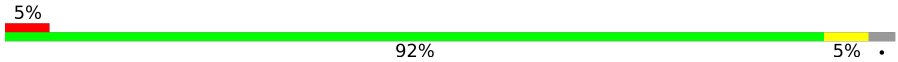
Chain I:

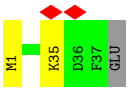




• Molecule 8: Photosystem II reaction center protein I

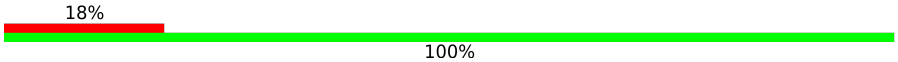
Chain i:

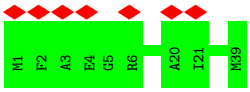




• Molecule 9: Photosystem II reaction center protein J

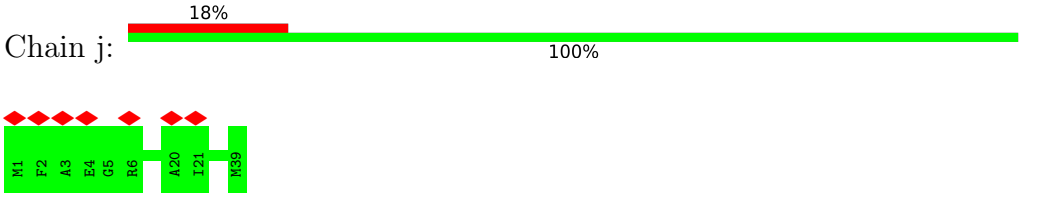
Chain J:





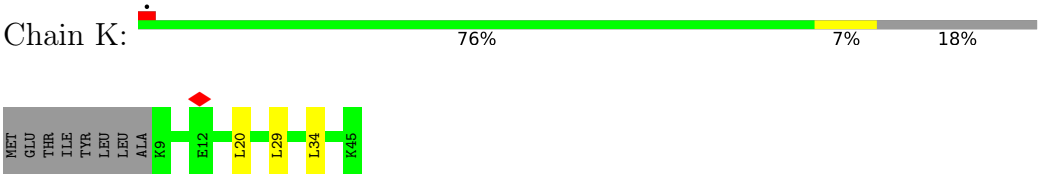
• Molecule 9: Photosystem II reaction center protein J

Chain j:



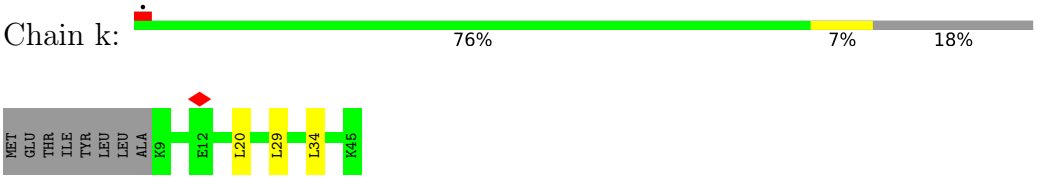
• Molecule 10: Photosystem II reaction center protein K

Chain K:



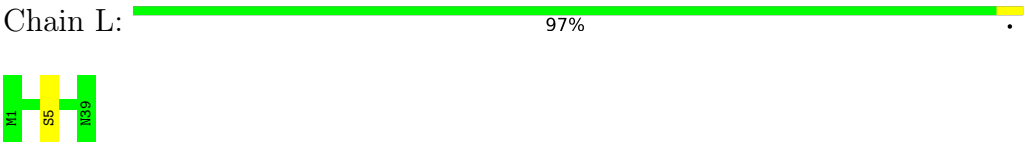
• Molecule 10: Photosystem II reaction center protein K

Chain k:



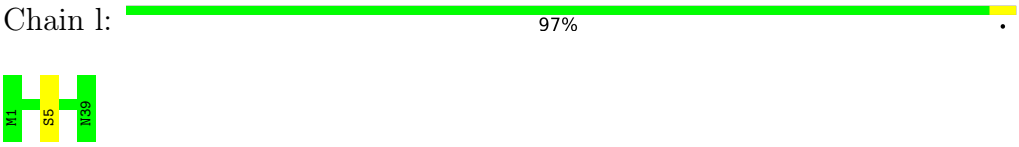
• Molecule 11: Photosystem II reaction center protein L

Chain L:



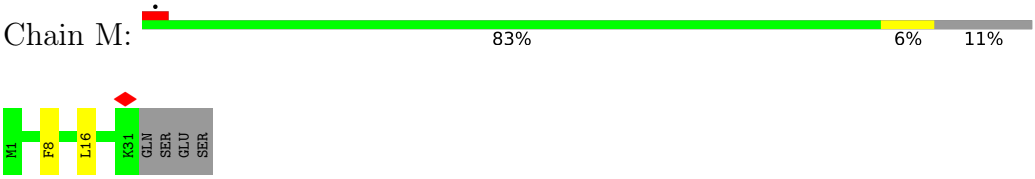
• Molecule 11: Photosystem II reaction center protein L

Chain l:



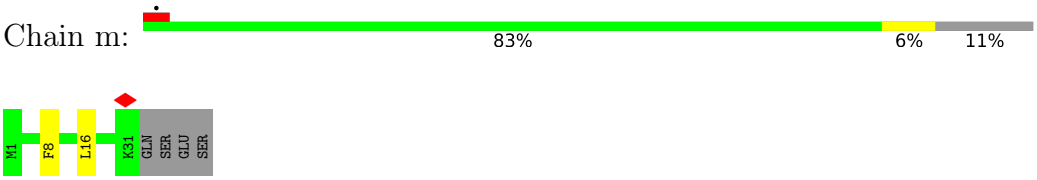
• Molecule 12: Photosystem II reaction center protein M

Chain M:



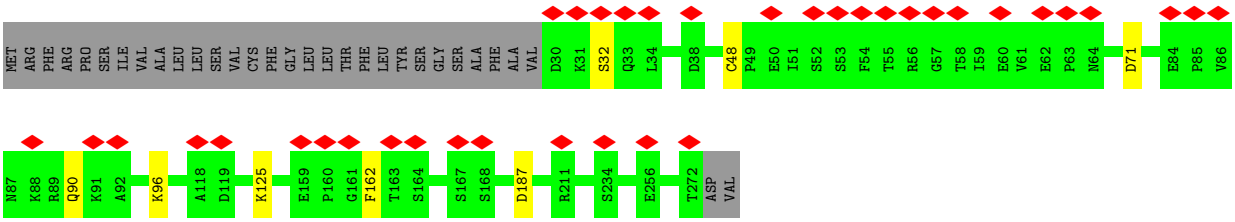
• Molecule 12: Photosystem II reaction center protein M

Chain m:



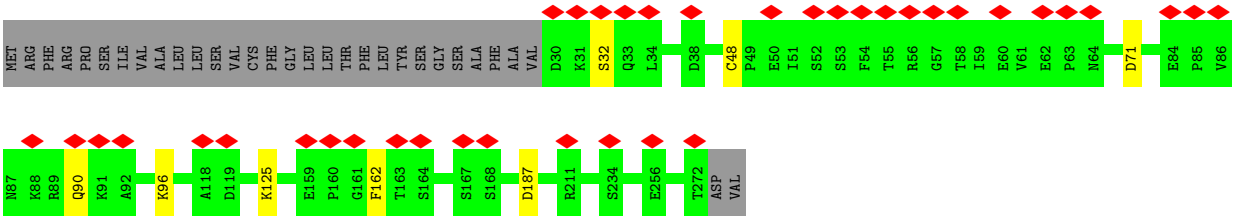
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



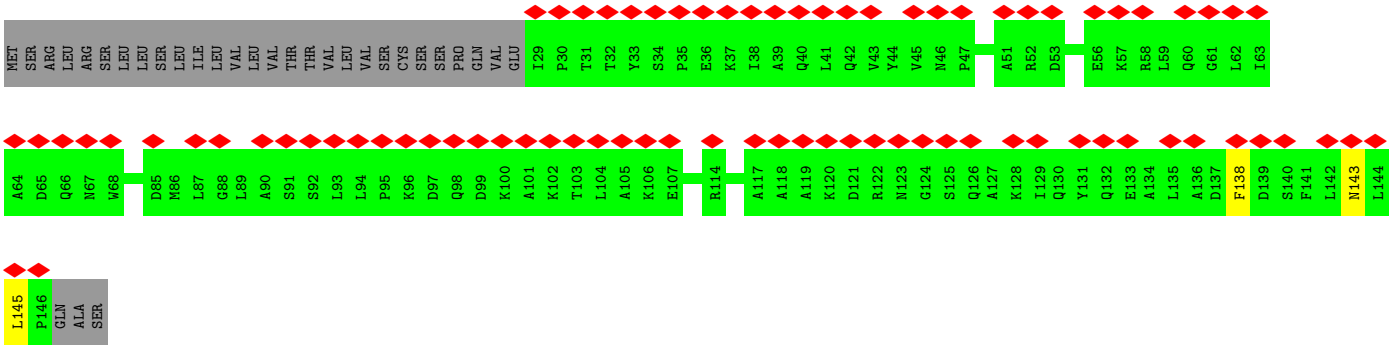
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



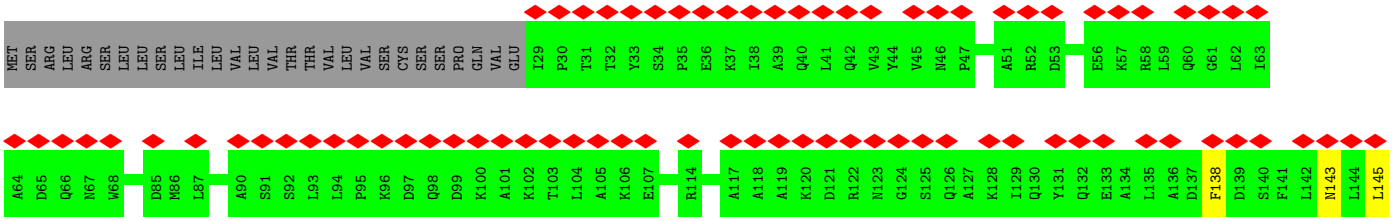
• Molecule 14: Sll1638 protein

Chain Q:



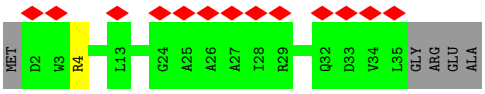
• Molecule 14: Sll1638 protein

Chain q:



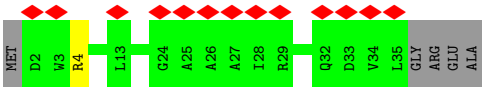
• Molecule 15: Photosystem II protein Y

Chain R:



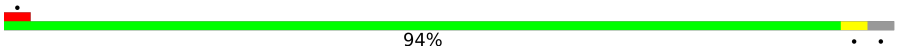
• Molecule 15: Photosystem II protein Y

Chain r:



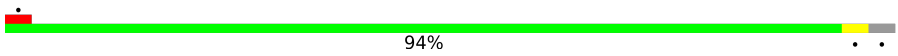
• Molecule 16: Photosystem II reaction center protein T

Chain T:



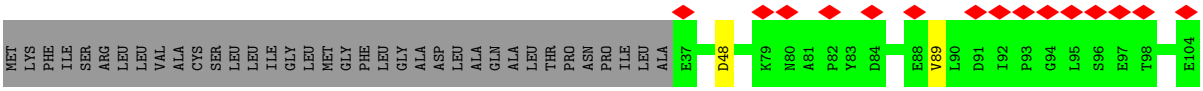
• Molecule 16: Photosystem II reaction center protein T

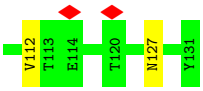
Chain t:



• Molecule 17: Photosystem II 12 kDa extrinsic protein

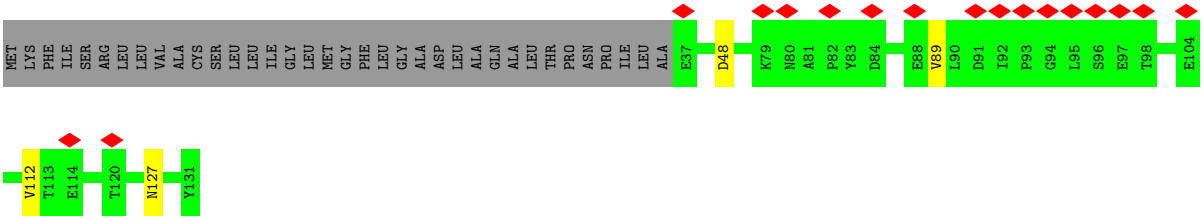
Chain U:



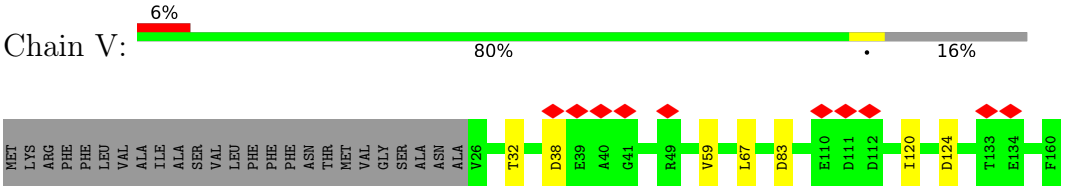


• Molecule 17: Photosystem II 12 kDa extrinsic protein

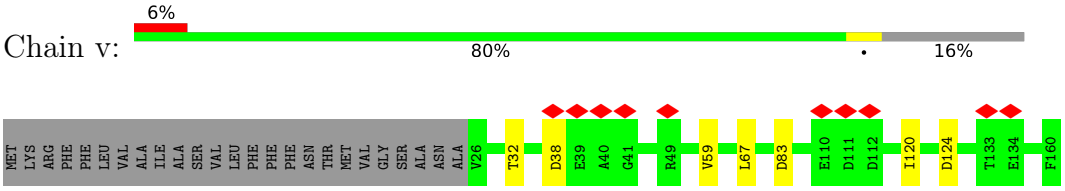
Chain u:



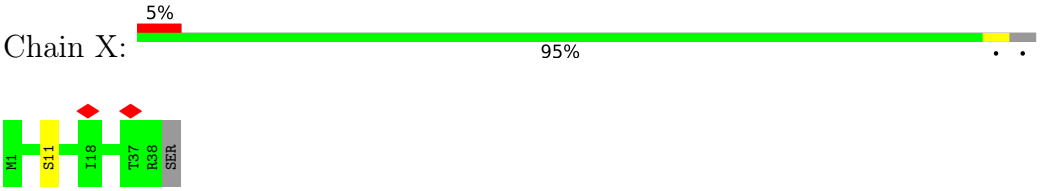
• Molecule 18: Cytochrome c-550



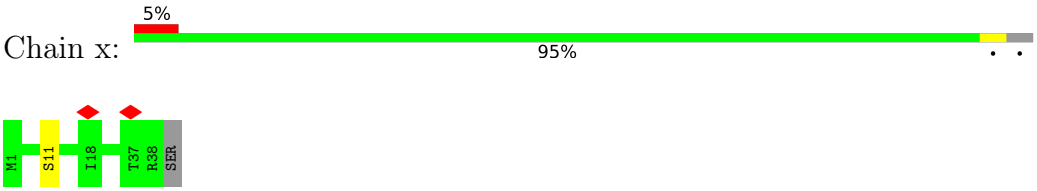
• Molecule 18: Cytochrome c-550



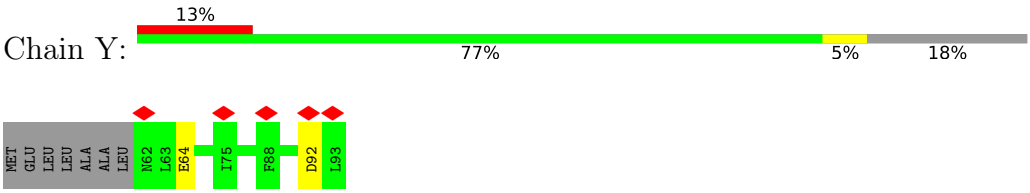
• Molecule 19: Photosystem II reaction center X protein



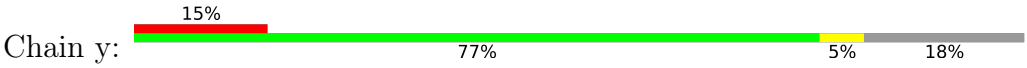
• Molecule 19: Photosystem II reaction center X protein

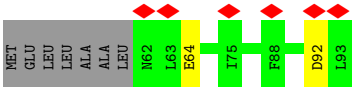


• Molecule 20: Photosystem II reaction center protein Ycf12

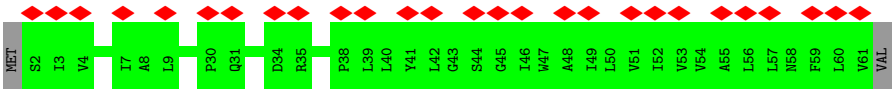


• Molecule 20: Photosystem II reaction center protein Ycf12

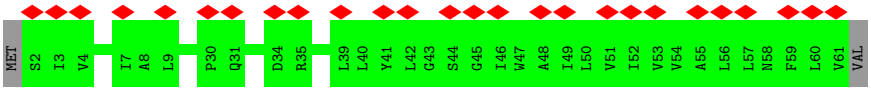




• Molecule 21: Photosystem II reaction center protein Z



• Molecule 21: Photosystem II reaction center protein Z



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129229	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 ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00432	Depositor
Map size (Å)	297.0, 297.0, 297.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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, FE2, BCT, OEX, LHG, BCR, DGD, CL, CLA, PL9, LMT, LMG, FME, HEM, PHO, CA, RRX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.42	0/2724	0.62	2/3710 (0.1%)
1	a	0.42	0/2724	0.62	2/3710 (0.1%)
2	B	0.37	0/4091	0.57	1/5568 (0.0%)
2	b	0.38	0/4091	0.57	1/5568 (0.0%)
3	C	0.38	0/3608	0.60	1/4912 (0.0%)
3	c	0.38	0/3608	0.60	1/4912 (0.0%)
4	D	0.39	0/2823	0.60	2/3843 (0.1%)
4	d	0.39	0/2823	0.60	2/3843 (0.1%)
5	E	0.40	0/664	0.71	2/906 (0.2%)
5	e	0.40	0/664	0.71	2/906 (0.2%)
6	F	0.38	0/288	0.59	0/393
6	f	0.38	0/288	0.59	0/393
7	H	0.34	0/506	0.58	0/687
7	h	0.34	0/506	0.58	0/687
8	I	0.33	0/294	0.56	0/397
8	i	0.33	0/294	0.56	0/397
9	J	0.30	0/278	0.55	0/375
9	j	0.30	0/278	0.55	0/375
10	K	0.41	0/310	0.94	3/424 (0.7%)
10	k	0.42	0/310	0.94	3/424 (0.7%)
11	L	0.40	0/322	0.53	0/435
11	l	0.40	0/322	0.53	0/435
12	M	0.35	0/239	0.67	1/325 (0.3%)
12	m	0.35	0/239	0.67	1/325 (0.3%)
13	O	0.35	0/1911	0.64	1/2590 (0.0%)
13	o	0.35	0/1911	0.64	1/2590 (0.0%)
14	Q	0.28	0/925	0.54	1/1250 (0.1%)
14	q	0.28	0/925	0.54	1/1250 (0.1%)
15	R	0.27	0/262	0.59	0/361
15	r	0.27	0/262	0.59	0/361
16	T	0.34	0/236	0.48	0/321

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	t	0.34	0/236	0.48	0/321
17	U	0.32	0/751	0.58	0/1018
17	u	0.32	0/751	0.58	0/1018
18	V	0.33	0/1086	0.60	1/1476 (0.1%)
18	v	0.34	0/1086	0.60	1/1476 (0.1%)
19	X	0.32	0/293	0.59	0/399
19	x	0.31	0/293	0.59	0/399
20	Y	0.37	0/247	0.60	0/335
20	y	0.37	0/247	0.60	0/335
21	Z	0.36	0/472	0.48	0/649
21	z	0.36	0/472	0.48	0/649
All	All	0.37	0/44660	0.60	30/60748 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	a	0	2
All	All	0	4

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	k	29	LEU	CA-CB-CG	7.40	132.33	115.30
10	K	29	LEU	CA-CB-CG	7.40	132.31	115.30
5	e	12	ASP	CB-CG-OD1	7.37	124.93	118.30
5	E	12	ASP	CB-CG-OD1	7.36	124.93	118.30
1	A	288	MET	CG-SD-CE	6.74	110.99	100.20
1	a	288	MET	CG-SD-CE	6.74	110.99	100.20
12	M	16	LEU	CA-CB-CG	6.37	129.94	115.30
12	m	16	LEU	CA-CB-CG	6.36	129.94	115.30
3	C	229	LEU	CA-CB-CG	6.05	129.21	115.30
3	c	229	LEU	CA-CB-CG	6.05	129.21	115.30
18	v	59	VAL	CG1-CB-CG2	-5.91	101.45	110.90
18	V	59	VAL	CG1-CB-CG2	-5.89	101.47	110.90
2	b	13	LEU	CA-CB-CG	5.80	128.65	115.30
2	B	13	LEU	CA-CB-CG	5.78	128.60	115.30
5	e	29	MET	CB-CG-SD	5.59	129.16	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	29	MET	CB-CG-SD	5.58	129.15	112.40
13	o	187	ASP	CB-CG-OD1	5.42	123.18	118.30
13	O	187	ASP	CB-CG-OD1	5.38	123.14	118.30
4	D	272	LEU	CA-CB-CG	5.36	127.62	115.30
4	d	272	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	308	ASP	CB-CG-OD1	5.29	123.06	118.30
10	K	20	LEU	CA-CB-CG	5.28	127.44	115.30
10	k	20	LEU	CA-CB-CG	5.28	127.44	115.30
1	a	308	ASP	CB-CG-OD1	5.27	123.05	118.30
14	Q	145	LEU	CB-CG-CD2	-5.13	102.27	111.00
14	q	145	LEU	CB-CG-CD2	-5.12	102.30	111.00
4	d	281	MET	CG-SD-CE	5.06	108.29	100.20
4	D	281	MET	CG-SD-CE	5.05	108.28	100.20
10	k	34	LEU	CA-CB-CG	5.05	126.91	115.30
10	K	34	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	ASP	Mainchain
1	a	342	ASP	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/360 (92%)	327 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	333/360 (92%)	327 (98%)	6 (2%)	0	100	100
2	B	504/507 (99%)	497 (99%)	7 (1%)	0	100	100
2	b	504/507 (99%)	497 (99%)	7 (1%)	0	100	100
3	C	448/460 (97%)	439 (98%)	9 (2%)	0	100	100
3	c	448/460 (97%)	439 (98%)	9 (2%)	0	100	100
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
5	E	76/81 (94%)	74 (97%)	2 (3%)	0	100	100
5	e	76/81 (94%)	74 (97%)	2 (3%)	0	100	100
6	F	33/44 (75%)	33 (100%)	0	0	100	100
6	f	33/44 (75%)	33 (100%)	0	0	100	100
7	H	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
7	h	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
8	I	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
8	i	35/38 (92%)	33 (94%)	2 (6%)	0	100	100
9	J	37/39 (95%)	37 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
10	k	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
11	L	37/39 (95%)	37 (100%)	0	0	100	100
11	l	37/39 (95%)	37 (100%)	0	0	100	100
12	M	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
12	m	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
13	O	241/274 (88%)	225 (93%)	15 (6%)	1 (0%)	34	29
13	o	241/274 (88%)	225 (93%)	15 (6%)	1 (0%)	34	29
14	Q	116/149 (78%)	112 (97%)	4 (3%)	0	100	100
14	q	116/149 (78%)	112 (97%)	4 (3%)	0	100	100
15	R	32/39 (82%)	32 (100%)	0	0	100	100
15	r	32/39 (82%)	32 (100%)	0	0	100	100
16	T	28/31 (90%)	28 (100%)	0	0	100	100
16	t	28/31 (90%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	U	93/131 (71%)	91 (98%)	2 (2%)	0	100	100
17	u	93/131 (71%)	91 (98%)	2 (2%)	0	100	100
18	V	133/160 (83%)	128 (96%)	5 (4%)	0	100	100
18	v	133/160 (83%)	128 (96%)	5 (4%)	0	100	100
19	X	36/39 (92%)	36 (100%)	0	0	100	100
19	x	36/39 (92%)	36 (100%)	0	0	100	100
20	Y	30/39 (77%)	30 (100%)	0	0	100	100
20	y	30/39 (77%)	30 (100%)	0	0	100	100
21	Z	58/62 (94%)	58 (100%)	0	0	100	100
21	z	58/62 (94%)	58 (100%)	0	0	100	100
All	All	5468/5976 (92%)	5340 (98%)	126 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	32	SER
13	o	32	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/293 (94%)	272 (99%)	2 (1%)	84	87
1	a	274/293 (94%)	272 (99%)	2 (1%)	84	87
2	B	403/404 (100%)	395 (98%)	8 (2%)	55	57
2	b	403/404 (100%)	395 (98%)	8 (2%)	55	57
3	C	351/361 (97%)	342 (97%)	9 (3%)	46	45
3	c	351/361 (97%)	342 (97%)	9 (3%)	46	45
4	D	277/285 (97%)	275 (99%)	2 (1%)	84	87
4	d	277/285 (97%)	275 (99%)	2 (1%)	84	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	70/73 (96%)	70 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	28/37 (76%)	28 (100%)	0	100	100
6	f	28/37 (76%)	28 (100%)	0	100	100
7	H	53/54 (98%)	51 (96%)	2 (4%)	33	30
7	h	53/54 (98%)	51 (96%)	2 (4%)	33	30
8	I	32/33 (97%)	31 (97%)	1 (3%)	40	38
8	i	32/33 (97%)	31 (97%)	1 (3%)	40	38
9	J	24/24 (100%)	24 (100%)	0	100	100
9	j	24/24 (100%)	24 (100%)	0	100	100
10	K	31/38 (82%)	31 (100%)	0	100	100
10	k	31/38 (82%)	31 (100%)	0	100	100
11	L	36/36 (100%)	35 (97%)	1 (3%)	43	42
11	l	36/36 (100%)	35 (97%)	1 (3%)	43	42
12	M	27/31 (87%)	26 (96%)	1 (4%)	34	31
12	m	27/31 (87%)	26 (96%)	1 (4%)	34	31
13	O	207/233 (89%)	201 (97%)	6 (3%)	42	40
13	o	207/233 (89%)	201 (97%)	6 (3%)	42	40
14	Q	93/128 (73%)	91 (98%)	2 (2%)	52	53
14	q	93/128 (73%)	91 (98%)	2 (2%)	52	53
15	R	26/29 (90%)	25 (96%)	1 (4%)	33	30
15	r	26/29 (90%)	25 (96%)	1 (4%)	33	30
16	T	24/25 (96%)	24 (100%)	0	100	100
16	t	24/25 (96%)	24 (100%)	0	100	100
17	U	83/111 (75%)	79 (95%)	4 (5%)	25	21
17	u	83/111 (75%)	79 (95%)	4 (5%)	25	21
18	V	117/137 (85%)	111 (95%)	6 (5%)	24	19
18	v	117/137 (85%)	111 (95%)	6 (5%)	24	19
19	X	32/33 (97%)	31 (97%)	1 (3%)	40	38
19	x	32/33 (97%)	31 (97%)	1 (3%)	40	38
20	Y	25/30 (83%)	23 (92%)	2 (8%)	12	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	y	25/30 (83%)	23 (92%)	2 (8%)	12 6
21	Z	49/52 (94%)	49 (100%)	0	100 100
21	z	49/52 (94%)	49 (100%)	0	100 100
All	All	4524/4894 (92%)	4428 (98%)	96 (2%)	56 54

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343[A]	LEU
1	A	343[B]	LEU
2	B	13	LEU
2	B	18	ARG
2	B	87	ASP
2	B	121	GLU
2	B	179	GLN
2	B	289	ASP
2	B	362	PHE
2	B	415	SER
3	C	54	MET
3	C	84	TRP
3	C	190	THR
3	C	217	MET
3	C	227	ILE
3	C	276	PHE
3	C	294	MET
3	C	342	THR
3	C	370	ASP
4	D	25	ASP
4	D	180	ARG
7	H	49	TYR
7	H	61	ASP
8	I	35	LYS
11	L	5	SER
12	M	8	PHE
13	O	48	CYS
13	O	71	ASP
13	O	90	GLN
13	O	96	LYS
13	O	125	LYS
13	O	162	PHE
14	Q	138	PHE

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Mol	Chain	Res	Type
14	Q	143	ASN
15	R	4	ARG
17	U	48	ASP
17	U	89	VAL
17	U	112	VAL
17	U	127	ASN
18	V	32	THR
18	V	38	ASP
18	V	67	LEU
18	V	83	ASP
18	V	120	ILE
18	V	124	ASP
19	X	11	SER
20	Y	64	GLU
20	Y	92	ASP
1	a	343[A]	LEU
1	a	343[B]	LEU
2	b	13	LEU
2	b	18	ARG
2	b	87	ASP
2	b	121	GLU
2	b	179	GLN
2	b	289	ASP
2	b	362	PHE
2	b	415	SER
3	c	54	MET
3	c	84	TRP
3	c	190	THR
3	c	217	MET
3	c	227	ILE
3	c	276	PHE
3	c	294	MET
3	c	342	THR
3	c	370	ASP
4	d	25	ASP
4	d	180	ARG
7	h	49	TYR
7	h	61	ASP
8	i	35	LYS
11	l	5	SER
12	m	8	PHE
13	o	48	CYS

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Mol	Chain	Res	Type
13	o	71	ASP
13	o	90	GLN
13	o	96	LYS
13	o	125	LYS
13	o	162	PHE
14	q	138	PHE
14	q	143	ASN
15	r	4	ARG
17	u	48	ASP
17	u	89	VAL
17	u	112	VAL
17	u	127	ASN
18	v	32	THR
18	v	38	ASP
18	v	67	LEU
18	v	83	ASP
18	v	120	ILE
18	v	124	ASP
19	x	11	SER
20	y	64	GLU
20	y	92	ASP

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

Mol	Chain	Res	Type
1	A	303	ASN
1	A	304	GLN
2	B	291	GLN
2	B	394	GLN
2	B	413	ASN
3	C	309	GLN
3	C	314	ASN
4	D	301	GLN
8	I	31	ASN
12	M	2	GLN
13	O	153	ASN
13	O	227	GLN
14	Q	143	ASN
17	U	56	ASN
17	U	127	ASN
18	V	50	GLN
1	a	303	ASN

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Mol	Chain	Res	Type
1	a	304	GLN
2	b	291	GLN
2	b	394	GLN
2	b	413	ASN
3	c	309	GLN
3	c	314	ASN
4	d	301	GLN
8	i	31	ASN
12	m	2	GLN
13	o	153	ASN
13	o	227	GLN
14	q	143	ASN
17	u	56	ASN
17	u	127	ASN
18	v	50	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
16	FME	t	1	16	8,9,10	0.85	0	7,9,11	1.12	1 (14%)
8	FME	I	1	8	8,9,10	0.95	0	7,9,11	1.17	1 (14%)
16	FME	T	1	16	8,9,10	0.85	0	7,9,11	1.12	1 (14%)
8	FME	i	1	8	8,9,10	0.95	0	7,9,11	1.17	1 (14%)
12	FME	m	1	12	8,9,10	0.95	0	7,9,11	0.88	0
12	FME	M	1	12	8,9,10	0.95	0	7,9,11	0.88	0
9	FME	J	1	9	6,7,10	0.81	0	2,7,11	0.79	0
9	FME	j	1	9	6,7,10	0.81	0	2,7,11	0.78	0

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
16	FME	t	1	16	-	4/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
16	FME	T	1	16	-	4/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
9	FME	J	1	9	-	2/5/6/11	-
9	FME	j	1	9	-	2/5/6/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	C-CA-N	2.54	114.31	109.73
8	I	1	FME	C-CA-N	2.52	114.28	109.73
16	T	1	FME	C-CA-N	2.12	113.55	109.73
16	t	1	FME	C-CA-N	2.12	113.55	109.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1	FME	N-CA-CB-CG
9	J	1	FME	CA-CB-CG-SD
16	T	1	FME	N-CA-CB-CG
9	j	1	FME	N-CA-CB-CG
9	j	1	FME	CA-CB-CG-SD
16	t	1	FME	N-CA-CB-CG
16	T	1	FME	CA-CB-CG-SD
16	t	1	FME	CA-CB-CG-SD
8	I	1	FME	CA-CB-CG-SD
8	i	1	FME	CA-CB-CG-SD
16	T	1	FME	C-CA-CB-CG
16	t	1	FME	C-CA-CB-CG
8	I	1	FME	C-CA-CB-CG
8	i	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
16	T	1	FME	CB-CG-SD-CE
16	t	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 232 ligands modelled in this entry, 12 are monoatomic - leaving 220 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	A	408	-	60,68,73	2.35	19 (31%)	70,107,113	2.75	22 (31%)
25	CLA	D	401	38	65,73,73	2.21	21 (32%)	76,113,113	2.63	25 (32%)
29	PL9	d	405	-	55,55,55	1.25	5 (9%)	68,69,69	1.45	10 (14%)
25	CLA	c	507	-	65,73,73	2.22	21 (32%)	76,113,113	2.60	24 (31%)
31	LMT	B	625	-	36,36,36	1.26	6 (16%)	47,47,47	1.04	1 (2%)
35	HEM	e	104	6,5	41,50,50	1.36	4 (9%)	45,82,82	1.92	11 (24%)
34	DGD	c	517	-	63,63,67	1.23	8 (12%)	77,77,81	1.07	5 (6%)
25	CLA	b	608	-	65,73,73	2.27	21 (32%)	76,113,113	2.56	24 (31%)
31	LMT	b	625	-	36,36,36	1.26	6 (16%)	47,47,47	1.04	1 (2%)
31	LMT	d	410	-	24,24,36	1.00	2 (8%)	29,29,47	1.20	4 (13%)
28	LMG	d	409	-	43,43,55	1.22	4 (9%)	51,51,63	1.11	3 (5%)
25	CLA	B	606	-	60,68,73	2.35	20 (33%)	70,107,113	2.58	24 (34%)
25	CLA	C	514	-	65,73,73	2.27	18 (27%)	76,113,113	2.52	23 (30%)
31	LMT	A	416	-	24,24,36	1.08	3 (12%)	29,29,47	1.00	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	LMT	D	412	-	36,36,36	1.20	5 (13%)	47,47,47	0.94	2 (4%)
33	LHG	D	406	-	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
28	LMG	a	414	-	36,36,55	1.11	2 (5%)	44,44,63	1.18	3 (6%)
31	LMT	I	101	-	24,24,36	1.08	2 (8%)	29,29,47	1.05	1 (3%)
25	CLA	C	506	-	55,63,73	2.43	20 (36%)	64,101,113	2.89	25 (39%)
30	SQD	c	501	-	53,54,54	0.94	6 (11%)	62,65,65	1.69	9 (14%)
31	LMT	k	105	-	36,36,36	1.23	6 (16%)	47,47,47	1.21	5 (10%)
25	CLA	b	603	-	65,73,73	2.25	19 (29%)	76,113,113	2.55	26 (34%)
25	CLA	B	610	38	65,73,73	2.26	21 (32%)	76,113,113	2.61	28 (36%)
25	CLA	B	611	-	65,73,73	2.20	19 (29%)	76,113,113	2.57	24 (31%)
30	SQD	b	620	-	53,54,54	0.40	0	62,65,65	0.45	0
31	LMT	e	103	-	36,36,36	1.25	7 (19%)	47,47,47	1.55	6 (12%)
25	CLA	B	612	-	65,73,73	2.25	19 (29%)	76,113,113	2.58	24 (31%)
31	LMT	y	101	-	21,21,36	1.12	2 (9%)	26,26,47	1.04	1 (3%)
34	DGD	h	104	-	63,63,67	1.23	8 (12%)	77,77,81	0.96	3 (3%)
26	PHO	d	402	-	51,69,69	1.00	4 (7%)	47,99,99	1.31	7 (14%)
31	LMT	j	101	-	24,24,36	1.05	2 (8%)	29,29,47	1.18	3 (10%)
25	CLA	B	607	38	65,73,73	2.17	19 (29%)	76,113,113	2.63	26 (34%)
25	CLA	c	502	-	65,73,73	2.23	19 (29%)	76,113,113	2.62	25 (32%)
32	BCT	A	417	-	2,3,3	1.28	0	2,3,3	4.14	1 (50%)
27	BCR	B	618	-	41,41,41	2.89	6 (14%)	56,56,56	6.30	19 (33%)
25	CLA	C	507	-	65,73,73	2.22	21 (32%)	76,113,113	2.60	24 (31%)
25	CLA	c	510	-	65,73,73	2.26	21 (32%)	76,113,113	2.64	25 (32%)
30	SQD	a	413	-	47,48,54	1.00	5 (10%)	56,59,65	1.92	13 (23%)
27	BCR	A	409	-	41,41,41	2.84	6 (14%)	56,56,56	6.32	19 (33%)
25	CLA	C	511	-	65,73,73	2.23	20 (30%)	76,113,113	2.69	30 (39%)
33	LHG	e	102	-	39,39,48	1.03	2 (5%)	42,45,54	1.10	3 (7%)
34	DGD	C	517	-	63,63,67	1.23	8 (12%)	77,77,81	1.07	5 (6%)
25	CLA	a	406	38	65,73,73	2.24	20 (30%)	76,113,113	2.62	23 (30%)
31	LMT	E	101	-	22,22,36	1.11	2 (9%)	27,27,47	1.15	3 (11%)
31	LMT	A	415	-	36,36,36	1.22	5 (13%)	47,47,47	1.00	2 (4%)
30	SQD	k	101	-	41,41,54	1.04	3 (7%)	49,49,65	1.77	9 (18%)
33	LHG	b	628	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	3 (5%)
28	LMG	D	409	-	43,43,55	1.22	4 (9%)	51,51,63	1.11	3 (5%)
31	LMT	m	101	-	36,36,36	1.20	6 (16%)	47,47,47	1.02	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	LMG	C	519	-	51,51,55	1.35	7 (13%)	59,59,63	1.11	3 (5%)
33	LHG	D	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.06	4 (7%)
29	PL9	a	411	-	55,55,55	1.11	3 (5%)	68,69,69	1.48	11 (16%)
25	CLA	A	406	38	65,73,73	2.24	20 (30%)	76,113,113	2.62	23 (30%)
31	LMT	Y	101	-	21,21,36	1.12	2 (9%)	26,26,47	1.04	1 (3%)
27	BCR	f	101	-	41,41,41	2.79	6 (14%)	56,56,56	6.47	22 (39%)
25	CLA	d	401	38	65,73,73	2.21	21 (32%)	76,113,113	2.63	25 (32%)
31	LMT	b	624	-	24,24,36	1.05	2 (8%)	29,29,47	0.90	0
27	BCR	k	102	-	41,41,41	2.80	6 (14%)	56,56,56	6.72	21 (37%)
25	CLA	B	615	-	65,73,73	2.19	19 (29%)	76,113,113	2.70	25 (32%)
30	SQD	A	413	-	47,48,54	1.00	5 (10%)	56,59,65	1.92	13 (23%)
31	LMT	B	626	-	24,24,36	1.02	2 (8%)	29,29,47	0.90	0
31	LMT	M	102	-	24,24,36	1.08	2 (8%)	29,29,47	1.07	1 (3%)
34	DGD	c	516	-	63,63,67	1.23	8 (12%)	77,77,81	0.92	2 (2%)
31	LMT	H	102	-	24,24,36	1.09	2 (8%)	29,29,47	1.11	2 (6%)
31	LMT	C	524	-	36,36,36	1.21	5 (13%)	47,47,47	1.17	3 (6%)
31	LMT	x	102	-	22,22,36	1.12	2 (9%)	27,27,47	1.04	1 (3%)
34	DGD	C	516	-	63,63,67	1.23	8 (12%)	77,77,81	0.92	2 (2%)
31	LMT	X	104	-	19,19,36	1.22	3 (15%)	24,24,47	1.05	1 (4%)
25	CLA	C	509	-	65,73,73	2.23	19 (29%)	76,113,113	2.49	25 (32%)
25	CLA	D	404	-	65,73,73	2.22	20 (30%)	76,113,113	2.57	23 (30%)
25	CLA	b	611	-	65,73,73	2.20	19 (29%)	76,113,113	2.57	24 (31%)
30	SQD	K	101	-	41,41,54	1.04	3 (7%)	49,49,65	1.77	9 (18%)
31	LMT	B	629	-	36,36,36	1.21	5 (13%)	47,47,47	0.99	0
31	LMT	e	101	-	22,22,36	1.11	2 (9%)	27,27,47	1.15	3 (11%)
31	LMT	i	103	-	36,36,36	1.21	6 (16%)	47,47,47	0.93	1 (2%)
25	CLA	C	510	-	65,73,73	2.26	21 (32%)	76,113,113	2.64	25 (32%)
25	CLA	b	605	-	65,73,73	2.18	19 (29%)	76,113,113	2.72	23 (30%)
27	BCR	k	103	-	41,41,41	2.84	6 (14%)	56,56,56	6.40	25 (44%)
25	CLA	c	512	3	65,73,73	2.25	19 (29%)	76,113,113	2.76	26 (34%)
25	CLA	b	607	38	65,73,73	2.17	19 (29%)	76,113,113	2.62	26 (34%)
31	LMT	X	105	-	19,19,36	1.14	2 (10%)	24,24,47	0.99	0
26	PHO	a	407	-	51,69,69	1.05	4 (7%)	47,99,99	1.12	4 (8%)
25	CLA	b	613	-	65,73,73	2.16	20 (30%)	76,113,113	2.66	24 (31%)
27	BCR	Z	101	-	41,41,41	2.82	6 (14%)	56,56,56	6.34	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	d	403	-	65,73,73	2.21	18 (27%)	76,113,113	2.75	22 (28%)
31	LMT	x	101	-	24,24,36	1.06	2 (8%)	29,29,47	1.06	1 (3%)
31	LMT	a	416	-	24,24,36	1.08	3 (12%)	29,29,47	1.00	1 (3%)
34	DGD	H	104	-	63,63,67	1.23	8 (12%)	77,77,81	0.96	3 (3%)
31	LMT	B	623	-	36,36,36	1.21	5 (13%)	47,47,47	1.09	4 (8%)
31	LMT	b	626	-	24,24,36	1.02	2 (8%)	29,29,47	0.90	0
31	LMT	K	105	-	36,36,36	1.23	6 (16%)	47,47,47	1.21	5 (10%)
31	LMT	x	103	-	22,22,36	1.03	2 (9%)	27,27,47	1.28	3 (11%)
27	BCR	z	101	-	41,41,41	2.82	6 (14%)	56,56,56	6.34	20 (35%)
27	BCR	K	103	-	41,41,41	2.84	6 (14%)	56,56,56	6.41	26 (46%)
31	LMT	T	101	-	24,24,36	1.11	2 (8%)	29,29,47	1.15	2 (6%)
27	BCR	b	617	-	41,41,41	2.90	6 (14%)	56,56,56	6.37	16 (28%)
31	LMT	d	411	-	36,36,36	1.20	5 (13%)	47,47,47	0.91	0
31	LMT	c	525	-	21,21,36	1.02	1 (4%)	26,26,47	1.28	2 (7%)
25	CLA	B	609	-	65,73,73	2.26	20 (30%)	76,113,113	2.56	23 (30%)
25	CLA	C	503	-	65,73,73	2.19	18 (27%)	76,113,113	2.56	27 (35%)
28	LMG	H	105	-	47,47,55	1.32	6 (12%)	55,55,63	1.37	7 (12%)
25	CLA	b	606	-	60,68,73	2.35	20 (33%)	70,107,113	2.59	24 (34%)
25	CLA	c	506	-	55,63,73	2.43	20 (36%)	64,101,113	2.89	25 (39%)
25	CLA	C	512	3	65,73,73	2.25	19 (29%)	76,113,113	2.76	26 (34%)
27	BCR	b	618	-	41,41,41	2.89	6 (14%)	56,56,56	6.30	19 (33%)
31	LMT	I	102	-	24,24,36	1.05	2 (8%)	29,29,47	1.07	1 (3%)
31	LMT	i	101	-	24,24,36	1.07	2 (8%)	29,29,47	1.05	1 (3%)
31	LMT	x	105	-	19,19,36	1.14	2 (10%)	24,24,47	0.99	0
31	LMT	i	102	-	24,24,36	1.05	2 (8%)	29,29,47	1.07	1 (3%)
31	LMT	D	411	-	36,36,36	1.20	5 (13%)	47,47,47	0.91	0
28	LMG	B	621	-	51,51,55	1.35	7 (13%)	59,59,63	1.02	2 (3%)
33	LHG	d	406	-	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
31	LMT	X	101	-	24,24,36	1.06	2 (8%)	29,29,47	1.06	1 (3%)
28	LMG	b	621	-	51,51,55	1.35	7 (13%)	59,59,63	1.02	2 (3%)
25	CLA	b	609	-	65,73,73	2.26	20 (30%)	76,113,113	2.55	23 (30%)
26	PHO	D	402	-	51,69,69	1.00	4 (7%)	47,99,99	1.30	7 (14%)
31	LMT	B	624	-	24,24,36	1.05	2 (8%)	29,29,47	0.90	1 (3%)
31	LMT	i	104	-	22,22,36	1.07	2 (9%)	27,27,47	1.04	0
25	CLA	B	602	-	65,73,73	2.20	18 (27%)	76,113,113	2.55	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	A	405	-	65,73,73	2.16	19 (29%)	76,113,113	2.62	25 (32%)
29	PL9	A	411	-	55,55,55	1.12	3 (5%)	68,69,69	1.48	11 (16%)
31	LMT	t	101	-	24,24,36	1.10	2 (8%)	29,29,47	1.15	2 (6%)
33	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	0.95	2 (3%)
25	CLA	B	608	-	65,73,73	2.27	21 (32%)	76,113,113	2.56	24 (31%)
25	CLA	c	508	38	65,73,73	2.21	20 (30%)	76,113,113	2.58	25 (32%)
25	CLA	c	503	-	65,73,73	2.19	18 (27%)	76,113,113	2.56	27 (35%)
25	CLA	d	404	-	65,73,73	2.22	20 (30%)	76,113,113	2.57	23 (30%)
28	LMG	c	519	-	51,51,55	1.35	7 (13%)	59,59,63	1.11	3 (5%)
31	LMT	X	103	-	22,22,36	1.03	2 (9%)	27,27,47	1.28	3 (11%)
27	BCR	F	101	-	41,41,41	2.79	6 (14%)	56,56,56	6.47	22 (39%)
25	CLA	a	408	-	60,68,73	2.35	19 (31%)	70,107,113	2.74	22 (31%)
31	LMT	I	104	-	22,22,36	1.07	2 (9%)	27,27,47	1.04	0
31	LMT	f	103	-	36,36,36	1.23	5 (13%)	47,47,47	1.01	2 (4%)
25	CLA	B	601	38	45,53,73	2.55	21 (46%)	52,89,113	3.01	20 (38%)
33	LHG	B	628	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	3 (5%)
31	LMT	C	525	-	21,21,36	1.03	2 (9%)	26,26,47	1.28	2 (7%)
25	CLA	c	504	-	65,73,73	2.26	21 (32%)	76,113,113	2.63	24 (31%)
30	SQD	A	412	-	53,54,54	0.96	3 (5%)	62,65,65	1.78	14 (22%)
33	LHG	b	627	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	2 (3%)
22	OEX	A	401	3,1,38	0,15,15	-	-	-		
31	LMT	I	103	-	36,36,36	1.21	6 (16%)	47,47,47	0.92	1 (2%)
34	DGD	c	518	-	63,63,67	1.23	7 (11%)	77,77,81	1.04	3 (3%)
29	PL9	D	405	-	55,55,55	1.25	5 (9%)	68,69,69	1.45	10 (14%)
28	LMG	A	414	-	36,36,55	1.11	2 (5%)	44,44,63	1.18	3 (6%)
25	CLA	c	505	38	65,73,73	2.19	19 (29%)	76,113,113	2.68	27 (35%)
25	CLA	b	615	-	65,73,73	2.19	19 (29%)	76,113,113	2.71	25 (32%)
27	BCR	B	619	-	41,41,41	2.91	6 (14%)	56,56,56	6.39	22 (39%)
25	CLA	B	604	-	65,73,73	2.19	18 (27%)	76,113,113	2.60	27 (35%)
25	CLA	C	505	38	65,73,73	2.19	19 (29%)	76,113,113	2.68	27 (35%)
25	CLA	b	610	38	65,73,73	2.26	21 (32%)	76,113,113	2.60	27 (35%)
25	CLA	B	603	-	65,73,73	2.25	19 (29%)	76,113,113	2.55	26 (34%)
33	LHG	z	102	-	35,35,48	1.14	2 (5%)	39,40,54	1.13	3 (7%)
27	BCR	C	515	-	41,41,41	2.87	6 (14%)	56,56,56	6.44	18 (32%)
30	SQD	B	620	-	53,54,54	0.39	0	62,65,65	0.45	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	LMT	F	103	-	36,36,36	1.22	5 (13%)	47,47,47	1.01	2 (4%)
25	CLA	b	612	-	65,73,73	2.26	19 (29%)	76,113,113	2.59	24 (31%)
32	BCT	a	417	-	2,3,3	1.28	0	2,3,3	4.14	1 (50%)
31	LMT	b	629	-	36,36,36	1.21	5 (13%)	47,47,47	0.99	0
25	CLA	b	601	38	45,53,73	2.55	21 (46%)	52,89,113	3.01	20 (38%)
25	CLA	b	614	-	65,73,73	2.24	19 (29%)	76,113,113	2.61	24 (31%)
26	PHO	A	407	-	51,69,69	1.04	4 (7%)	47,99,99	1.12	4 (8%)
27	BCR	B	617	-	41,41,41	2.90	6 (14%)	56,56,56	6.37	16 (28%)
36	RRX	h	101	-	42,42,42	1.63	8 (19%)	57,58,58	1.48	9 (15%)
25	CLA	c	511	-	65,73,73	2.23	20 (30%)	76,113,113	2.69	30 (39%)
25	CLA	C	504	-	65,73,73	2.26	21 (32%)	76,113,113	2.63	24 (31%)
31	LMT	c	524	-	36,36,36	1.21	5 (13%)	47,47,47	1.16	3 (6%)
31	LMT	m	102	-	24,24,36	1.08	2 (8%)	29,29,47	1.08	1 (3%)
30	SQD	F	102	-	33,34,54	1.19	5 (15%)	42,45,65	2.04	11 (26%)
31	LMT	X	102	-	22,22,36	1.11	2 (9%)	27,27,47	1.05	1 (3%)
33	LHG	d	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.06	4 (7%)
25	CLA	B	613	-	65,73,73	2.16	20 (30%)	76,113,113	2.66	24 (31%)
33	LHG	Z	102	-	35,35,48	1.14	2 (5%)	39,40,54	1.14	3 (7%)
25	CLA	B	616	-	60,68,73	2.28	18 (30%)	70,107,113	2.74	27 (38%)
35	HEM	E	104	6,5	41,50,50	1.35	4 (9%)	45,82,82	1.92	11 (24%)
31	LMT	b	623	-	36,36,36	1.21	5 (13%)	47,47,47	1.09	4 (8%)
36	RRX	H	101	-	42,42,42	1.62	8 (19%)	57,58,58	1.49	9 (15%)
35	HEM	v	201	18	41,50,50	1.50	8 (19%)	45,82,82	2.20	11 (24%)
31	LMT	E	103	-	36,36,36	1.25	7 (19%)	47,47,47	1.55	6 (12%)
25	CLA	b	604	-	65,73,73	2.18	18 (27%)	76,113,113	2.60	27 (35%)
22	OEX	a	401	3,1,38	0,15,15	-	-	-		
30	SQD	h	103	-	53,54,54	0.94	5 (9%)	62,65,65	1.61	8 (12%)
31	LMT	J	101	-	24,24,36	1.05	2 (8%)	29,29,47	1.18	3 (10%)
31	LMT	D	410	-	24,24,36	1.01	2 (8%)	29,29,47	1.20	4 (13%)
30	SQD	f	102	-	33,34,54	1.19	5 (15%)	42,45,65	2.04	11 (26%)
33	LHG	E	102	-	39,39,48	1.03	2 (5%)	42,45,54	1.10	3 (7%)
34	DGD	C	518	-	63,63,67	1.23	8 (12%)	77,77,81	1.04	3 (3%)
33	LHG	D	408	-	48,48,48	0.91	2 (4%)	51,54,54	0.95	2 (3%)
27	BCR	a	409	-	41,41,41	2.85	6 (14%)	56,56,56	6.32	19 (33%)
31	LMT	a	415	-	36,36,36	1.22	5 (13%)	47,47,47	1.00	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	C	513	-	50,58,73	2.55	19 (38%)	58,95,113	2.97	19 (32%)
28	LMG	c	523	-	49,49,55	1.34	6 (12%)	57,57,63	1.20	4 (7%)
31	LMT	x	104	-	19,19,36	1.22	3 (15%)	24,24,47	1.05	1 (4%)
27	BCR	c	515	-	41,41,41	2.87	6 (14%)	56,56,56	6.43	18 (32%)
30	SQD	C	501	-	53,54,54	0.93	6 (11%)	62,65,65	1.69	9 (14%)
28	LMG	C	523	-	49,49,55	1.34	6 (12%)	57,57,63	1.20	4 (7%)
31	LMT	c	522	-	24,24,36	1.16	5 (20%)	29,29,47	1.31	4 (13%)
33	LHG	B	627	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	2 (3%)
25	CLA	B	614	-	65,73,73	2.23	19 (29%)	76,113,113	2.61	24 (31%)
35	HEM	V	201	18	41,50,50	1.50	8 (19%)	45,82,82	2.20	11 (24%)
31	LMT	d	412	-	36,36,36	1.20	5 (13%)	47,47,47	0.94	2 (4%)
25	CLA	C	502	-	65,73,73	2.23	19 (29%)	76,113,113	2.62	25 (32%)
25	CLA	c	513	-	50,58,73	2.55	19 (38%)	58,95,113	2.97	19 (32%)
31	LMT	M	101	-	36,36,36	1.20	6 (16%)	47,47,47	1.02	2 (4%)
30	SQD	H	103	-	53,54,54	0.94	5 (9%)	62,65,65	1.61	8 (12%)
25	CLA	D	403	-	65,73,73	2.21	18 (27%)	76,113,113	2.75	22 (28%)
28	LMG	a	410	-	51,51,55	1.36	8 (15%)	59,59,63	1.09	3 (5%)
25	CLA	c	509	-	65,73,73	2.23	19 (29%)	76,113,113	2.48	25 (32%)
25	CLA	c	514	-	65,73,73	2.27	18 (27%)	76,113,113	2.51	24 (31%)
25	CLA	a	405	-	65,73,73	2.16	19 (29%)	76,113,113	2.62	25 (32%)
25	CLA	C	508	38	65,73,73	2.21	20 (30%)	76,113,113	2.58	25 (32%)
25	CLA	b	602	-	65,73,73	2.20	18 (27%)	76,113,113	2.55	24 (31%)
27	BCR	b	619	-	41,41,41	2.91	6 (14%)	56,56,56	6.39	22 (39%)
30	SQD	a	412	-	53,54,54	0.96	3 (5%)	62,65,65	1.78	14 (22%)
31	LMT	h	102	-	24,24,36	1.09	2 (8%)	29,29,47	1.11	2 (6%)
25	CLA	b	616	-	60,68,73	2.28	18 (30%)	70,107,113	2.74	27 (38%)
31	LMT	C	522	-	24,24,36	1.17	5 (20%)	29,29,47	1.31	4 (13%)
28	LMG	h	105	-	47,47,55	1.32	6 (12%)	55,55,63	1.37	7 (12%)
28	LMG	A	410	-	51,51,55	1.36	8 (15%)	59,59,63	1.09	3 (5%)
25	CLA	B	605	-	65,73,73	2.18	19 (29%)	76,113,113	2.72	23 (30%)
27	BCR	K	102	-	41,41,41	2.79	6 (14%)	56,56,56	6.72	21 (37%)

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
25	CLA	A	408	-	1/1/14/20	14/31/109/115	-
25	CLA	D	401	38	1/1/15/20	11/37/115/115	-
29	PL9	d	405	-	-	9/53/73/73	0/1/1/1
25	CLA	c	507	-	1/1/15/20	15/37/115/115	-
31	LMT	B	625	-	-	11/21/61/61	0/2/2/2
35	HEM	e	104	6,5	-	4/12/54/54	-
34	DGD	c	517	-	-	17/51/91/95	0/2/2/2
25	CLA	b	608	-	1/1/15/20	10/37/115/115	-
31	LMT	b	625	-	-	11/21/61/61	0/2/2/2
31	LMT	d	410	-	-	8/15/35/61	0/1/1/2
28	LMG	d	409	-	-	14/38/58/70	0/1/1/1
25	CLA	B	606	-	1/1/14/20	9/31/109/115	-
25	CLA	C	514	-	1/1/15/20	20/37/115/115	-
31	LMT	A	416	-	-	5/15/35/61	0/1/1/2
31	LMT	D	412	-	-	7/21/61/61	0/2/2/2
33	LHG	D	406	-	-	25/53/53/53	-
28	LMG	a	414	-	-	6/31/51/70	0/1/1/1
31	LMT	I	101	-	-	11/15/35/61	0/1/1/2
25	CLA	C	506	-	1/1/13/20	9/25/103/115	-
30	SQD	c	501	-	-	29/49/69/69	0/1/1/1
31	LMT	k	105	-	-	12/21/61/61	0/2/2/2
25	CLA	b	603	-	1/1/15/20	18/37/115/115	-
25	CLA	B	610	38	1/1/15/20	8/37/115/115	-
25	CLA	B	611	-	1/1/15/20	10/37/115/115	-
30	SQD	b	620	-	-	24/49/69/69	0/1/1/1
31	LMT	e	103	-	-	8/21/61/61	0/2/2/2
25	CLA	B	612	-	1/1/15/20	11/37/115/115	-
31	LMT	y	101	-	-	7/12/32/61	0/1/1/2
34	DGD	h	104	-	-	11/51/91/95	0/2/2/2
26	PHO	d	402	-	-	4/37/103/103	0/5/6/6
31	LMT	j	101	-	-	11/15/35/61	0/1/1/2
25	CLA	B	607	38	1/1/15/20	13/37/115/115	-
25	CLA	c	502	-	1/1/15/20	12/37/115/115	-
27	BCR	B	618	-	-	10/29/63/63	0/2/2/2
25	CLA	C	507	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	510	-	1/1/15/20	12/37/115/115	-
30	SQD	a	413	-	-	22/43/63/69	0/1/1/1
27	BCR	A	409	-	-	9/29/63/63	0/2/2/2
25	CLA	C	511	-	1/1/15/20	14/37/115/115	-
33	LHG	e	102	-	-	30/44/44/53	-
34	DGD	C	517	-	-	17/51/91/95	0/2/2/2
25	CLA	a	406	38	1/1/15/20	16/37/115/115	-
31	LMT	E	101	-	-	5/13/33/61	0/1/1/2
31	LMT	A	415	-	-	11/21/61/61	0/2/2/2
30	SQD	k	101	-	-	21/35/55/69	0/1/1/1
33	LHG	b	628	-	-	25/53/53/53	-
28	LMG	D	409	-	-	14/38/58/70	0/1/1/1
31	LMT	m	101	-	-	10/21/61/61	0/2/2/2
28	LMG	C	519	-	-	18/46/66/70	0/1/1/1
33	LHG	D	407	-	-	26/53/53/53	-
29	PL9	a	411	-	-	18/53/73/73	0/1/1/1
25	CLA	A	406	38	1/1/15/20	16/37/115/115	-
31	LMT	Y	101	-	-	7/12/32/61	0/1/1/2
27	BCR	f	101	-	-	9/29/63/63	0/2/2/2
25	CLA	d	401	38	1/1/15/20	11/37/115/115	-
31	LMT	b	624	-	-	9/15/35/61	0/1/1/2
27	BCR	k	102	-	-	15/29/63/63	0/2/2/2
25	CLA	B	615	-	1/1/15/20	13/37/115/115	-
30	SQD	A	413	-	-	22/43/63/69	0/1/1/1
31	LMT	B	626	-	-	5/15/35/61	0/1/1/2
31	LMT	M	102	-	-	4/15/35/61	0/1/1/2
34	DGD	c	516	-	-	14/51/91/95	0/2/2/2
31	LMT	H	102	-	-	9/15/35/61	0/1/1/2
31	LMT	C	524	-	-	10/21/61/61	0/2/2/2
31	LMT	x	102	-	-	9/12/32/61	0/1/1/2
34	DGD	C	516	-	-	14/51/91/95	0/2/2/2
31	LMT	X	104	-	-	7/10/30/61	0/1/1/2
25	CLA	C	509	-	1/1/15/20	11/37/115/115	-
25	CLA	D	404	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	611	-	1/1/15/20	10/37/115/115	-
30	SQD	K	101	-	-	21/35/55/69	0/1/1/1
31	LMT	B	629	-	-	11/21/61/61	0/2/2/2
31	LMT	e	101	-	-	5/13/33/61	0/1/1/2
31	LMT	i	103	-	-	8/21/61/61	0/2/2/2
25	CLA	C	510	-	1/1/15/20	12/37/115/115	-
25	CLA	b	605	-	1/1/15/20	12/37/115/115	-
27	BCR	k	103	-	-	8/29/63/63	0/2/2/2
25	CLA	c	512	3	1/1/15/20	21/37/115/115	-
25	CLA	b	607	38	1/1/15/20	13/37/115/115	-
31	LMT	X	105	-	-	6/10/30/61	0/1/1/2
26	PHO	a	407	-	-	9/37/103/103	0/5/6/6
25	CLA	b	613	-	1/1/15/20	8/37/115/115	-
27	BCR	Z	101	-	-	9/29/63/63	0/2/2/2
25	CLA	d	403	-	1/1/15/20	9/37/115/115	-
31	LMT	x	101	-	-	6/15/35/61	0/1/1/2
31	LMT	a	416	-	-	5/15/35/61	0/1/1/2
34	DGD	H	104	-	-	11/51/91/95	0/2/2/2
31	LMT	B	623	-	-	11/21/61/61	0/2/2/2
31	LMT	b	626	-	-	5/15/35/61	0/1/1/2
31	LMT	K	105	-	-	12/21/61/61	0/2/2/2
31	LMT	x	103	-	-	3/13/33/61	0/1/1/2
27	BCR	z	101	-	-	9/29/63/63	0/2/2/2
27	BCR	K	103	-	-	8/29/63/63	0/2/2/2
31	LMT	T	101	-	-	11/15/35/61	0/1/1/2
27	BCR	b	617	-	-	7/29/63/63	0/2/2/2
31	LMT	d	411	-	-	11/21/61/61	0/2/2/2
31	LMT	c	525	-	-	8/12/32/61	0/1/1/2
25	CLA	B	609	-	1/1/15/20	15/37/115/115	-
25	CLA	C	503	-	1/1/15/20	11/37/115/115	-
28	LMG	H	105	-	-	17/42/62/70	0/1/1/1
25	CLA	b	606	-	1/1/14/20	9/31/109/115	-
25	CLA	c	506	-	1/1/13/20	9/25/103/115	-
25	CLA	C	512	3	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	b	618	-	-	10/29/63/63	0/2/2/2
31	LMT	I	102	-	-	8/15/35/61	0/1/1/2
31	LMT	i	101	-	-	11/15/35/61	0/1/1/2
31	LMT	x	105	-	-	6/10/30/61	0/1/1/2
31	LMT	i	102	-	-	8/15/35/61	0/1/1/2
31	LMT	D	411	-	-	11/21/61/61	0/2/2/2
28	LMG	B	621	-	-	7/46/66/70	0/1/1/1
33	LHG	d	406	-	-	25/53/53/53	-
31	LMT	X	101	-	-	6/15/35/61	0/1/1/2
28	LMG	b	621	-	-	7/46/66/70	0/1/1/1
25	CLA	b	609	-	1/1/15/20	15/37/115/115	-
26	PHO	D	402	-	-	4/37/103/103	0/5/6/6
31	LMT	B	624	-	-	9/15/35/61	0/1/1/2
31	LMT	i	104	-	-	9/13/33/61	0/1/1/2
25	CLA	B	602	-	1/1/15/20	18/37/115/115	-
25	CLA	A	405	-	1/1/15/20	9/37/115/115	-
29	PL9	A	411	-	-	18/53/73/73	0/1/1/1
31	LMT	t	101	-	-	11/15/35/61	0/1/1/2
33	LHG	d	408	-	-	25/53/53/53	-
25	CLA	B	608	-	1/1/15/20	10/37/115/115	-
25	CLA	c	508	38	1/1/15/20	12/37/115/115	-
25	CLA	c	503	-	1/1/15/20	11/37/115/115	-
25	CLA	d	404	-	1/1/15/20	11/37/115/115	-
28	LMG	c	519	-	-	18/46/66/70	0/1/1/1
31	LMT	X	103	-	-	3/13/33/61	0/1/1/2
27	BCR	F	101	-	-	9/29/63/63	0/2/2/2
25	CLA	a	408	-	1/1/14/20	14/31/109/115	-
31	LMT	I	104	-	-	9/13/33/61	0/1/1/2
31	LMT	f	103	-	-	11/21/61/61	0/2/2/2
25	CLA	B	601	38	1/1/11/20	4/13/91/115	-
33	LHG	B	628	-	-	25/53/53/53	-
31	LMT	C	525	-	-	8/12/32/61	0/1/1/2
25	CLA	c	504	-	1/1/15/20	6/37/115/115	-
30	SQD	A	412	-	-	26/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	b	627	-	-	30/53/53/53	-
31	LMT	I	103	-	-	8/21/61/61	0/2/2/2
34	DGD	c	518	-	-	15/51/91/95	0/2/2/2
29	PL9	D	405	-	-	9/53/73/73	0/1/1/1
28	LMG	A	414	-	-	6/31/51/70	0/1/1/1
25	CLA	c	505	38	1/1/15/20	13/37/115/115	-
25	CLA	b	615	-	1/1/15/20	13/37/115/115	-
27	BCR	B	619	-	-	11/29/63/63	0/2/2/2
25	CLA	B	604	-	1/1/15/20	13/37/115/115	-
25	CLA	C	505	38	1/1/15/20	13/37/115/115	-
25	CLA	b	610	38	1/1/15/20	8/37/115/115	-
25	CLA	B	603	-	1/1/15/20	18/37/115/115	-
33	LHG	z	102	-	-	24/37/37/53	-
27	BCR	C	515	-	-	9/29/63/63	0/2/2/2
30	SQD	B	620	-	-	24/49/69/69	0/1/1/1
31	LMT	F	103	-	-	11/21/61/61	0/2/2/2
25	CLA	b	612	-	1/1/15/20	11/37/115/115	-
31	LMT	b	629	-	-	11/21/61/61	0/2/2/2
25	CLA	b	601	38	1/1/11/20	4/13/91/115	-
27	BCR	B	617	-	-	7/29/63/63	0/2/2/2
25	CLA	b	614	-	1/1/15/20	16/37/115/115	-
26	PHO	A	407	-	-	9/37/103/103	0/5/6/6
36	RRX	h	101	-	-	16/29/65/65	0/2/2/2
25	CLA	c	511	-	1/1/15/20	14/37/115/115	-
25	CLA	C	504	-	1/1/15/20	6/37/115/115	-
31	LMT	c	524	-	-	10/21/61/61	0/2/2/2
31	LMT	m	102	-	-	4/15/35/61	0/1/1/2
30	SQD	F	102	-	-	16/29/49/69	0/1/1/1
31	LMT	X	102	-	-	9/12/32/61	0/1/1/2
33	LHG	d	407	-	-	26/53/53/53	-
25	CLA	B	613	-	1/1/15/20	8/37/115/115	-
33	LHG	Z	102	-	-	24/37/37/53	-
25	CLA	B	616	-	1/1/14/20	17/31/109/115	-
35	HEM	E	104	6,5	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	b	623	-	-	11/21/61/61	0/2/2/2
36	RRX	H	101	-	-	16/29/65/65	0/2/2/2
35	HEM	v	201	18	-	2/12/54/54	-
31	LMT	E	103	-	-	8/21/61/61	0/2/2/2
25	CLA	b	604	-	1/1/15/20	13/37/115/115	-
31	LMT	J	101	-	-	11/15/35/61	0/1/1/2
30	SQD	h	103	-	-	16/49/69/69	0/1/1/1
31	LMT	D	410	-	-	8/15/35/61	0/1/1/2
30	SQD	f	102	-	-	16/29/49/69	0/1/1/1
33	LHG	E	102	-	-	30/44/44/53	-
34	DGD	C	518	-	-	15/51/91/95	0/2/2/2
33	LHG	D	408	-	-	25/53/53/53	-
27	BCR	a	409	-	-	9/29/63/63	0/2/2/2
31	LMT	a	415	-	-	10/21/61/61	0/2/2/2
25	CLA	C	513	-	1/1/12/20	7/19/97/115	-
28	LMG	c	523	-	-	17/44/64/70	0/1/1/1
31	LMT	x	104	-	-	7/10/30/61	0/1/1/2
27	BCR	c	515	-	-	9/29/63/63	0/2/2/2
30	SQD	C	501	-	-	29/49/69/69	0/1/1/1
28	LMG	C	523	-	-	17/44/64/70	0/1/1/1
31	LMT	c	522	-	-	7/15/35/61	0/1/1/2
33	LHG	B	627	-	-	30/53/53/53	-
25	CLA	B	614	-	1/1/15/20	16/37/115/115	-
35	HEM	V	201	18	-	2/12/54/54	-
31	LMT	d	412	-	-	7/21/61/61	0/2/2/2
25	CLA	C	502	-	1/1/15/20	12/37/115/115	-
25	CLA	c	513	-	1/1/12/20	7/19/97/115	-
31	LMT	M	101	-	-	10/21/61/61	0/2/2/2
30	SQD	H	103	-	-	16/49/69/69	0/1/1/1
25	CLA	D	403	-	1/1/15/20	9/37/115/115	-
28	LMG	a	410	-	-	21/46/66/70	0/1/1/1
25	CLA	c	509	-	1/1/15/20	11/37/115/115	-
25	CLA	c	514	-	1/1/15/20	20/37/115/115	-
25	CLA	a	405	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	508	38	1/1/15/20	12/37/115/115	-
25	CLA	b	602	-	1/1/15/20	18/37/115/115	-
27	BCR	b	619	-	-	11/29/63/63	0/2/2/2
30	SQD	a	412	-	-	26/49/69/69	0/1/1/1
31	LMT	h	102	-	-	9/15/35/61	0/1/1/2
25	CLA	b	616	-	1/1/14/20	17/31/109/115	-
31	LMT	C	522	-	-	7/15/35/61	0/1/1/2
28	LMG	h	105	-	-	17/42/62/70	0/1/1/1
28	LMG	A	410	-	-	21/46/66/70	0/1/1/1
25	CLA	B	605	-	1/1/15/20	12/37/115/115	-
27	BCR	K	102	-	-	15/29/63/63	0/2/2/2

All (1988) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Z	101	BCR	C8-C9	-8.68	1.27	1.45
27	z	101	BCR	C8-C9	-8.68	1.27	1.45
27	B	619	BCR	C8-C9	-8.44	1.27	1.45
27	b	619	BCR	C8-C9	-8.44	1.27	1.45
27	B	617	BCR	C8-C9	-8.44	1.27	1.45
27	b	617	BCR	C8-C9	-8.44	1.27	1.45
27	B	618	BCR	C8-C9	-8.44	1.27	1.45
27	b	618	BCR	C8-C9	-8.44	1.27	1.45
27	C	515	BCR	C8-C9	-8.33	1.28	1.45
27	c	515	BCR	C8-C9	-8.33	1.28	1.45
27	B	619	BCR	C11-C10	-8.29	1.17	1.43
27	b	619	BCR	C11-C10	-8.29	1.17	1.43
27	B	617	BCR	C11-C10	-8.23	1.17	1.43
27	b	617	BCR	C11-C10	-8.23	1.17	1.43
27	K	103	BCR	C8-C9	-8.21	1.28	1.45
27	k	103	BCR	C8-C9	-8.21	1.28	1.45
27	A	409	BCR	C8-C9	-8.17	1.28	1.45
27	a	409	BCR	C8-C9	-8.17	1.28	1.45
27	B	618	BCR	C11-C10	-8.17	1.18	1.43
27	b	618	BCR	C11-C10	-8.17	1.18	1.43
27	C	515	BCR	C11-C10	-8.16	1.18	1.43
27	c	515	BCR	C11-C10	-8.15	1.18	1.43
27	K	103	BCR	C11-C10	-8.15	1.18	1.43
27	k	103	BCR	C11-C10	-8.15	1.18	1.43
27	A	409	BCR	C11-C10	-8.08	1.18	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	409	BCR	C11-C10	-8.08	1.18	1.43
27	K	102	BCR	C8-C9	-8.04	1.28	1.45
27	k	102	BCR	C8-C9	-8.04	1.28	1.45
25	C	504	CLA	MG-NA	8.01	2.25	2.06
25	c	504	CLA	MG-NA	8.01	2.25	2.06
27	F	101	BCR	C8-C9	-8.01	1.28	1.45
27	f	101	BCR	C8-C9	-8.01	1.28	1.45
27	F	101	BCR	C11-C10	-7.97	1.18	1.43
27	f	101	BCR	C11-C10	-7.97	1.18	1.43
27	B	619	BCR	C10-C9	-7.96	1.25	1.35
27	b	619	BCR	C10-C9	-7.96	1.25	1.35
27	b	617	BCR	C10-C9	-7.95	1.25	1.35
27	Z	101	BCR	C11-C10	-7.94	1.18	1.43
27	z	101	BCR	C11-C10	-7.94	1.18	1.43
27	B	617	BCR	C10-C9	-7.92	1.25	1.35
27	K	102	BCR	C11-C10	-7.91	1.18	1.43
27	k	102	BCR	C11-C10	-7.91	1.18	1.43
27	C	515	BCR	C10-C9	-7.90	1.25	1.35
27	c	515	BCR	C10-C9	-7.90	1.25	1.35
27	K	102	BCR	C20-C21	-7.79	1.19	1.43
27	k	102	BCR	C20-C21	-7.79	1.19	1.43
25	B	609	CLA	MG-NA	7.76	2.24	2.06
25	b	609	CLA	MG-NA	7.76	2.24	2.06
27	B	618	BCR	C10-C9	-7.71	1.25	1.35
27	b	618	BCR	C10-C9	-7.71	1.25	1.35
27	A	409	BCR	C10-C9	-7.70	1.25	1.35
27	a	409	BCR	C10-C9	-7.70	1.25	1.35
25	B	606	CLA	MG-NA	7.68	2.24	2.06
25	b	606	CLA	MG-NA	7.67	2.24	2.06
27	K	103	BCR	C10-C9	-7.65	1.25	1.35
27	k	103	BCR	C10-C9	-7.65	1.25	1.35
25	C	508	CLA	MG-NA	7.64	2.24	2.06
25	c	508	CLA	MG-NA	7.64	2.24	2.06
27	B	618	BCR	C20-C21	-7.60	1.19	1.43
27	b	618	BCR	C20-C21	-7.60	1.19	1.43
25	B	601	CLA	MG-NA	7.60	2.24	2.06
25	b	601	CLA	MG-NA	7.60	2.24	2.06
25	B	610	CLA	MG-NA	7.58	2.24	2.06
25	b	610	CLA	MG-NA	7.58	2.24	2.06
27	F	101	BCR	C10-C9	-7.56	1.25	1.35
27	f	101	BCR	C10-C9	-7.56	1.25	1.35
27	B	617	BCR	C20-C21	-7.56	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	617	BCR	C20-C21	-7.56	1.20	1.43
27	B	619	BCR	C20-C21	-7.55	1.20	1.43
27	b	619	BCR	C20-C21	-7.55	1.20	1.43
27	A	409	BCR	C20-C21	-7.54	1.20	1.43
27	a	409	BCR	C20-C21	-7.54	1.20	1.43
27	B	618	BCR	C16-C17	-7.54	1.20	1.43
27	b	618	BCR	C16-C17	-7.54	1.20	1.43
27	C	515	BCR	C20-C21	-7.51	1.20	1.43
27	c	515	BCR	C20-C21	-7.51	1.20	1.43
27	B	619	BCR	C16-C17	-7.47	1.20	1.43
27	b	619	BCR	C16-C17	-7.47	1.20	1.43
25	B	604	CLA	MG-NA	7.47	2.24	2.06
25	c	507	CLA	MG-NA	7.46	2.24	2.06
25	C	507	CLA	MG-NA	7.46	2.24	2.06
25	b	603	CLA	MG-NA	7.46	2.24	2.06
25	B	603	CLA	MG-NA	7.45	2.24	2.06
25	b	604	CLA	MG-NA	7.45	2.24	2.06
25	B	608	CLA	MG-NA	7.44	2.23	2.06
25	C	509	CLA	MG-NA	7.44	2.23	2.06
27	C	515	BCR	C16-C17	-7.43	1.20	1.43
25	b	608	CLA	MG-NA	7.43	2.23	2.06
27	k	103	BCR	C20-C21	-7.43	1.20	1.43
27	c	515	BCR	C16-C17	-7.42	1.20	1.43
27	B	617	BCR	C16-C17	-7.42	1.20	1.43
27	b	617	BCR	C16-C17	-7.42	1.20	1.43
25	c	509	CLA	MG-NA	7.42	2.23	2.06
27	z	101	BCR	C16-C17	-7.42	1.20	1.43
27	K	103	BCR	C20-C21	-7.40	1.20	1.43
27	A	409	BCR	C16-C17	-7.40	1.20	1.43
27	a	409	BCR	C16-C17	-7.40	1.20	1.43
25	c	512	CLA	MG-NA	7.39	2.23	2.06
27	Z	101	BCR	C16-C17	-7.39	1.20	1.43
25	C	512	CLA	MG-NA	7.39	2.23	2.06
27	K	103	BCR	C16-C17	-7.39	1.20	1.43
27	k	103	BCR	C16-C17	-7.39	1.20	1.43
25	B	602	CLA	MG-NA	7.39	2.23	2.06
25	b	602	CLA	MG-NA	7.39	2.23	2.06
25	C	510	CLA	MG-NA	7.37	2.23	2.06
25	C	513	CLA	MG-NA	7.36	2.23	2.06
25	c	513	CLA	MG-NA	7.36	2.23	2.06
27	Z	101	BCR	C20-C21	-7.35	1.20	1.43
27	z	101	BCR	C20-C21	-7.35	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	MG-NA	7.35	2.23	2.06
25	c	510	CLA	MG-NA	7.34	2.23	2.06
25	B	611	CLA	MG-NA	7.33	2.23	2.06
25	b	611	CLA	MG-NA	7.33	2.23	2.06
25	c	502	CLA	MG-NA	7.33	2.23	2.06
27	F	101	BCR	C20-C21	-7.32	1.20	1.43
27	f	101	BCR	C20-C21	-7.32	1.20	1.43
25	a	406	CLA	MG-NA	7.32	2.23	2.06
25	C	511	CLA	MG-NA	7.31	2.23	2.06
25	c	511	CLA	MG-NA	7.31	2.23	2.06
25	A	406	CLA	MG-NA	7.28	2.23	2.06
27	z	101	BCR	C10-C9	-7.28	1.26	1.35
27	F	101	BCR	C16-C17	-7.27	1.20	1.43
27	f	101	BCR	C16-C17	-7.27	1.20	1.43
27	k	102	BCR	C10-C9	-7.25	1.26	1.35
25	B	615	CLA	MG-NA	7.24	2.23	2.06
25	b	615	CLA	MG-NA	7.24	2.23	2.06
25	C	514	CLA	MG-NA	7.24	2.23	2.06
25	c	514	CLA	MG-NA	7.24	2.23	2.06
27	K	102	BCR	C10-C9	-7.24	1.26	1.35
27	Z	101	BCR	C10-C9	-7.23	1.26	1.35
27	k	102	BCR	C16-C17	-7.22	1.21	1.43
25	c	506	CLA	MG-NA	7.22	2.23	2.06
25	D	404	CLA	MG-NA	7.22	2.23	2.06
25	d	404	CLA	MG-NA	7.22	2.23	2.06
27	K	102	BCR	C16-C17	-7.22	1.21	1.43
25	a	408	CLA	MG-NA	7.21	2.23	2.06
25	C	506	CLA	MG-NA	7.21	2.23	2.06
25	B	614	CLA	MG-NA	7.20	2.23	2.06
25	b	614	CLA	MG-NA	7.20	2.23	2.06
25	A	408	CLA	MG-NA	7.18	2.23	2.06
25	B	612	CLA	MG-NA	7.15	2.23	2.06
25	b	612	CLA	MG-NA	7.15	2.23	2.06
25	C	503	CLA	MG-NA	7.14	2.23	2.06
25	c	503	CLA	MG-NA	7.14	2.23	2.06
25	B	613	CLA	MG-NA	7.05	2.23	2.06
25	b	613	CLA	MG-NA	7.05	2.23	2.06
25	B	605	CLA	MG-NA	7.03	2.23	2.06
25	b	605	CLA	MG-NA	7.03	2.23	2.06
25	B	607	CLA	MG-NA	6.95	2.22	2.06
25	b	607	CLA	MG-NA	6.95	2.22	2.06
25	D	403	CLA	MG-NA	6.95	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	CLA	MG-NA	6.95	2.22	2.06
25	C	505	CLA	MG-NA	6.94	2.22	2.06
25	D	401	CLA	MG-NA	6.93	2.22	2.06
25	c	505	CLA	MG-NA	6.93	2.22	2.06
25	d	401	CLA	MG-NA	6.89	2.22	2.06
25	B	616	CLA	MG-NA	6.85	2.22	2.06
25	b	616	CLA	MG-NA	6.85	2.22	2.06
25	A	405	CLA	MG-NA	6.78	2.22	2.06
25	a	405	CLA	MG-NA	6.78	2.22	2.06
25	d	403	CLA	C3B-C2B	5.60	1.48	1.40
25	A	408	CLA	C3B-C2B	5.59	1.48	1.40
25	a	408	CLA	C3B-C2B	5.59	1.48	1.40
25	D	403	CLA	C3B-C2B	5.58	1.48	1.40
25	C	514	CLA	C3B-C2B	5.58	1.48	1.40
25	c	514	CLA	C3B-C2B	5.58	1.48	1.40
25	B	612	CLA	C3B-C2B	5.38	1.47	1.40
25	b	612	CLA	C3B-C2B	5.38	1.47	1.40
25	B	605	CLA	C3B-C2B	5.32	1.47	1.40
25	b	605	CLA	C3B-C2B	5.32	1.47	1.40
25	C	504	CLA	C3B-C2B	5.31	1.47	1.40
25	c	504	CLA	C3B-C2B	5.31	1.47	1.40
25	c	512	CLA	C3B-C2B	5.21	1.47	1.40
25	C	512	CLA	C3B-C2B	5.21	1.47	1.40
25	C	514	CLA	O2D-CGD	5.20	1.45	1.33
25	c	514	CLA	O2D-CGD	5.20	1.45	1.33
25	C	514	CLA	CHC-C1C	5.20	1.48	1.35
25	C	505	CLA	O2A-C1	5.20	1.60	1.46
25	a	408	CLA	O2A-C1	5.20	1.60	1.46
25	A	408	CLA	O2A-C1	5.19	1.60	1.46
25	D	401	CLA	O2A-C1	5.19	1.60	1.46
25	d	401	CLA	O2A-C1	5.19	1.60	1.46
25	c	514	CLA	CHC-C1C	5.19	1.48	1.35
25	c	505	CLA	O2A-C1	5.19	1.60	1.46
25	b	610	CLA	O2A-C1	5.17	1.60	1.46
25	C	502	CLA	C3B-C2B	5.17	1.47	1.40
25	c	502	CLA	C3B-C2B	5.17	1.47	1.40
25	B	610	CLA	O2A-C1	5.17	1.60	1.46
25	B	614	CLA	C3B-C2B	5.15	1.47	1.40
25	b	614	CLA	C3B-C2B	5.15	1.47	1.40
25	C	509	CLA	O2D-CGD	5.15	1.45	1.33
25	c	509	CLA	O2D-CGD	5.15	1.45	1.33
25	B	607	CLA	O2A-C1	5.14	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	607	CLA	O2A-C1	5.14	1.60	1.46
25	c	510	CLA	O2A-C1	5.14	1.60	1.46
25	B	611	CLA	O2D-CGD	5.14	1.45	1.33
25	b	611	CLA	O2D-CGD	5.14	1.45	1.33
25	b	606	CLA	O2D-CGD	5.13	1.45	1.33
25	C	508	CLA	O2A-C1	5.12	1.60	1.46
25	A	406	CLA	O2D-CGD	5.12	1.45	1.33
25	a	406	CLA	O2D-CGD	5.12	1.45	1.33
25	C	510	CLA	O2A-C1	5.11	1.60	1.46
25	A	405	CLA	C3B-C2B	5.11	1.47	1.40
25	a	405	CLA	C3B-C2B	5.11	1.47	1.40
25	C	513	CLA	O2A-C1	5.11	1.60	1.46
25	B	606	CLA	O2D-CGD	5.11	1.45	1.33
25	c	513	CLA	O2A-C1	5.10	1.60	1.46
25	A	406	CLA	O2A-C1	5.10	1.60	1.46
25	c	508	CLA	O2A-C1	5.10	1.60	1.46
25	c	503	CLA	O2D-CGD	5.10	1.45	1.33
25	B	602	CLA	CHC-C1C	5.09	1.48	1.35
25	b	602	CLA	CHC-C1C	5.09	1.48	1.35
25	C	507	CLA	O2D-CGD	5.08	1.45	1.33
25	c	507	CLA	O2D-CGD	5.08	1.45	1.33
25	b	614	CLA	O2A-C1	5.08	1.60	1.46
25	C	504	CLA	O2A-C1	5.08	1.60	1.46
25	c	504	CLA	O2A-C1	5.08	1.60	1.46
25	B	603	CLA	O2A-C1	5.07	1.60	1.46
25	b	603	CLA	O2A-C1	5.07	1.60	1.46
25	C	503	CLA	O2D-CGD	5.07	1.45	1.33
25	C	514	CLA	O2A-C1	5.07	1.60	1.46
25	a	406	CLA	O2A-C1	5.07	1.60	1.46
25	B	601	CLA	O2D-CGD	5.07	1.45	1.33
25	b	601	CLA	O2D-CGD	5.07	1.45	1.33
25	c	509	CLA	CHC-C1C	5.06	1.47	1.35
25	C	512	CLA	O2D-CGD	5.06	1.45	1.33
25	c	512	CLA	O2D-CGD	5.06	1.45	1.33
25	B	610	CLA	C3B-C2B	5.06	1.47	1.40
25	B	606	CLA	CHC-C1C	5.06	1.47	1.35
25	b	606	CLA	CHC-C1C	5.06	1.47	1.35
25	C	509	CLA	CHC-C1C	5.06	1.47	1.35
25	b	612	CLA	O2D-CGD	5.05	1.45	1.33
25	B	614	CLA	O2A-C1	5.05	1.60	1.46
25	c	514	CLA	O2A-C1	5.05	1.60	1.46
25	c	502	CLA	O2D-CGD	5.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	509	CLA	O2A-C1	5.05	1.60	1.46
25	A	405	CLA	CHC-C1C	5.05	1.47	1.35
25	a	405	CLA	CHC-C1C	5.05	1.47	1.35
25	B	612	CLA	O2D-CGD	5.04	1.45	1.33
25	b	607	CLA	O2D-CGD	5.04	1.45	1.33
25	C	506	CLA	O2D-CGD	5.04	1.45	1.33
25	c	506	CLA	O2D-CGD	5.04	1.45	1.33
25	C	513	CLA	C3B-C2B	5.04	1.47	1.40
25	c	513	CLA	C3B-C2B	5.04	1.47	1.40
25	A	405	CLA	O2D-CGD	5.04	1.45	1.33
25	a	405	CLA	O2D-CGD	5.04	1.45	1.33
25	C	503	CLA	O2A-C1	5.04	1.60	1.46
25	c	503	CLA	O2A-C1	5.04	1.60	1.46
25	C	504	CLA	CHC-C1C	5.04	1.47	1.35
25	c	504	CLA	CHC-C1C	5.04	1.47	1.35
25	D	401	CLA	O2D-CGD	5.03	1.45	1.33
25	B	607	CLA	O2D-CGD	5.03	1.45	1.33
25	B	609	CLA	O2D-CGD	5.03	1.45	1.33
25	C	502	CLA	O2D-CGD	5.03	1.45	1.33
25	b	609	CLA	O2D-CGD	5.03	1.45	1.33
25	b	610	CLA	C3B-C2B	5.02	1.47	1.40
25	c	509	CLA	O2A-C1	5.02	1.60	1.46
25	B	602	CLA	O2A-C1	5.02	1.60	1.46
25	b	602	CLA	O2A-C1	5.02	1.60	1.46
25	D	403	CLA	CHC-C1C	5.02	1.47	1.35
25	d	403	CLA	CHC-C1C	5.02	1.47	1.35
25	d	401	CLA	O2D-CGD	5.01	1.45	1.33
25	D	404	CLA	CHC-C1C	5.01	1.47	1.35
25	d	404	CLA	CHC-C1C	5.01	1.47	1.35
25	D	403	CLA	C1D-ND	-5.00	1.31	1.37
25	d	403	CLA	C1D-ND	-5.00	1.31	1.37
25	b	606	CLA	O2A-C1	5.00	1.60	1.46
25	B	606	CLA	O2A-C1	5.00	1.60	1.46
25	B	608	CLA	O2A-C1	5.00	1.60	1.46
25	b	608	CLA	O2A-C1	5.00	1.60	1.46
25	B	615	CLA	C3B-C2B	5.00	1.47	1.40
25	b	615	CLA	C3B-C2B	5.00	1.47	1.40
25	B	605	CLA	O2D-CGD	4.99	1.45	1.33
25	b	605	CLA	O2D-CGD	4.99	1.45	1.33
25	B	608	CLA	O2D-CGD	4.99	1.45	1.33
25	C	506	CLA	CHC-C1C	4.99	1.47	1.35
25	c	506	CLA	CHC-C1C	4.99	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	608	CLA	O2D-CGD	4.98	1.45	1.33
25	b	612	CLA	CHC-C1C	4.98	1.47	1.35
25	B	612	CLA	CHC-C1C	4.98	1.47	1.35
25	B	616	CLA	O2D-CGD	4.98	1.45	1.33
25	b	616	CLA	O2D-CGD	4.98	1.45	1.33
25	c	505	CLA	O2D-CGD	4.98	1.45	1.33
25	B	604	CLA	O2D-CGD	4.98	1.45	1.33
25	b	604	CLA	O2D-CGD	4.98	1.45	1.33
25	C	505	CLA	O2D-CGD	4.97	1.45	1.33
25	B	616	CLA	C3B-C2B	4.97	1.47	1.40
25	b	616	CLA	C3B-C2B	4.97	1.47	1.40
25	b	616	CLA	O2A-C1	4.96	1.60	1.46
25	C	513	CLA	O2D-CGD	4.96	1.45	1.33
25	c	513	CLA	O2D-CGD	4.96	1.45	1.33
25	C	512	CLA	CHC-C1C	4.96	1.47	1.35
25	D	404	CLA	O2A-C1	4.96	1.60	1.46
25	d	404	CLA	O2A-C1	4.96	1.60	1.46
25	B	605	CLA	CHC-C1C	4.95	1.47	1.35
25	b	605	CLA	CHC-C1C	4.95	1.47	1.35
25	c	512	CLA	CHC-C1C	4.95	1.47	1.35
25	B	613	CLA	O2A-C1	4.95	1.60	1.46
25	b	613	CLA	O2A-C1	4.95	1.60	1.46
25	b	612	CLA	C1D-ND	-4.95	1.31	1.37
25	B	610	CLA	O2D-CGD	4.95	1.45	1.33
25	b	610	CLA	O2D-CGD	4.95	1.45	1.33
25	C	507	CLA	O2A-C1	4.95	1.60	1.46
25	c	507	CLA	O2A-C1	4.95	1.60	1.46
25	b	609	CLA	O2A-C1	4.95	1.60	1.46
25	B	609	CLA	O2A-C1	4.94	1.60	1.46
25	B	612	CLA	C1D-ND	-4.94	1.31	1.37
25	B	614	CLA	CHC-C1C	4.94	1.47	1.35
25	b	614	CLA	CHC-C1C	4.94	1.47	1.35
25	C	502	CLA	CHC-C1C	4.94	1.47	1.35
25	C	512	CLA	O2A-C1	4.94	1.60	1.46
25	c	512	CLA	O2A-C1	4.94	1.60	1.46
25	B	616	CLA	O2A-C1	4.93	1.60	1.46
25	A	408	CLA	CHC-C1C	4.92	1.47	1.35
25	a	408	CLA	CHC-C1C	4.92	1.47	1.35
25	A	408	CLA	O2D-CGD	4.92	1.45	1.33
25	a	408	CLA	O2D-CGD	4.92	1.45	1.33
25	c	502	CLA	CHC-C1C	4.92	1.47	1.35
25	B	615	CLA	O2A-C1	4.91	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	615	CLA	O2A-C1	4.91	1.60	1.46
25	c	511	CLA	O2D-CGD	4.91	1.45	1.33
25	C	502	CLA	O2A-C1	4.91	1.60	1.46
25	c	502	CLA	O2A-C1	4.89	1.59	1.46
25	B	604	CLA	O2A-C1	4.89	1.59	1.46
25	b	604	CLA	O2A-C1	4.89	1.59	1.46
25	B	603	CLA	O2D-CGD	4.89	1.45	1.33
25	b	603	CLA	O2D-CGD	4.89	1.45	1.33
25	C	511	CLA	O2D-CGD	4.88	1.45	1.33
25	B	605	CLA	O2A-C1	4.88	1.59	1.46
25	b	605	CLA	O2A-C1	4.88	1.59	1.46
25	C	506	CLA	C3B-C2B	4.86	1.47	1.40
25	c	506	CLA	C3B-C2B	4.86	1.47	1.40
25	D	401	CLA	C3B-C2B	4.85	1.47	1.40
25	d	401	CLA	C3B-C2B	4.85	1.47	1.40
25	D	404	CLA	O2D-CGD	4.85	1.45	1.33
25	d	404	CLA	O2D-CGD	4.85	1.45	1.33
25	C	511	CLA	O2A-C1	4.85	1.59	1.46
25	c	511	CLA	O2A-C1	4.85	1.59	1.46
25	B	613	CLA	O2D-CGD	4.84	1.45	1.33
25	b	613	CLA	O2D-CGD	4.84	1.45	1.33
25	B	615	CLA	O2D-CGD	4.83	1.45	1.33
25	b	615	CLA	O2D-CGD	4.83	1.45	1.33
25	A	405	CLA	O2A-C1	4.83	1.59	1.46
25	a	405	CLA	O2A-C1	4.83	1.59	1.46
25	C	506	CLA	O2A-C1	4.82	1.59	1.46
25	c	511	CLA	C3B-C2B	4.82	1.47	1.40
25	C	508	CLA	O2D-CGD	4.82	1.45	1.33
25	c	508	CLA	O2D-CGD	4.82	1.45	1.33
25	c	506	CLA	O2A-C1	4.81	1.59	1.46
25	C	511	CLA	C3B-C2B	4.79	1.47	1.40
25	b	612	CLA	O2A-C1	4.78	1.59	1.46
25	A	405	CLA	C3D-C4D	-4.77	1.33	1.44
25	a	405	CLA	C3D-C4D	-4.77	1.33	1.44
25	B	615	CLA	CHC-C1C	4.77	1.47	1.35
25	b	615	CLA	CHC-C1C	4.77	1.47	1.35
25	c	505	CLA	C3B-C2B	4.76	1.47	1.40
25	B	612	CLA	O2A-C1	4.76	1.59	1.46
25	d	403	CLA	O2A-C1	4.76	1.59	1.46
25	B	614	CLA	O2D-CGD	4.75	1.44	1.33
25	b	614	CLA	O2D-CGD	4.75	1.44	1.33
25	D	403	CLA	O2A-C1	4.75	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	608	CLA	CHC-C1C	4.73	1.47	1.35
25	B	603	CLA	C3D-C4D	-4.72	1.33	1.44
25	b	608	CLA	CHC-C1C	4.72	1.47	1.35
25	b	609	CLA	CHC-C1C	4.72	1.47	1.35
25	B	602	CLA	O2D-CGD	4.72	1.44	1.33
25	b	602	CLA	O2D-CGD	4.72	1.44	1.33
25	B	609	CLA	CHC-C1C	4.71	1.47	1.35
25	D	403	CLA	O2D-CGD	4.71	1.44	1.33
25	C	506	CLA	C3D-C4D	-4.70	1.33	1.44
25	c	506	CLA	C3D-C4D	-4.70	1.33	1.44
25	b	607	CLA	CHC-C1C	4.70	1.47	1.35
25	C	505	CLA	C3B-C2B	4.70	1.46	1.40
25	B	607	CLA	CHC-C1C	4.69	1.47	1.35
25	d	403	CLA	O2D-CGD	4.69	1.44	1.33
25	b	603	CLA	C3D-C4D	-4.69	1.33	1.44
25	A	406	CLA	CHC-C1C	4.69	1.47	1.35
29	D	405	PL9	C7-C3	-4.69	1.46	1.51
29	d	405	PL9	C7-C3	-4.68	1.46	1.51
25	B	608	CLA	C3B-C2B	4.68	1.46	1.40
25	b	608	CLA	C3B-C2B	4.68	1.46	1.40
25	C	509	CLA	C3B-C2B	4.68	1.46	1.40
25	c	509	CLA	C3B-C2B	4.68	1.46	1.40
25	A	406	CLA	C3B-C2B	4.67	1.46	1.40
25	a	406	CLA	CHC-C1C	4.67	1.46	1.35
25	B	611	CLA	O2A-C1	4.67	1.59	1.46
25	b	611	CLA	O2A-C1	4.67	1.59	1.46
25	C	510	CLA	O2D-CGD	4.67	1.44	1.33
25	c	510	CLA	O2D-CGD	4.67	1.44	1.33
25	c	511	CLA	CHC-C1C	4.67	1.46	1.35
25	B	601	CLA	CHC-C1C	4.66	1.46	1.35
25	b	601	CLA	CHC-C1C	4.66	1.46	1.35
25	C	511	CLA	CHC-C1C	4.66	1.46	1.35
25	D	401	CLA	C3C-C2C	4.65	1.46	1.36
25	d	401	CLA	C3C-C2C	4.65	1.46	1.36
25	D	401	CLA	CHC-C1C	4.65	1.46	1.35
25	d	401	CLA	CHC-C1C	4.65	1.46	1.35
25	a	406	CLA	C3B-C2B	4.65	1.46	1.40
25	B	603	CLA	CHC-C1C	4.64	1.46	1.35
25	B	610	CLA	CHC-C1C	4.64	1.46	1.35
25	b	610	CLA	CHC-C1C	4.64	1.46	1.35
25	c	510	CLA	C3B-C2B	4.64	1.46	1.40
25	C	504	CLA	C3C-C2C	4.63	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	504	CLA	C3C-C2C	4.63	1.46	1.36
25	C	510	CLA	C3B-C2B	4.62	1.46	1.40
25	b	603	CLA	CHC-C1C	4.62	1.46	1.35
25	B	608	CLA	CHD-C1D	4.62	1.47	1.38
25	b	608	CLA	CHD-C1D	4.62	1.47	1.38
25	C	503	CLA	CHC-C1C	4.62	1.46	1.35
25	c	503	CLA	CHC-C1C	4.62	1.46	1.35
25	C	513	CLA	CHC-C1C	4.61	1.46	1.35
25	c	513	CLA	CHC-C1C	4.61	1.46	1.35
25	C	504	CLA	O2D-CGD	4.61	1.44	1.33
25	c	504	CLA	O2D-CGD	4.61	1.44	1.33
25	C	508	CLA	CHC-C1C	4.61	1.46	1.35
25	c	508	CLA	CHC-C1C	4.61	1.46	1.35
25	B	609	CLA	C3B-C2B	4.61	1.46	1.40
25	B	606	CLA	C3B-C2B	4.60	1.46	1.40
25	b	606	CLA	C3B-C2B	4.60	1.46	1.40
25	C	505	CLA	CHC-C1C	4.60	1.46	1.35
25	c	505	CLA	CHC-C1C	4.60	1.46	1.35
25	C	510	CLA	CHC-C1C	4.59	1.46	1.35
25	c	510	CLA	CHC-C1C	4.59	1.46	1.35
25	b	606	CLA	CHD-C1D	4.59	1.47	1.38
25	B	613	CLA	C3B-C2B	4.57	1.46	1.40
25	b	613	CLA	C3B-C2B	4.57	1.46	1.40
25	B	602	CLA	C3C-C2C	4.57	1.46	1.36
25	b	602	CLA	C3C-C2C	4.57	1.46	1.36
25	A	406	CLA	C3D-C4D	-4.57	1.33	1.44
25	a	406	CLA	C3D-C4D	-4.57	1.33	1.44
25	B	613	CLA	CHC-C1C	4.57	1.46	1.35
25	b	613	CLA	CHC-C1C	4.57	1.46	1.35
25	b	609	CLA	C3B-C2B	4.57	1.46	1.40
25	c	507	CLA	C3C-C2C	4.57	1.46	1.36
25	B	602	CLA	C3B-C2B	4.56	1.46	1.40
25	B	606	CLA	CHD-C1D	4.55	1.47	1.38
25	d	404	CLA	CHD-C1D	4.55	1.47	1.38
25	C	507	CLA	C3C-C2C	4.55	1.46	1.36
25	a	406	CLA	CHD-C1D	4.55	1.47	1.38
25	B	611	CLA	CHC-C1C	4.55	1.46	1.35
25	b	611	CLA	CHC-C1C	4.55	1.46	1.35
25	D	404	CLA	CHD-C1D	4.54	1.47	1.38
25	b	602	CLA	C3B-C2B	4.54	1.46	1.40
25	C	507	CLA	CHD-C1D	4.53	1.47	1.38
25	c	507	CLA	CHD-C1D	4.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	406	CLA	CHD-C1D	4.53	1.47	1.38
25	A	406	CLA	C3C-C2C	4.53	1.46	1.36
25	C	502	CLA	CHD-C1D	4.53	1.47	1.38
25	c	502	CLA	CHD-C1D	4.53	1.47	1.38
25	B	612	CLA	C3D-C4D	-4.52	1.34	1.44
25	B	608	CLA	C3D-C4D	-4.52	1.34	1.44
25	b	608	CLA	C3D-C4D	-4.52	1.34	1.44
25	b	612	CLA	C3D-C4D	-4.51	1.34	1.44
25	C	505	CLA	CHD-C1D	4.51	1.47	1.38
25	B	611	CLA	C3B-C2B	4.51	1.46	1.40
25	b	611	CLA	C3B-C2B	4.51	1.46	1.40
25	b	604	CLA	CHC-C1C	4.51	1.46	1.35
25	B	602	CLA	CHD-C1D	4.50	1.47	1.38
25	b	602	CLA	CHD-C1D	4.50	1.47	1.38
25	D	404	CLA	C3C-C2C	4.50	1.46	1.36
25	d	404	CLA	C3C-C2C	4.50	1.46	1.36
25	c	505	CLA	CHD-C1D	4.50	1.47	1.38
25	B	604	CLA	C3D-C4D	-4.50	1.34	1.44
25	a	406	CLA	C3C-C2C	4.50	1.46	1.36
25	c	508	CLA	C3D-C4D	-4.50	1.34	1.44
25	C	508	CLA	C3D-C4D	-4.49	1.34	1.44
25	B	604	CLA	CHC-C1C	4.49	1.46	1.35
25	b	604	CLA	C3D-C4D	-4.49	1.34	1.44
25	B	606	CLA	C3D-C4D	-4.49	1.34	1.44
25	b	606	CLA	C3D-C4D	-4.49	1.34	1.44
25	C	514	CLA	C3C-C2C	4.48	1.46	1.36
25	c	514	CLA	C3C-C2C	4.48	1.46	1.36
25	C	512	CLA	C3C-C2C	4.47	1.46	1.36
25	c	512	CLA	C3C-C2C	4.47	1.46	1.36
25	B	610	CLA	C3C-C2C	4.46	1.46	1.36
25	b	610	CLA	C3C-C2C	4.46	1.46	1.36
25	D	403	CLA	C3C-C2C	4.46	1.46	1.36
25	d	403	CLA	C3C-C2C	4.46	1.46	1.36
25	b	603	CLA	C3B-C2B	4.46	1.46	1.40
25	C	503	CLA	C3D-C4D	-4.46	1.34	1.44
25	c	503	CLA	C3D-C4D	-4.46	1.34	1.44
25	C	511	CLA	C3D-C4D	-4.46	1.34	1.44
25	c	511	CLA	C3D-C4D	-4.46	1.34	1.44
25	C	503	CLA	C3C-C2C	4.45	1.46	1.36
25	c	503	CLA	C3C-C2C	4.45	1.46	1.36
25	B	610	CLA	C3D-C4D	-4.45	1.34	1.44
25	b	610	CLA	C3D-C4D	-4.45	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	C3B-C2B	4.44	1.46	1.40
25	C	509	CLA	C3C-C2C	4.44	1.46	1.36
25	c	509	CLA	C3C-C2C	4.44	1.46	1.36
25	C	506	CLA	C3C-C2C	4.44	1.46	1.36
25	A	408	CLA	C3C-C2C	4.44	1.46	1.36
25	D	404	CLA	C3D-C4D	-4.44	1.34	1.44
25	d	404	CLA	C3D-C4D	-4.44	1.34	1.44
25	c	506	CLA	C3C-C2C	4.43	1.46	1.36
25	B	604	CLA	CHD-C1D	4.43	1.47	1.38
25	C	503	CLA	C3B-C2B	4.43	1.46	1.40
25	c	503	CLA	C3B-C2B	4.43	1.46	1.40
25	d	404	CLA	C3B-C2B	4.43	1.46	1.40
25	B	601	CLA	C3B-C2B	4.43	1.46	1.40
25	b	601	CLA	C3B-C2B	4.43	1.46	1.40
25	a	408	CLA	C3C-C2C	4.42	1.46	1.36
25	B	616	CLA	CHD-C1D	4.42	1.47	1.38
25	b	616	CLA	CHD-C1D	4.42	1.47	1.38
25	C	509	CLA	CHD-C1D	4.42	1.47	1.38
25	c	509	CLA	CHD-C1D	4.42	1.47	1.38
25	B	601	CLA	C3C-C2C	4.41	1.46	1.36
25	b	601	CLA	C3C-C2C	4.41	1.46	1.36
28	H	105	LMG	O8-C28	4.41	1.46	1.33
25	B	609	CLA	CHD-C1D	4.41	1.47	1.38
25	b	609	CLA	CHD-C1D	4.41	1.47	1.38
28	h	105	LMG	O8-C28	4.40	1.46	1.33
25	D	404	CLA	C3B-C2B	4.40	1.46	1.40
25	b	604	CLA	CHD-C1D	4.40	1.46	1.38
25	B	603	CLA	C3C-C2C	4.39	1.46	1.36
25	b	603	CLA	C3C-C2C	4.39	1.46	1.36
28	a	410	LMG	O8-C28	4.38	1.46	1.33
25	C	510	CLA	CHD-C1D	4.38	1.46	1.38
25	c	510	CLA	CHD-C1D	4.38	1.46	1.38
25	d	401	CLA	CHD-C1D	4.38	1.46	1.38
25	b	606	CLA	C3C-C2C	4.38	1.46	1.36
25	B	606	CLA	C3C-C2C	4.38	1.46	1.36
33	Z	102	LHG	O8-C23	4.37	1.46	1.33
33	z	102	LHG	O8-C23	4.37	1.46	1.33
25	c	507	CLA	C3D-C4D	-4.37	1.34	1.44
25	D	401	CLA	CHD-C1D	4.37	1.46	1.38
28	A	410	LMG	O8-C28	4.37	1.46	1.33
25	C	502	CLA	C3D-C4D	-4.37	1.34	1.44
25	c	502	CLA	C3D-C4D	-4.37	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	614	CLA	C3D-C4D	-4.37	1.34	1.44
25	b	614	CLA	C3D-C4D	-4.37	1.34	1.44
25	C	513	CLA	C3C-C2C	4.36	1.46	1.36
25	C	502	CLA	C3C-C2C	4.36	1.46	1.36
25	C	511	CLA	CHD-C1D	4.35	1.46	1.38
25	c	511	CLA	CHD-C1D	4.35	1.46	1.38
25	B	616	CLA	C1C-NC	-4.35	1.31	1.37
25	c	513	CLA	C3C-C2C	4.34	1.46	1.36
25	c	502	CLA	C3C-C2C	4.34	1.46	1.36
25	B	609	CLA	C3D-C4D	-4.34	1.34	1.44
25	C	506	CLA	CHD-C1D	4.33	1.46	1.38
25	c	506	CLA	CHD-C1D	4.33	1.46	1.38
25	C	507	CLA	C3D-C4D	-4.33	1.34	1.44
33	B	627	LHG	O7-C7	4.32	1.46	1.34
25	A	408	CLA	CHD-C1D	4.32	1.46	1.38
25	B	615	CLA	C3D-C4D	-4.32	1.34	1.44
25	b	615	CLA	C3D-C4D	-4.32	1.34	1.44
25	C	508	CLA	C3C-C2C	4.32	1.45	1.36
28	a	414	LMG	O8-C28	4.32	1.46	1.33
28	C	523	LMG	O8-C28	4.31	1.45	1.33
28	c	523	LMG	O8-C28	4.31	1.45	1.33
25	B	607	CLA	C3D-C4D	-4.31	1.34	1.44
25	b	607	CLA	C3D-C4D	-4.31	1.34	1.44
25	b	609	CLA	C3D-C4D	-4.31	1.34	1.44
25	C	511	CLA	C3C-C2C	4.31	1.45	1.36
25	c	511	CLA	C3C-C2C	4.31	1.45	1.36
25	A	408	CLA	C3D-C4D	-4.31	1.34	1.44
25	C	510	CLA	C3C-C2C	4.31	1.45	1.36
25	c	510	CLA	C3C-C2C	4.31	1.45	1.36
25	b	616	CLA	C1C-NC	-4.31	1.31	1.37
25	B	613	CLA	C3D-C4D	-4.31	1.34	1.44
25	b	613	CLA	C3D-C4D	-4.31	1.34	1.44
25	a	408	CLA	CHD-C1D	4.30	1.46	1.38
25	D	403	CLA	C3D-C4D	-4.30	1.34	1.44
25	d	403	CLA	C3D-C4D	-4.30	1.34	1.44
25	B	613	CLA	C3C-C2C	4.30	1.45	1.36
25	b	613	CLA	C3C-C2C	4.30	1.45	1.36
33	b	627	LHG	O7-C7	4.29	1.46	1.34
25	c	508	CLA	C3C-C2C	4.29	1.45	1.36
28	A	414	LMG	O8-C28	4.29	1.45	1.33
25	B	610	CLA	CHD-C1D	4.28	1.46	1.38
25	b	610	CLA	CHD-C1D	4.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	E	102	LHG	O8-C23	4.28	1.45	1.33
25	D	401	CLA	C3D-C4D	-4.28	1.34	1.44
25	b	602	CLA	C3D-C4D	-4.28	1.34	1.44
25	d	401	CLA	C3D-C4D	-4.28	1.34	1.44
25	a	408	CLA	C3D-C4D	-4.28	1.34	1.44
25	c	503	CLA	CHD-C1D	4.27	1.46	1.38
28	c	519	LMG	O8-C28	4.27	1.45	1.33
25	C	503	CLA	CHD-C1D	4.27	1.46	1.38
25	C	512	CLA	C3D-C4D	-4.27	1.34	1.44
25	c	512	CLA	C3D-C4D	-4.27	1.34	1.44
25	B	601	CLA	CHD-C1D	4.27	1.46	1.38
25	b	601	CLA	CHD-C1D	4.27	1.46	1.38
35	V	201	HEM	C1B-NB	-4.26	1.33	1.40
35	v	201	HEM	C1B-NB	-4.26	1.33	1.40
25	C	507	CLA	CHC-C1C	4.26	1.45	1.35
25	c	507	CLA	CHC-C1C	4.26	1.45	1.35
25	B	602	CLA	C3D-C4D	-4.26	1.34	1.44
28	C	519	LMG	O8-C28	4.26	1.45	1.33
33	e	102	LHG	O8-C23	4.25	1.45	1.33
25	c	504	CLA	C3D-C4D	-4.25	1.34	1.44
25	B	607	CLA	C3C-C2C	4.25	1.45	1.36
25	b	607	CLA	C3C-C2C	4.25	1.45	1.36
25	C	504	CLA	C3D-C4D	-4.24	1.34	1.44
25	B	616	CLA	CHC-C1C	4.24	1.45	1.35
25	b	616	CLA	CHC-C1C	4.24	1.45	1.35
25	B	605	CLA	C3D-C4D	-4.24	1.34	1.44
25	b	605	CLA	C3D-C4D	-4.24	1.34	1.44
25	C	508	CLA	CHD-C1D	4.23	1.46	1.38
25	c	508	CLA	CHD-C1D	4.23	1.46	1.38
25	B	611	CLA	C3D-C4D	-4.22	1.34	1.44
25	b	611	CLA	C3D-C4D	-4.22	1.34	1.44
25	B	616	CLA	C3D-C4D	-4.22	1.34	1.44
25	b	616	CLA	C3D-C4D	-4.22	1.34	1.44
33	B	628	LHG	O8-C23	4.22	1.45	1.33
33	b	628	LHG	O8-C23	4.22	1.45	1.33
28	c	523	LMG	O7-C10	4.22	1.46	1.34
25	B	608	CLA	C3C-C2C	4.22	1.45	1.36
25	b	608	CLA	C3C-C2C	4.22	1.45	1.36
25	c	505	CLA	C3D-C4D	-4.21	1.34	1.44
25	C	505	CLA	C3D-C4D	-4.21	1.34	1.44
25	C	512	CLA	CHD-C1D	4.20	1.46	1.38
28	C	523	LMG	O7-C10	4.20	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	621	LMG	O8-C28	4.20	1.45	1.33
28	b	621	LMG	O8-C28	4.20	1.45	1.33
28	a	414	LMG	O7-C10	4.19	1.46	1.34
25	B	604	CLA	C3B-C2B	4.18	1.46	1.40
25	b	604	CLA	C3B-C2B	4.18	1.46	1.40
25	C	514	CLA	C3D-C4D	-4.17	1.34	1.44
25	c	514	CLA	C3D-C4D	-4.17	1.34	1.44
25	c	512	CLA	CHD-C1D	4.17	1.46	1.38
28	A	414	LMG	O7-C10	4.17	1.46	1.34
25	C	509	CLA	C3D-C4D	-4.16	1.34	1.44
25	c	509	CLA	C3D-C4D	-4.16	1.34	1.44
33	z	102	LHG	O7-C7	4.16	1.46	1.34
33	Z	102	LHG	O7-C7	4.16	1.46	1.34
25	B	614	CLA	C3C-C2C	4.16	1.45	1.36
25	b	614	CLA	C3C-C2C	4.16	1.45	1.36
34	c	517	DGD	O1G-C1A	4.15	1.45	1.33
25	B	605	CLA	C3C-C2C	4.15	1.45	1.36
33	B	627	LHG	O8-C23	4.15	1.45	1.33
33	b	627	LHG	O8-C23	4.15	1.45	1.33
34	C	517	DGD	O1G-C1A	4.15	1.45	1.33
25	b	605	CLA	C3C-C2C	4.14	1.45	1.36
28	H	105	LMG	O7-C10	4.13	1.46	1.34
28	h	105	LMG	O7-C10	4.13	1.45	1.34
28	A	410	LMG	O7-C10	4.12	1.45	1.34
28	a	410	LMG	O7-C10	4.12	1.45	1.34
25	B	608	CLA	C1D-ND	-4.12	1.32	1.37
25	b	608	CLA	C1D-ND	-4.12	1.32	1.37
25	C	504	CLA	CHD-C1D	4.12	1.46	1.38
25	c	504	CLA	CHD-C1D	4.12	1.46	1.38
25	B	609	CLA	C3C-C2C	4.11	1.45	1.36
25	b	609	CLA	C3C-C2C	4.11	1.45	1.36
25	B	603	CLA	C1D-ND	-4.10	1.32	1.37
25	b	603	CLA	C1D-ND	-4.10	1.32	1.37
25	B	601	CLA	C3D-C4D	-4.09	1.34	1.44
25	B	616	CLA	C3C-C2C	4.09	1.45	1.36
25	b	616	CLA	C3C-C2C	4.08	1.45	1.36
25	B	615	CLA	C3C-C2C	4.08	1.45	1.36
25	C	514	CLA	CHD-C1D	4.08	1.46	1.38
33	D	408	LHG	O7-C7	4.07	1.45	1.34
33	d	408	LHG	O7-C7	4.07	1.45	1.34
34	C	516	DGD	O2G-C1B	4.07	1.45	1.34
25	B	604	CLA	C3C-C2C	4.07	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	604	CLA	C3C-C2C	4.07	1.45	1.36
28	b	621	LMG	O7-C10	4.07	1.45	1.34
28	D	409	LMG	O7-C10	4.06	1.45	1.34
28	d	409	LMG	O7-C10	4.06	1.45	1.34
25	b	615	CLA	C3C-C2C	4.06	1.45	1.36
33	D	406	LHG	O8-C23	4.06	1.45	1.33
33	d	406	LHG	O8-C23	4.06	1.45	1.33
25	b	601	CLA	C3D-C4D	-4.06	1.35	1.44
25	c	514	CLA	CHD-C1D	4.06	1.46	1.38
28	B	621	LMG	O7-C10	4.06	1.45	1.34
28	D	409	LMG	O8-C28	4.06	1.45	1.33
25	B	612	CLA	C3C-C2C	4.06	1.45	1.36
25	b	612	CLA	C3C-C2C	4.06	1.45	1.36
34	c	516	DGD	O2G-C1B	4.05	1.45	1.34
28	d	409	LMG	O8-C28	4.05	1.45	1.33
25	B	607	CLA	CHD-C1D	4.05	1.46	1.38
25	b	607	CLA	CHD-C1D	4.05	1.46	1.38
25	C	510	CLA	C3D-C4D	-4.05	1.35	1.44
25	c	510	CLA	C3D-C4D	-4.05	1.35	1.44
25	A	406	CLA	CHD-C4C	4.05	1.48	1.39
25	a	406	CLA	CHD-C4C	4.05	1.48	1.39
28	C	519	LMG	O7-C10	4.04	1.45	1.34
28	c	519	LMG	O7-C10	4.04	1.45	1.34
25	B	611	CLA	CHD-C1D	4.04	1.46	1.38
25	B	603	CLA	CHD-C1D	4.04	1.46	1.38
25	b	603	CLA	CHD-C1D	4.04	1.46	1.38
25	B	613	CLA	CHD-C1D	4.03	1.46	1.38
25	b	613	CLA	CHD-C1D	4.03	1.46	1.38
25	C	505	CLA	C3C-C2C	4.03	1.45	1.36
25	c	505	CLA	C3C-C2C	4.03	1.45	1.36
33	d	407	LHG	O8-C23	4.03	1.45	1.33
33	D	407	LHG	O8-C23	4.03	1.45	1.33
34	H	104	DGD	O2G-C1B	4.02	1.45	1.34
34	h	104	DGD	O2G-C1B	4.02	1.45	1.34
34	H	104	DGD	O1G-C1A	4.02	1.45	1.33
34	h	104	DGD	O1G-C1A	4.02	1.45	1.33
34	C	518	DGD	O1G-C1A	4.02	1.45	1.33
34	c	518	DGD	O1G-C1A	4.02	1.45	1.33
25	B	616	CLA	CHD-C4C	4.01	1.48	1.39
25	b	616	CLA	CHD-C4C	4.01	1.48	1.39
25	B	614	CLA	CHD-C1D	4.01	1.46	1.38
25	b	614	CLA	CHD-C1D	4.01	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	518	DGD	O2G-C1B	4.01	1.45	1.34
34	C	516	DGD	O1G-C1A	4.00	1.45	1.33
34	c	516	DGD	O1G-C1A	4.00	1.45	1.33
25	b	611	CLA	CHD-C1D	3.99	1.46	1.38
34	C	518	DGD	O2G-C1B	3.99	1.45	1.34
25	c	505	CLA	CHD-C4C	3.98	1.48	1.39
25	b	615	CLA	CHD-C1D	3.98	1.46	1.38
25	C	505	CLA	CHD-C4C	3.98	1.48	1.39
25	C	510	CLA	CHD-C4C	3.97	1.48	1.39
25	c	510	CLA	CHD-C4C	3.97	1.48	1.39
25	b	602	CLA	CHD-C4C	3.97	1.48	1.39
33	D	408	LHG	O8-C23	3.97	1.44	1.33
33	d	408	LHG	O8-C23	3.97	1.44	1.33
25	C	513	CLA	C1D-ND	-3.97	1.32	1.37
25	C	513	CLA	C3D-C4D	-3.97	1.35	1.44
25	B	607	CLA	C3B-C2B	3.96	1.45	1.40
25	b	607	CLA	C3B-C2B	3.96	1.45	1.40
25	B	602	CLA	CHD-C4C	3.96	1.48	1.39
25	c	513	CLA	C3D-C4D	-3.94	1.35	1.44
25	B	615	CLA	CHD-C1D	3.93	1.46	1.38
33	d	407	LHG	O7-C7	3.92	1.45	1.34
25	c	513	CLA	C1D-ND	-3.92	1.33	1.37
34	C	517	DGD	O2G-C1B	3.91	1.45	1.34
34	c	517	DGD	O2G-C1B	3.91	1.45	1.34
33	D	407	LHG	O7-C7	3.91	1.45	1.34
25	D	404	CLA	CHD-C4C	3.90	1.48	1.39
25	d	404	CLA	CHD-C4C	3.90	1.48	1.39
33	E	102	LHG	O7-C7	3.89	1.45	1.34
33	e	102	LHG	O7-C7	3.89	1.45	1.34
25	A	405	CLA	CHD-C1D	3.89	1.46	1.38
25	a	405	CLA	CHD-C1D	3.89	1.46	1.38
25	C	511	CLA	C1D-ND	-3.88	1.33	1.37
25	c	511	CLA	C1D-ND	-3.88	1.33	1.37
25	b	605	CLA	CHD-C1D	3.88	1.45	1.38
35	V	201	HEM	C4D-ND	-3.87	1.33	1.40
35	v	201	HEM	C4D-ND	-3.87	1.33	1.40
25	B	605	CLA	CHD-C1D	3.87	1.45	1.38
25	D	401	CLA	CHD-C4C	3.87	1.48	1.39
25	d	401	CLA	CHD-C4C	3.87	1.48	1.39
25	C	513	CLA	CHD-C1D	3.86	1.45	1.38
25	c	513	CLA	CHD-C1D	3.86	1.45	1.38
33	B	628	LHG	O7-C7	3.86	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	628	LHG	O7-C7	3.86	1.45	1.34
25	C	511	CLA	CHD-C4C	3.85	1.48	1.39
25	c	511	CLA	CHD-C4C	3.84	1.48	1.39
36	h	101	RRX	C21-C22	3.84	1.40	1.35
25	C	508	CLA	C1D-ND	-3.83	1.33	1.37
25	c	508	CLA	C1D-ND	-3.83	1.33	1.37
25	B	606	CLA	CHD-C4C	3.82	1.48	1.39
25	C	510	CLA	OBD-CAD	3.81	1.29	1.22
25	c	510	CLA	OBD-CAD	3.81	1.29	1.22
25	C	502	CLA	CHD-C4C	3.81	1.47	1.39
25	c	502	CLA	CHD-C4C	3.81	1.47	1.39
36	H	101	RRX	C21-C22	3.81	1.40	1.35
33	d	406	LHG	O7-C7	3.79	1.45	1.34
25	b	606	CLA	CHD-C4C	3.79	1.47	1.39
25	C	507	CLA	CHD-C4C	3.79	1.47	1.39
25	c	507	CLA	CHD-C4C	3.79	1.47	1.39
33	D	406	LHG	O7-C7	3.78	1.45	1.34
25	B	611	CLA	C1D-ND	-3.77	1.33	1.37
25	b	611	CLA	C1D-ND	-3.77	1.33	1.37
25	B	607	CLA	CHD-C4C	3.76	1.47	1.39
25	b	607	CLA	CHD-C4C	3.76	1.47	1.39
25	c	508	CLA	CHD-C4C	3.75	1.47	1.39
25	C	508	CLA	CHD-C4C	3.75	1.47	1.39
25	B	613	CLA	CHD-C4C	3.73	1.47	1.39
25	b	613	CLA	CHD-C4C	3.73	1.47	1.39
25	c	512	CLA	OBD-CAD	3.72	1.28	1.22
25	C	508	CLA	C3B-C2B	3.72	1.45	1.40
25	c	508	CLA	C3B-C2B	3.72	1.45	1.40
25	C	512	CLA	OBD-CAD	3.72	1.28	1.22
25	C	510	CLA	C1D-ND	-3.71	1.33	1.37
25	c	510	CLA	C1D-ND	-3.71	1.33	1.37
25	A	408	CLA	CHD-C4C	3.69	1.47	1.39
25	C	509	CLA	CHD-C4C	3.69	1.47	1.39
25	a	408	CLA	CHD-C4C	3.69	1.47	1.39
25	c	509	CLA	CHD-C4C	3.69	1.47	1.39
25	b	605	CLA	C1D-ND	-3.68	1.33	1.37
25	A	406	CLA	OBD-CAD	3.67	1.28	1.22
25	a	406	CLA	OBD-CAD	3.67	1.28	1.22
25	c	512	CLA	CHD-C4C	3.67	1.47	1.39
25	C	512	CLA	CHD-C4C	3.67	1.47	1.39
36	h	101	RRX	C14-C13	3.66	1.40	1.35
25	C	506	CLA	C1D-ND	-3.66	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	C1D-ND	-3.66	1.33	1.37
25	B	613	CLA	C1D-ND	-3.66	1.33	1.37
25	B	605	CLA	C1D-ND	-3.65	1.33	1.37
25	b	611	CLA	C3C-C2C	3.64	1.44	1.36
25	B	604	CLA	CHD-C4C	3.64	1.47	1.39
25	b	613	CLA	C1D-ND	-3.64	1.33	1.37
25	B	611	CLA	C3C-C2C	3.63	1.44	1.36
27	b	619	BCR	C11-C12	-3.63	1.25	1.34
25	b	604	CLA	CHD-C4C	3.62	1.47	1.39
29	A	411	PL9	C7-C3	-3.62	1.47	1.51
29	a	411	PL9	C7-C3	-3.62	1.47	1.51
25	B	601	CLA	OBD-CAD	3.62	1.28	1.22
25	b	601	CLA	OBD-CAD	3.62	1.28	1.22
25	C	513	CLA	OBD-CAD	3.62	1.28	1.22
25	c	513	CLA	OBD-CAD	3.62	1.28	1.22
35	e	104	HEM	C1B-NB	-3.62	1.34	1.40
35	E	104	HEM	C4D-ND	-3.61	1.34	1.40
25	b	603	CLA	MG-ND	-3.61	1.98	2.05
35	e	104	HEM	C4D-ND	-3.61	1.34	1.40
25	B	603	CLA	MG-ND	-3.61	1.98	2.05
27	B	619	BCR	C11-C12	-3.61	1.25	1.34
36	H	101	RRX	C17-C18	3.60	1.40	1.35
27	B	617	BCR	C11-C12	-3.60	1.25	1.34
27	b	617	BCR	C11-C12	-3.60	1.25	1.34
25	a	408	CLA	OBD-CAD	3.60	1.28	1.22
36	H	101	RRX	C14-C13	3.60	1.40	1.35
25	C	506	CLA	CHD-C4C	3.59	1.47	1.39
25	c	506	CLA	CHD-C4C	3.59	1.47	1.39
25	C	504	CLA	CHD-C4C	3.59	1.47	1.39
25	B	609	CLA	OBD-CAD	3.58	1.28	1.22
25	c	504	CLA	CHD-C4C	3.58	1.47	1.39
25	B	609	CLA	C1D-ND	-3.58	1.33	1.37
36	h	101	RRX	C17-C18	3.58	1.40	1.35
25	B	615	CLA	OBD-CAD	3.57	1.28	1.22
25	b	615	CLA	OBD-CAD	3.57	1.28	1.22
25	c	503	CLA	CHD-C4C	3.57	1.47	1.39
25	B	615	CLA	C1D-ND	-3.57	1.33	1.37
25	b	615	CLA	C1D-ND	-3.57	1.33	1.37
35	E	104	HEM	C1B-NB	-3.57	1.34	1.40
25	C	514	CLA	OBD-CAD	3.56	1.28	1.22
25	c	514	CLA	OBD-CAD	3.56	1.28	1.22
25	A	408	CLA	OBD-CAD	3.56	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	CLA	CHD-C4C	3.56	1.47	1.39
25	b	601	CLA	CHD-C4C	3.56	1.47	1.39
25	c	506	CLA	OBD-CAD	3.56	1.28	1.22
25	c	513	CLA	CHD-C4C	3.55	1.47	1.39
25	c	505	CLA	OBD-CAD	3.55	1.28	1.22
25	c	511	CLA	OBD-CAD	3.55	1.28	1.22
25	b	609	CLA	C1D-ND	-3.55	1.33	1.37
25	C	503	CLA	CHD-C4C	3.54	1.47	1.39
25	B	611	CLA	C1C-NC	-3.54	1.32	1.37
25	b	611	CLA	C1C-NC	-3.54	1.32	1.37
25	b	609	CLA	OBD-CAD	3.54	1.28	1.22
25	B	614	CLA	CHD-C4C	3.53	1.47	1.39
25	b	614	CLA	CHD-C4C	3.53	1.47	1.39
25	B	608	CLA	CHD-C4C	3.53	1.47	1.39
25	B	609	CLA	CHD-C4C	3.53	1.47	1.39
25	b	608	CLA	CHD-C4C	3.53	1.47	1.39
36	H	101	RRX	C10-C9	3.53	1.40	1.35
36	h	101	RRX	C10-C9	3.53	1.40	1.35
25	C	511	CLA	OBD-CAD	3.53	1.28	1.22
25	b	614	CLA	C1D-ND	-3.53	1.33	1.37
25	C	505	CLA	OBD-CAD	3.53	1.28	1.22
25	b	609	CLA	CHD-C4C	3.53	1.47	1.39
27	C	515	BCR	C11-C12	-3.52	1.25	1.34
27	c	515	BCR	C11-C12	-3.52	1.25	1.34
25	C	513	CLA	CHD-C4C	3.52	1.47	1.39
25	C	506	CLA	OBD-CAD	3.51	1.28	1.22
25	C	514	CLA	CHD-C4C	3.51	1.47	1.39
25	c	514	CLA	CHD-C4C	3.51	1.47	1.39
25	A	405	CLA	C1D-ND	-3.51	1.33	1.37
25	a	405	CLA	C1D-ND	-3.51	1.33	1.37
25	B	614	CLA	C1D-ND	-3.50	1.33	1.37
25	b	616	CLA	C1D-ND	-3.50	1.33	1.37
25	B	603	CLA	CHD-C4C	3.50	1.47	1.39
25	D	404	CLA	OBD-CAD	3.49	1.28	1.22
25	d	404	CLA	OBD-CAD	3.49	1.28	1.22
25	B	616	CLA	C1D-ND	-3.49	1.33	1.37
25	B	602	CLA	OBD-CAD	3.49	1.28	1.22
25	b	602	CLA	OBD-CAD	3.49	1.28	1.22
25	B	614	CLA	OBD-CAD	3.49	1.28	1.22
25	b	614	CLA	OBD-CAD	3.49	1.28	1.22
25	b	603	CLA	CHD-C4C	3.49	1.47	1.39
27	B	618	BCR	C11-C12	-3.48	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	513	CLA	C3D-C2D	3.48	1.48	1.39
25	c	513	CLA	C3D-C2D	3.48	1.48	1.39
27	b	618	BCR	C11-C12	-3.48	1.25	1.34
25	B	605	CLA	CHD-C4C	3.47	1.47	1.39
25	b	605	CLA	CHD-C4C	3.47	1.47	1.39
25	B	607	CLA	C1C-NC	-3.47	1.32	1.37
25	b	607	CLA	C1C-NC	-3.47	1.32	1.37
25	C	512	CLA	C1D-ND	-3.47	1.33	1.37
27	K	103	BCR	C11-C12	-3.45	1.25	1.34
25	b	615	CLA	CHD-C4C	3.45	1.47	1.39
25	B	605	CLA	OBD-CAD	3.45	1.28	1.22
27	k	103	BCR	C11-C12	-3.43	1.25	1.34
25	B	607	CLA	OBD-CAD	3.43	1.28	1.22
25	b	605	CLA	OBD-CAD	3.43	1.28	1.22
25	b	607	CLA	OBD-CAD	3.43	1.28	1.22
25	B	615	CLA	CHD-C4C	3.42	1.47	1.39
25	B	612	CLA	CHD-C1D	3.41	1.45	1.38
25	b	612	CLA	CHD-C1D	3.41	1.45	1.38
25	c	514	CLA	C1D-ND	-3.41	1.33	1.37
25	b	606	CLA	C1D-ND	-3.40	1.33	1.37
25	C	514	CLA	C1D-ND	-3.40	1.33	1.37
25	B	608	CLA	OBD-CAD	3.40	1.28	1.22
25	b	608	CLA	OBD-CAD	3.40	1.28	1.22
25	C	508	CLA	OBD-CAD	3.40	1.28	1.22
25	c	508	CLA	OBD-CAD	3.40	1.28	1.22
25	B	606	CLA	C1D-ND	-3.40	1.33	1.37
25	B	611	CLA	OBD-CAD	3.40	1.28	1.22
25	b	611	CLA	OBD-CAD	3.40	1.28	1.22
25	C	507	CLA	OBD-CAD	3.39	1.28	1.22
25	c	507	CLA	OBD-CAD	3.39	1.28	1.22
25	c	512	CLA	C1D-ND	-3.39	1.33	1.37
25	C	503	CLA	C1C-NC	-3.37	1.32	1.37
25	c	503	CLA	C1C-NC	-3.37	1.32	1.37
25	B	606	CLA	OBD-CAD	3.36	1.28	1.22
25	b	606	CLA	OBD-CAD	3.36	1.28	1.22
25	C	508	CLA	MG-ND	-3.36	1.99	2.05
27	A	409	BCR	C11-C12	-3.35	1.25	1.34
27	a	409	BCR	C11-C12	-3.35	1.25	1.34
25	B	610	CLA	CHD-C4C	3.34	1.46	1.39
25	b	610	CLA	CHD-C4C	3.34	1.46	1.39
25	c	508	CLA	MG-ND	-3.34	1.99	2.05
25	B	610	CLA	OBD-CAD	3.33	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	MG-NC	3.33	2.14	2.06
25	c	510	CLA	MG-NC	3.33	2.14	2.06
25	C	507	CLA	C1C-NC	-3.33	1.32	1.37
25	c	507	CLA	C1C-NC	-3.33	1.32	1.37
25	b	611	CLA	CHD-C4C	3.33	1.46	1.39
25	b	610	CLA	OBD-CAD	3.32	1.28	1.22
25	a	405	CLA	C3C-C2C	3.32	1.43	1.36
28	H	105	LMG	C37-C36	-3.31	1.33	1.51
25	D	403	CLA	CHD-C4C	3.31	1.46	1.39
25	B	612	CLA	MG-NC	3.31	2.14	2.06
25	b	612	CLA	MG-NC	3.31	2.14	2.06
27	Z	101	BCR	C11-C12	-3.31	1.26	1.34
27	z	101	BCR	C11-C12	-3.31	1.26	1.34
28	h	105	LMG	C37-C36	-3.31	1.33	1.51
25	B	611	CLA	CHD-C4C	3.30	1.46	1.39
25	C	509	CLA	C1D-ND	-3.30	1.33	1.37
25	c	509	CLA	C1D-ND	-3.30	1.33	1.37
28	H	105	LMG	C40-C39	-3.30	1.33	1.51
28	h	105	LMG	C40-C39	-3.30	1.33	1.51
34	H	104	DGD	CAA-C9A	-3.30	1.33	1.51
34	h	104	DGD	CAA-C9A	-3.30	1.33	1.51
28	C	523	LMG	C22-C21	-3.30	1.33	1.51
28	c	523	LMG	C22-C21	-3.30	1.33	1.51
34	c	518	DGD	CDA-CCA	-3.30	1.33	1.51
25	A	405	CLA	C3C-C2C	3.29	1.43	1.36
25	C	509	CLA	OBD-CAD	3.29	1.28	1.22
25	c	509	CLA	OBD-CAD	3.29	1.28	1.22
34	C	518	DGD	CDA-CCA	-3.29	1.33	1.51
34	C	518	DGD	CAA-C9A	-3.29	1.33	1.51
34	c	518	DGD	CAA-C9A	-3.29	1.33	1.51
25	A	405	CLA	CHD-C4C	3.28	1.46	1.39
34	C	516	DGD	CAB-C9B	-3.28	1.33	1.51
34	c	516	DGD	CAB-C9B	-3.28	1.33	1.51
25	B	604	CLA	OBD-CAD	3.28	1.28	1.22
25	b	604	CLA	OBD-CAD	3.28	1.28	1.22
25	B	610	CLA	C1C-NC	-3.28	1.32	1.37
28	C	523	LMG	C37-C36	-3.28	1.33	1.51
28	c	523	LMG	C37-C36	-3.28	1.33	1.51
28	C	519	LMG	C22-C21	-3.28	1.33	1.51
28	c	519	LMG	C22-C21	-3.28	1.33	1.51
25	d	403	CLA	CHD-C4C	3.28	1.46	1.39
25	C	509	CLA	C3D-C2D	3.27	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	518	DGD	CDB-CCB	-3.27	1.33	1.51
34	c	518	DGD	CDB-CCB	-3.27	1.33	1.51
28	B	621	LMG	C40-C39	-3.27	1.33	1.51
28	b	621	LMG	C40-C39	-3.27	1.33	1.51
25	b	610	CLA	C1C-NC	-3.27	1.32	1.37
34	H	104	DGD	CAB-C9B	-3.27	1.33	1.51
34	h	104	DGD	CAB-C9B	-3.27	1.33	1.51
28	B	621	LMG	C37-C36	-3.26	1.33	1.51
28	b	621	LMG	C37-C36	-3.26	1.33	1.51
25	D	403	CLA	OBD-CAD	3.26	1.28	1.22
25	d	403	CLA	OBD-CAD	3.26	1.28	1.22
25	D	401	CLA	OBD-CAD	3.26	1.28	1.22
25	d	401	CLA	OBD-CAD	3.26	1.28	1.22
25	a	405	CLA	CHD-C4C	3.26	1.46	1.39
25	B	616	CLA	OBD-CAD	3.26	1.28	1.22
25	b	616	CLA	OBD-CAD	3.26	1.28	1.22
28	B	621	LMG	C19-C18	-3.26	1.33	1.51
28	b	621	LMG	C19-C18	-3.26	1.33	1.51
25	c	509	CLA	C3D-C2D	3.26	1.48	1.39
27	F	101	BCR	C11-C12	-3.25	1.26	1.34
27	f	101	BCR	C11-C12	-3.25	1.26	1.34
25	c	503	CLA	OBD-CAD	3.25	1.28	1.22
25	C	513	CLA	MG-NC	3.25	2.14	2.06
28	a	410	LMG	C22-C21	-3.25	1.33	1.51
34	C	517	DGD	CDA-CCA	-3.25	1.33	1.51
34	c	517	DGD	CDA-CCA	-3.25	1.33	1.51
28	b	621	LMG	C22-C21	-3.25	1.33	1.51
28	A	410	LMG	C22-C21	-3.24	1.33	1.51
34	H	104	DGD	CDA-CCA	-3.24	1.33	1.51
34	h	104	DGD	CDA-CCA	-3.24	1.33	1.51
25	C	503	CLA	OBD-CAD	3.24	1.28	1.22
25	B	603	CLA	OBD-CAD	3.24	1.28	1.22
25	A	408	CLA	C1D-ND	-3.24	1.33	1.37
25	a	408	CLA	C1D-ND	-3.24	1.33	1.37
34	C	516	DGD	CAA-C9A	-3.24	1.33	1.51
34	c	516	DGD	CAA-C9A	-3.24	1.33	1.51
25	b	603	CLA	OBD-CAD	3.24	1.28	1.22
34	H	104	DGD	CDB-CCB	-3.24	1.33	1.51
34	h	104	DGD	CDB-CCB	-3.24	1.33	1.51
25	B	610	CLA	C1D-ND	-3.24	1.33	1.37
25	b	610	CLA	C1D-ND	-3.24	1.33	1.37
28	B	621	LMG	C22-C21	-3.24	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	410	LMG	C40-C39	-3.23	1.33	1.51
28	a	410	LMG	C40-C39	-3.23	1.33	1.51
34	C	516	DGD	CDB-CCB	-3.23	1.33	1.51
34	c	516	DGD	CDB-CCB	-3.23	1.33	1.51
28	C	519	LMG	C19-C18	-3.23	1.33	1.51
28	A	410	LMG	C37-C36	-3.23	1.33	1.51
28	a	410	LMG	C37-C36	-3.23	1.33	1.51
25	B	604	CLA	C1D-ND	-3.23	1.33	1.37
25	b	604	CLA	C1D-ND	-3.23	1.33	1.37
28	C	523	LMG	C40-C39	-3.23	1.33	1.51
30	a	412	SQD	O48-C23	3.23	1.42	1.33
34	C	518	DGD	CAB-C9B	-3.23	1.33	1.51
34	c	518	DGD	CAB-C9B	-3.23	1.33	1.51
25	D	401	CLA	C1C-NC	-3.23	1.33	1.37
25	d	401	CLA	C1C-NC	-3.23	1.33	1.37
28	c	519	LMG	C19-C18	-3.22	1.33	1.51
34	C	516	DGD	CDA-CCA	-3.22	1.33	1.51
34	c	516	DGD	CDA-CCA	-3.22	1.33	1.51
28	C	519	LMG	C37-C36	-3.22	1.33	1.51
28	c	519	LMG	C37-C36	-3.22	1.33	1.51
25	c	502	CLA	OBD-CAD	3.22	1.28	1.22
25	D	401	CLA	C1D-ND	-3.22	1.33	1.37
25	d	401	CLA	C1D-ND	-3.22	1.33	1.37
25	B	612	CLA	OBD-CAD	3.22	1.28	1.22
25	b	612	CLA	OBD-CAD	3.22	1.28	1.22
34	c	517	DGD	CAA-C9A	-3.22	1.33	1.51
25	B	604	CLA	C1C-NC	-3.22	1.33	1.37
25	b	604	CLA	C1C-NC	-3.22	1.33	1.37
30	A	412	SQD	O48-C23	3.21	1.42	1.33
25	c	513	CLA	MG-NC	3.21	2.13	2.06
28	c	523	LMG	C40-C39	-3.21	1.33	1.51
34	C	517	DGD	CDB-CCB	-3.21	1.33	1.51
34	c	517	DGD	CDB-CCB	-3.21	1.33	1.51
25	C	502	CLA	OBD-CAD	3.21	1.28	1.22
25	C	503	CLA	C1D-ND	-3.21	1.33	1.37
25	c	503	CLA	C1D-ND	-3.21	1.33	1.37
25	C	504	CLA	MG-NC	3.20	2.13	2.06
25	c	504	CLA	MG-NC	3.20	2.13	2.06
28	D	409	LMG	C40-C39	-3.20	1.33	1.51
28	d	409	LMG	C40-C39	-3.20	1.33	1.51
34	C	517	DGD	CAA-C9A	-3.20	1.33	1.51
34	c	517	DGD	CAB-C9B	-3.20	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	410	LMG	C19-C18	-3.20	1.33	1.51
28	a	410	LMG	C19-C18	-3.20	1.33	1.51
29	D	405	PL9	C3-C4	-3.20	1.44	1.49
29	d	405	PL9	C3-C4	-3.20	1.44	1.49
36	H	101	RRX	C8-C9	-3.19	1.39	1.45
36	h	101	RRX	C8-C9	-3.19	1.39	1.45
25	B	607	CLA	C1D-ND	-3.19	1.33	1.37
25	b	607	CLA	C1D-ND	-3.19	1.33	1.37
28	D	409	LMG	C37-C36	-3.19	1.33	1.51
28	d	409	LMG	C37-C36	-3.19	1.33	1.51
34	C	517	DGD	CAB-C9B	-3.19	1.33	1.51
25	B	609	CLA	MG-NC	3.18	2.13	2.06
25	b	609	CLA	MG-NC	3.18	2.13	2.06
28	C	519	LMG	C40-C39	-3.18	1.33	1.51
28	c	519	LMG	C40-C39	-3.18	1.33	1.51
25	b	610	CLA	MG-NC	3.17	2.13	2.06
30	K	101	SQD	O48-C23	3.17	1.42	1.33
30	k	101	SQD	O48-C23	3.17	1.42	1.33
25	C	514	CLA	C3D-C2D	3.16	1.47	1.39
25	c	514	CLA	C3D-C2D	3.16	1.47	1.39
28	C	523	LMG	C19-C18	-3.15	1.33	1.51
28	c	523	LMG	C19-C18	-3.15	1.33	1.51
30	A	413	SQD	O48-C23	3.15	1.42	1.33
30	a	413	SQD	O48-C23	3.15	1.42	1.33
25	C	505	CLA	C1D-ND	-3.14	1.33	1.37
25	c	505	CLA	C1D-ND	-3.14	1.33	1.37
30	F	102	SQD	O48-C23	3.14	1.42	1.33
25	B	601	CLA	C1D-ND	-3.14	1.33	1.37
25	b	601	CLA	C1D-ND	-3.14	1.33	1.37
25	B	610	CLA	MG-NC	3.14	2.13	2.06
30	f	102	SQD	O48-C23	3.14	1.42	1.33
25	B	612	CLA	MG-ND	-3.13	1.99	2.05
25	b	612	CLA	MG-ND	-3.13	1.99	2.05
25	B	601	CLA	MG-NC	3.13	2.13	2.06
25	b	601	CLA	MG-NC	3.13	2.13	2.06
25	C	504	CLA	OBD-CAD	3.13	1.27	1.22
25	c	504	CLA	OBD-CAD	3.13	1.27	1.22
25	C	507	CLA	C3B-C2B	3.11	1.44	1.40
25	c	507	CLA	C3B-C2B	3.11	1.44	1.40
25	C	507	CLA	C1D-ND	-3.11	1.34	1.37
25	D	404	CLA	C1D-ND	-3.11	1.34	1.37
25	c	507	CLA	C1D-ND	-3.11	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	CLA	C1D-ND	-3.11	1.34	1.37
25	c	510	CLA	C1C-NC	-3.09	1.33	1.37
25	B	614	CLA	MG-NC	3.09	2.13	2.06
25	b	604	CLA	MG-ND	-3.09	1.99	2.05
25	b	614	CLA	MG-NC	3.09	2.13	2.06
27	K	102	BCR	C11-C12	-3.09	1.26	1.34
27	k	102	BCR	C11-C12	-3.09	1.26	1.34
25	c	508	CLA	C1C-NC	-3.08	1.33	1.37
25	B	615	CLA	MG-NC	3.08	2.13	2.06
25	b	615	CLA	MG-NC	3.08	2.13	2.06
25	C	507	CLA	C3D-C2D	3.08	1.47	1.39
25	c	507	CLA	C3D-C2D	3.08	1.47	1.39
30	H	103	SQD	O48-C23	3.07	1.42	1.33
25	d	404	CLA	C3D-C2D	3.07	1.47	1.39
25	A	405	CLA	C1C-NC	-3.07	1.33	1.37
25	a	405	CLA	C1C-NC	-3.07	1.33	1.37
30	h	103	SQD	O48-C23	3.06	1.42	1.33
25	C	508	CLA	C1C-NC	-3.06	1.33	1.37
25	B	614	CLA	C1C-NC	-3.06	1.33	1.37
25	b	614	CLA	C1C-NC	-3.06	1.33	1.37
25	A	406	CLA	C1D-ND	-3.06	1.34	1.37
25	a	406	CLA	C1D-ND	-3.06	1.34	1.37
25	B	604	CLA	MG-ND	-3.05	1.99	2.05
25	b	608	CLA	C1B-NB	-3.05	1.32	1.35
25	C	510	CLA	C1C-NC	-3.05	1.33	1.37
25	B	616	CLA	C3D-C2D	3.05	1.47	1.39
25	b	615	CLA	C3D-C2D	3.05	1.47	1.39
25	B	608	CLA	C1B-NB	-3.04	1.32	1.35
30	F	102	SQD	O47-C7	3.04	1.42	1.34
30	f	102	SQD	O47-C7	3.04	1.42	1.34
25	D	404	CLA	C3D-C2D	3.04	1.47	1.39
25	B	609	CLA	C3D-C2D	3.04	1.47	1.39
25	b	616	CLA	C3D-C2D	3.03	1.47	1.39
25	B	615	CLA	C3D-C2D	3.01	1.47	1.39
25	b	609	CLA	C3D-C2D	3.01	1.47	1.39
25	a	408	CLA	C3D-C2D	3.01	1.47	1.39
25	A	405	CLA	OBD-CAD	3.00	1.27	1.22
25	a	405	CLA	OBD-CAD	3.00	1.27	1.22
25	B	603	CLA	MG-NC	3.00	2.13	2.06
25	b	603	CLA	MG-NC	3.00	2.13	2.06
25	A	408	CLA	C3D-C2D	3.00	1.47	1.39
25	b	612	CLA	CHD-C4C	3.00	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	512	CLA	MG-NC	2.99	2.13	2.06
25	c	512	CLA	MG-NC	2.99	2.13	2.06
25	B	612	CLA	CHD-C4C	2.99	1.46	1.39
30	c	501	SQD	O48-C23	2.99	1.42	1.33
30	C	501	SQD	O48-C23	2.98	1.42	1.33
25	c	504	CLA	C1D-ND	-2.98	1.34	1.37
25	C	510	CLA	C3D-C2D	2.98	1.47	1.39
25	c	510	CLA	C3D-C2D	2.98	1.47	1.39
25	A	408	CLA	MG-NC	2.98	2.13	2.06
25	C	503	CLA	MG-ND	-2.97	1.99	2.05
25	C	504	CLA	C1D-ND	-2.97	1.34	1.37
25	b	605	CLA	C1C-NC	-2.97	1.33	1.37
25	C	505	CLA	C3D-C2D	2.97	1.47	1.39
30	a	413	SQD	O47-C7	2.96	1.42	1.34
25	B	605	CLA	C1C-NC	-2.96	1.33	1.37
25	B	613	CLA	C3D-C2D	2.96	1.47	1.39
25	b	613	CLA	C3D-C2D	2.96	1.47	1.39
25	c	505	CLA	C3D-C2D	2.96	1.47	1.39
25	c	503	CLA	MG-ND	-2.96	1.99	2.05
25	a	408	CLA	MG-NC	2.96	2.13	2.06
25	C	502	CLA	C1D-ND	-2.94	1.34	1.37
25	c	502	CLA	C1D-ND	-2.94	1.34	1.37
36	H	101	RRX	C23-C22	-2.93	1.39	1.45
36	h	101	RRX	C23-C22	-2.93	1.39	1.45
30	A	413	SQD	O47-C7	2.93	1.42	1.34
25	B	602	CLA	C3D-C2D	2.93	1.47	1.39
25	b	606	CLA	C3D-C2D	2.93	1.47	1.39
25	C	509	CLA	C1C-NC	-2.92	1.33	1.37
25	c	509	CLA	C1C-NC	-2.92	1.33	1.37
25	b	602	CLA	C3D-C2D	2.92	1.47	1.39
25	C	506	CLA	C1C-NC	-2.92	1.33	1.37
25	c	506	CLA	C1C-NC	-2.92	1.33	1.37
25	b	604	CLA	MG-NC	2.92	2.13	2.06
25	C	502	CLA	C3D-C2D	2.92	1.47	1.39
25	c	502	CLA	C3D-C2D	2.92	1.47	1.39
25	B	602	CLA	MG-NC	2.92	2.13	2.06
25	b	602	CLA	MG-NC	2.92	2.13	2.06
25	C	503	CLA	C3D-C2D	2.92	1.47	1.39
25	c	503	CLA	C3D-C2D	2.92	1.47	1.39
25	C	513	CLA	C4D-CHA	2.91	1.48	1.38
25	B	606	CLA	C3D-C2D	2.91	1.47	1.39
25	B	610	CLA	C3D-C2D	2.91	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	610	CLA	C3D-C2D	2.91	1.47	1.39
25	B	608	CLA	MG-NC	2.90	2.13	2.06
25	b	608	CLA	MG-NC	2.90	2.13	2.06
25	B	610	CLA	MG-ND	-2.90	2.00	2.05
25	C	507	CLA	MG-NC	2.90	2.13	2.06
25	c	507	CLA	MG-NC	2.90	2.13	2.06
25	C	514	CLA	MG-NC	2.90	2.13	2.06
25	c	514	CLA	MG-NC	2.90	2.13	2.06
25	D	401	CLA	C3D-C2D	2.90	1.47	1.39
25	d	401	CLA	C3D-C2D	2.90	1.47	1.39
25	D	403	CLA	MG-ND	-2.90	2.00	2.05
25	d	403	CLA	MG-ND	-2.90	2.00	2.05
31	H	102	LMT	O2'-C2'	-2.90	1.36	1.43
31	h	102	LMT	O2'-C2'	-2.90	1.36	1.43
25	A	406	CLA	C1C-NC	-2.89	1.33	1.37
25	a	406	CLA	C1C-NC	-2.89	1.33	1.37
25	B	613	CLA	C4D-CHA	2.89	1.48	1.38
25	b	613	CLA	C4D-CHA	2.89	1.48	1.38
25	B	611	CLA	C3D-C2D	2.89	1.47	1.39
25	b	611	CLA	C3D-C2D	2.89	1.47	1.39
25	C	511	CLA	MG-ND	-2.89	2.00	2.05
30	H	103	SQD	O47-C7	2.89	1.42	1.34
30	h	103	SQD	O47-C7	2.89	1.42	1.34
25	c	513	CLA	MG-ND	-2.89	2.00	2.05
25	c	513	CLA	C4D-CHA	2.89	1.48	1.38
25	B	604	CLA	MG-NC	2.89	2.13	2.06
25	C	513	CLA	MG-ND	-2.88	2.00	2.05
25	c	511	CLA	MG-ND	-2.88	2.00	2.05
25	B	603	CLA	C1C-NC	-2.88	1.33	1.37
25	b	603	CLA	C1C-NC	-2.88	1.33	1.37
25	B	607	CLA	C3D-C2D	2.88	1.47	1.39
25	b	607	CLA	C3D-C2D	2.88	1.47	1.39
31	D	412	LMT	O3'-C3'	-2.87	1.36	1.43
31	d	412	LMT	O3'-C3'	-2.87	1.36	1.43
25	C	502	CLA	MG-NC	2.87	2.13	2.06
25	c	502	CLA	MG-NC	2.87	2.13	2.06
25	c	511	CLA	MG-NC	2.87	2.13	2.06
25	b	610	CLA	MG-ND	-2.87	2.00	2.05
25	C	504	CLA	C4D-CHA	2.86	1.48	1.38
25	c	504	CLA	C4D-CHA	2.86	1.48	1.38
30	A	412	SQD	O47-C7	2.86	1.42	1.34
30	a	412	SQD	O47-C7	2.86	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	CLA	C3D-C2D	2.86	1.46	1.39
25	b	601	CLA	C3D-C2D	2.86	1.46	1.39
25	C	514	CLA	C1C-NC	-2.86	1.33	1.37
25	c	514	CLA	C1C-NC	-2.86	1.33	1.37
25	c	507	CLA	C4D-CHA	2.85	1.48	1.38
25	C	511	CLA	MG-NC	2.85	2.13	2.06
25	C	507	CLA	MG-ND	-2.85	2.00	2.05
25	C	505	CLA	C1C-NC	-2.84	1.33	1.37
25	c	505	CLA	C1C-NC	-2.84	1.33	1.37
25	b	606	CLA	C1C-NC	-2.84	1.33	1.37
25	C	507	CLA	C4D-CHA	2.84	1.48	1.38
25	D	404	CLA	MG-NC	2.84	2.13	2.06
25	c	507	CLA	MG-ND	-2.83	2.00	2.05
25	B	611	CLA	C1B-NB	-2.83	1.32	1.35
25	b	611	CLA	C1B-NB	-2.83	1.32	1.35
25	C	506	CLA	MG-ND	-2.83	2.00	2.05
35	e	104	HEM	FE-NB	2.83	2.10	1.96
25	b	609	CLA	C4D-CHA	2.83	1.48	1.38
35	V	201	HEM	C4B-NB	-2.82	1.33	1.38
35	v	201	HEM	C4B-NB	-2.82	1.33	1.38
35	E	104	HEM	FE-NB	2.82	2.10	1.96
25	d	404	CLA	MG-NC	2.81	2.13	2.06
25	B	609	CLA	C4D-CHA	2.81	1.48	1.38
25	B	606	CLA	C1C-NC	-2.81	1.33	1.37
25	a	406	CLA	C3D-C2D	2.81	1.46	1.39
25	c	510	CLA	C4D-CHA	2.81	1.48	1.38
30	K	101	SQD	O47-C7	2.81	1.42	1.34
30	k	101	SQD	O47-C7	2.81	1.42	1.34
25	c	508	CLA	C3D-C2D	2.80	1.46	1.39
25	c	506	CLA	MG-ND	-2.80	2.00	2.05
25	B	608	CLA	C3D-C2D	2.80	1.46	1.39
25	C	510	CLA	C4D-CHA	2.80	1.48	1.38
25	B	613	CLA	C1C-NC	-2.80	1.33	1.37
25	b	613	CLA	C1C-NC	-2.80	1.33	1.37
25	A	405	CLA	MG-ND	-2.80	2.00	2.05
25	C	508	CLA	C3D-C2D	2.79	1.46	1.39
25	A	406	CLA	C3D-C2D	2.79	1.46	1.39
25	B	614	CLA	MG-ND	-2.79	2.00	2.05
25	b	614	CLA	MG-ND	-2.79	2.00	2.05
25	b	608	CLA	C3D-C2D	2.79	1.46	1.39
25	a	405	CLA	MG-ND	-2.79	2.00	2.05
25	C	502	CLA	C1C-NC	-2.78	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	502	CLA	C1C-NC	-2.78	1.33	1.37
25	B	613	CLA	MG-ND	-2.78	2.00	2.05
25	b	613	CLA	MG-ND	-2.78	2.00	2.05
25	C	504	CLA	MG-ND	-2.78	2.00	2.05
25	c	504	CLA	MG-ND	-2.78	2.00	2.05
25	c	508	CLA	C4D-CHA	2.78	1.48	1.38
25	B	601	CLA	C1C-NC	-2.77	1.33	1.37
25	b	601	CLA	C1C-NC	-2.77	1.33	1.37
25	b	616	CLA	C4D-CHA	2.77	1.48	1.38
25	b	607	CLA	C4D-CHA	2.77	1.48	1.38
25	C	508	CLA	MG-NC	2.77	2.12	2.06
25	c	508	CLA	MG-NC	2.77	2.12	2.06
25	B	601	CLA	C4D-CHA	2.77	1.48	1.38
25	C	508	CLA	C4D-CHA	2.77	1.48	1.38
25	b	601	CLA	C4D-CHA	2.77	1.48	1.38
31	M	102	LMT	O3'-C3'	-2.77	1.36	1.43
31	m	102	LMT	O3'-C3'	-2.77	1.36	1.43
25	B	610	CLA	C4D-CHA	2.76	1.48	1.38
25	b	610	CLA	C4D-CHA	2.76	1.48	1.38
31	D	411	LMT	O3'-C3'	-2.76	1.36	1.43
31	d	411	LMT	O3'-C3'	-2.76	1.36	1.43
31	i	103	LMT	O3'-C3'	-2.76	1.36	1.43
25	B	616	CLA	C4D-CHA	2.76	1.48	1.38
25	C	512	CLA	C3D-C2D	2.75	1.46	1.39
25	c	512	CLA	C3D-C2D	2.75	1.46	1.39
25	B	607	CLA	C4D-CHA	2.75	1.48	1.38
25	A	406	CLA	MG-NC	2.75	2.12	2.06
31	I	103	LMT	O3'-C3'	-2.74	1.36	1.43
25	D	403	CLA	C1C-NC	-2.73	1.33	1.37
25	C	512	CLA	MG-ND	-2.72	2.00	2.05
25	c	512	CLA	MG-ND	-2.72	2.00	2.05
25	B	615	CLA	C1C-NC	-2.72	1.33	1.37
25	C	510	CLA	C1B-CHB	2.72	1.48	1.41
25	c	510	CLA	C1B-CHB	2.72	1.48	1.41
25	b	604	CLA	C4D-CHA	2.72	1.48	1.38
25	a	406	CLA	MG-NC	2.72	2.12	2.06
31	A	416	LMT	O3'-C3'	-2.72	1.36	1.43
31	X	102	LMT	O3'-C3'	-2.71	1.36	1.43
31	x	102	LMT	O3'-C3'	-2.71	1.36	1.43
25	B	607	CLA	MG-ND	-2.71	2.00	2.05
31	X	101	LMT	O3'-C3'	-2.71	1.36	1.43
31	k	105	LMT	O3'-C3'	-2.71	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	MG-NC	2.71	2.12	2.06
25	b	613	CLA	MG-NC	2.71	2.12	2.06
25	B	615	CLA	C4D-CHA	2.70	1.48	1.38
25	b	607	CLA	MG-ND	-2.70	2.00	2.05
31	B	623	LMT	O3'-C3'	-2.70	1.36	1.43
31	b	623	LMT	O3'-C3'	-2.70	1.36	1.43
25	B	606	CLA	C4D-CHA	2.70	1.48	1.38
25	b	606	CLA	C4D-CHA	2.70	1.48	1.38
25	c	507	CLA	C4C-C3C	2.70	1.49	1.45
25	B	604	CLA	C4D-CHA	2.70	1.48	1.38
25	b	615	CLA	C4D-CHA	2.70	1.48	1.38
29	A	411	PL9	C3-C4	-2.70	1.45	1.49
25	B	609	CLA	MG-ND	-2.70	2.00	2.05
25	b	609	CLA	MG-ND	-2.70	2.00	2.05
25	b	611	CLA	MG-ND	-2.70	2.00	2.05
31	K	105	LMT	O3'-C3'	-2.70	1.36	1.43
25	B	612	CLA	C1B-CHB	2.70	1.48	1.41
25	b	612	CLA	C1B-CHB	2.70	1.48	1.41
31	I	101	LMT	O3'-C3'	-2.70	1.36	1.43
31	i	101	LMT	O3'-C3'	-2.70	1.36	1.43
25	c	511	CLA	C4D-CHA	2.70	1.48	1.38
31	C	525	LMT	O3'-C3'	-2.70	1.36	1.43
31	c	525	LMT	O3'-C3'	-2.70	1.36	1.43
29	A	411	PL9	C53-C6	-2.69	1.45	1.50
25	b	615	CLA	C1C-NC	-2.69	1.33	1.37
29	a	411	PL9	C53-C6	-2.69	1.45	1.50
25	A	408	CLA	C4D-CHA	2.69	1.48	1.38
25	a	408	CLA	C4D-CHA	2.69	1.48	1.38
25	C	509	CLA	MG-NC	2.69	2.12	2.06
25	c	509	CLA	MG-NC	2.69	2.12	2.06
25	B	611	CLA	MG-ND	-2.69	2.00	2.05
31	x	101	LMT	O3'-C3'	-2.69	1.36	1.43
31	b	629	LMT	O3'-C3'	-2.69	1.36	1.43
25	C	514	CLA	C4D-CHA	2.69	1.47	1.38
25	c	514	CLA	C4D-CHA	2.69	1.47	1.38
31	D	410	LMT	O3'-C3'	-2.69	1.36	1.43
31	J	101	LMT	O3'-C3'	-2.68	1.36	1.43
31	j	101	LMT	O3'-C3'	-2.68	1.36	1.43
25	C	505	CLA	MG-ND	-2.68	2.00	2.05
25	c	505	CLA	MG-ND	-2.68	2.00	2.05
25	C	507	CLA	C4C-C3C	2.68	1.49	1.45
31	F	103	LMT	O3'-C3'	-2.68	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	f	103	LMT	O3'-C3'	-2.68	1.36	1.43
25	B	609	CLA	C1C-NC	-2.68	1.33	1.37
25	b	609	CLA	C1C-NC	-2.68	1.33	1.37
25	d	403	CLA	C1C-NC	-2.68	1.33	1.37
25	C	512	CLA	C1C-NC	-2.68	1.33	1.37
25	c	512	CLA	C1C-NC	-2.68	1.33	1.37
25	C	511	CLA	C4D-CHA	2.68	1.47	1.38
31	a	416	LMT	O3'-C3'	-2.68	1.36	1.43
25	D	403	CLA	CHD-C1D	2.68	1.43	1.38
25	d	403	CLA	CHD-C1D	2.68	1.43	1.38
25	A	406	CLA	C4D-CHA	2.68	1.47	1.38
25	a	406	CLA	C4D-CHA	2.68	1.47	1.38
25	b	603	CLA	C1B-NB	-2.67	1.32	1.35
25	c	503	CLA	MG-NC	2.67	2.12	2.06
25	B	606	CLA	MG-ND	-2.67	2.00	2.05
25	b	606	CLA	MG-ND	-2.67	2.00	2.05
31	d	410	LMT	O3'-C3'	-2.67	1.36	1.43
25	C	510	CLA	MG-ND	-2.67	2.00	2.05
25	B	602	CLA	C4D-CHA	2.67	1.47	1.38
25	B	602	CLA	C1C-NC	-2.66	1.33	1.37
31	B	629	LMT	O3'-C3'	-2.66	1.36	1.43
25	C	503	CLA	C4D-CHA	2.66	1.47	1.38
25	c	503	CLA	C4D-CHA	2.66	1.47	1.38
25	b	602	CLA	C4D-CHA	2.66	1.47	1.38
25	B	601	CLA	MG-ND	-2.66	2.00	2.05
31	X	105	LMT	O3'-C3'	-2.66	1.36	1.43
31	x	105	LMT	O3'-C3'	-2.66	1.36	1.43
29	a	411	PL9	C3-C4	-2.66	1.45	1.49
25	B	613	CLA	OBD-CAD	2.66	1.27	1.22
25	b	613	CLA	OBD-CAD	2.66	1.27	1.22
25	B	606	CLA	MG-NC	2.66	2.12	2.06
25	b	606	CLA	MG-NC	2.66	2.12	2.06
25	B	603	CLA	C1B-NB	-2.66	1.32	1.35
25	C	503	CLA	MG-NC	2.66	2.12	2.06
25	C	509	CLA	MG-ND	-2.65	2.00	2.05
25	c	510	CLA	MG-ND	-2.65	2.00	2.05
25	c	509	CLA	MG-ND	-2.65	2.00	2.05
31	x	102	LMT	O2'-C2'	-2.65	1.36	1.43
25	b	602	CLA	C1C-NC	-2.65	1.33	1.37
25	C	505	CLA	C4D-CHA	2.65	1.47	1.38
25	c	505	CLA	C4D-CHA	2.65	1.47	1.38
25	C	506	CLA	MG-NC	2.64	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	514	CLA	C4B-CHC	2.64	1.48	1.41
25	c	514	CLA	C4B-CHC	2.64	1.48	1.41
25	B	616	CLA	MG-ND	-2.64	2.00	2.05
25	b	616	CLA	MG-ND	-2.64	2.00	2.05
26	A	407	PHO	CAC-C3C	-2.64	1.47	1.52
26	a	407	PHO	CAC-C3C	-2.64	1.47	1.52
31	I	102	LMT	O3'-C3'	-2.63	1.36	1.43
31	i	102	LMT	O3'-C3'	-2.63	1.36	1.43
25	b	611	CLA	C4D-CHA	2.63	1.47	1.38
25	c	502	CLA	C4D-CHA	2.63	1.47	1.38
31	B	624	LMT	O3'-C3'	-2.63	1.36	1.43
31	b	624	LMT	O3'-C3'	-2.63	1.36	1.43
31	X	102	LMT	O2'-C2'	-2.63	1.36	1.43
31	T	101	LMT	O3'-C3'	-2.63	1.36	1.43
31	t	101	LMT	O3'-C3'	-2.63	1.36	1.43
25	b	612	CLA	C3D-C2D	2.63	1.46	1.39
25	b	611	CLA	MG-NC	2.63	2.12	2.06
31	B	625	LMT	O2'-C2'	-2.63	1.36	1.43
31	b	625	LMT	O2'-C2'	-2.63	1.36	1.43
25	b	601	CLA	MG-ND	-2.63	2.00	2.05
31	A	415	LMT	O3'-C3'	-2.63	1.36	1.43
31	a	415	LMT	O3'-C3'	-2.63	1.36	1.43
25	A	408	CLA	C1C-NC	-2.63	1.33	1.37
25	a	408	CLA	C1C-NC	-2.63	1.33	1.37
25	C	502	CLA	MG-ND	-2.62	2.00	2.05
31	x	103	LMT	O3'-C3'	-2.62	1.36	1.43
25	B	611	CLA	C4D-CHA	2.62	1.47	1.38
25	C	504	CLA	C3D-C2D	2.62	1.46	1.39
25	c	504	CLA	C3D-C2D	2.62	1.46	1.39
31	I	104	LMT	O3'-C3'	-2.62	1.36	1.43
31	i	104	LMT	O3'-C3'	-2.62	1.36	1.43
25	B	608	CLA	C4D-CHA	2.62	1.47	1.38
25	b	608	CLA	C4D-CHA	2.62	1.47	1.38
31	X	103	LMT	O3'-C3'	-2.62	1.36	1.43
25	B	605	CLA	C3D-C2D	2.62	1.46	1.39
25	b	605	CLA	C3D-C2D	2.62	1.46	1.39
25	C	514	CLA	MG-ND	-2.61	2.00	2.05
25	c	514	CLA	MG-ND	-2.61	2.00	2.05
31	y	101	LMT	O3'-C3'	-2.61	1.36	1.43
25	B	611	CLA	MG-NC	2.61	2.12	2.06
26	d	402	PHO	CMC-C2C	-2.61	1.45	1.51
25	C	504	CLA	C1C-NC	-2.61	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	504	CLA	C1C-NC	-2.61	1.33	1.37
25	c	506	CLA	MG-NC	2.61	2.12	2.06
25	C	502	CLA	C4D-CHA	2.61	1.47	1.38
31	T	101	LMT	O2'-C2'	-2.60	1.36	1.43
31	t	101	LMT	O2'-C2'	-2.60	1.36	1.43
25	a	406	CLA	MG-ND	-2.60	2.00	2.05
31	Y	101	LMT	O3'-C3'	-2.60	1.36	1.43
25	B	612	CLA	C3D-C2D	2.60	1.46	1.39
25	D	404	CLA	C4D-CHA	2.60	1.47	1.38
25	d	404	CLA	C4D-CHA	2.60	1.47	1.38
25	A	406	CLA	MG-ND	-2.59	2.00	2.05
25	b	608	CLA	MG-ND	-2.59	2.00	2.05
25	C	512	CLA	C4D-CHA	2.59	1.47	1.38
25	c	512	CLA	C4D-CHA	2.59	1.47	1.38
25	c	502	CLA	MG-ND	-2.59	2.00	2.05
31	C	524	LMT	O3'-C3'	-2.59	1.36	1.43
31	c	524	LMT	O3'-C3'	-2.59	1.36	1.43
26	D	402	PHO	CMC-C2C	-2.59	1.45	1.51
31	B	626	LMT	O3'-C3'	-2.59	1.36	1.43
31	b	626	LMT	O3'-C3'	-2.59	1.36	1.43
25	B	608	CLA	MG-ND	-2.59	2.00	2.05
25	D	401	CLA	MG-ND	-2.58	2.00	2.05
25	d	401	CLA	MG-ND	-2.58	2.00	2.05
25	B	614	CLA	C4D-CHA	2.58	1.47	1.38
25	b	614	CLA	C4D-CHA	2.58	1.47	1.38
25	B	612	CLA	C4B-CHC	2.58	1.48	1.41
25	b	612	CLA	C4B-CHC	2.58	1.48	1.41
28	H	105	LMG	C19-C18	-2.58	1.33	1.51
28	h	105	LMG	C19-C18	-2.58	1.33	1.51
30	c	501	SQD	O47-C7	2.58	1.41	1.34
30	C	501	SQD	O47-C7	2.58	1.41	1.34
28	H	105	LMG	C43-C42	-2.58	1.33	1.51
28	h	105	LMG	C43-C42	-2.58	1.33	1.51
25	B	616	CLA	MG-NC	2.58	2.12	2.06
25	B	609	CLA	C1B-NB	-2.57	1.32	1.35
25	b	609	CLA	C1B-NB	-2.57	1.32	1.35
29	D	405	PL9	C7-C8	-2.57	1.46	1.50
29	d	405	PL9	C7-C8	-2.57	1.46	1.50
25	D	404	CLA	C1C-NC	-2.57	1.34	1.37
25	d	404	CLA	C1C-NC	-2.57	1.34	1.37
25	B	603	CLA	C4D-CHA	2.57	1.47	1.38
25	c	512	CLA	C1B-CHB	2.57	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	CLA	C4D-CHA	2.57	1.47	1.38
25	d	401	CLA	C4D-CHA	2.57	1.47	1.38
31	D	411	LMT	O2'-C2'	-2.57	1.36	1.43
31	d	411	LMT	O2'-C2'	-2.57	1.36	1.43
25	d	403	CLA	C4B-CHC	2.56	1.48	1.41
31	b	623	LMT	O2B-C2B	-2.56	1.36	1.43
31	E	101	LMT	O3'-C3'	-2.56	1.37	1.43
31	e	101	LMT	O3'-C3'	-2.56	1.37	1.43
25	D	403	CLA	C4B-CHC	2.56	1.48	1.41
25	B	607	CLA	MG-NC	2.55	2.12	2.06
25	C	513	CLA	C1B-CHB	2.55	1.48	1.41
25	c	513	CLA	C1B-CHB	2.55	1.48	1.41
25	b	616	CLA	MG-NC	2.55	2.12	2.06
25	B	612	CLA	C1C-NC	-2.55	1.34	1.37
25	b	612	CLA	C1C-NC	-2.55	1.34	1.37
25	b	610	CLA	C4B-CHC	2.55	1.48	1.41
31	H	102	LMT	O3'-C3'	-2.55	1.37	1.43
31	h	102	LMT	O3'-C3'	-2.55	1.37	1.43
25	B	610	CLA	C4B-CHC	2.55	1.48	1.41
25	b	603	CLA	C4D-CHA	2.55	1.47	1.38
31	C	522	LMT	O2'-C2'	-2.55	1.37	1.43
31	B	625	LMT	O3'-C3'	-2.55	1.37	1.43
31	b	625	LMT	O3'-C3'	-2.55	1.37	1.43
25	D	403	CLA	MG-NC	2.54	2.12	2.06
25	C	505	CLA	MG-NC	2.54	2.12	2.06
25	c	505	CLA	MG-NC	2.54	2.12	2.06
31	X	101	LMT	O2'-C2'	-2.54	1.37	1.43
25	C	512	CLA	C4B-CHC	2.54	1.48	1.41
25	c	512	CLA	C4B-CHC	2.54	1.48	1.41
31	B	623	LMT	O2B-C2B	-2.54	1.37	1.43
25	D	403	CLA	C1B-CHB	2.54	1.48	1.41
25	d	403	CLA	C1B-CHB	2.54	1.48	1.41
25	C	512	CLA	C1B-CHB	2.54	1.48	1.41
25	d	403	CLA	MG-NC	2.54	2.12	2.06
25	b	602	CLA	C4B-CHC	2.54	1.48	1.41
31	x	101	LMT	O2'-C2'	-2.54	1.37	1.43
25	c	506	CLA	C4D-CHA	2.54	1.47	1.38
25	C	509	CLA	C4D-CHA	2.53	1.47	1.38
25	c	509	CLA	C4D-CHA	2.53	1.47	1.38
25	b	601	CLA	C4B-CHC	2.53	1.48	1.41
25	C	506	CLA	C4D-CHA	2.53	1.47	1.38
25	B	602	CLA	C4B-CHC	2.53	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	522	LMT	O2'-C2'	-2.53	1.37	1.43
25	B	601	CLA	C4B-CHC	2.53	1.48	1.41
25	B	604	CLA	C1B-CHB	2.52	1.48	1.41
25	C	511	CLA	C1B-CHB	2.52	1.48	1.41
25	c	511	CLA	C1B-CHB	2.52	1.48	1.41
25	b	604	CLA	C1B-CHB	2.52	1.48	1.41
25	b	607	CLA	MG-NC	2.52	2.12	2.06
25	a	405	CLA	C4B-CHC	2.51	1.48	1.41
25	A	405	CLA	C4B-CHC	2.51	1.48	1.41
29	d	405	PL9	C6-C1	-2.51	1.44	1.48
25	C	504	CLA	C4B-CHC	2.50	1.48	1.41
31	B	626	LMT	O2'-C2'	-2.50	1.37	1.43
31	b	626	LMT	O2'-C2'	-2.50	1.37	1.43
31	B	625	LMT	O3B-C3B	-2.50	1.37	1.43
31	b	625	LMT	O3B-C3B	-2.50	1.37	1.43
25	c	504	CLA	C4B-CHC	2.50	1.47	1.41
25	A	405	CLA	MG-NC	2.50	2.12	2.06
25	a	405	CLA	MG-NC	2.50	2.12	2.06
25	B	605	CLA	MG-NC	2.50	2.12	2.06
25	b	605	CLA	MG-NC	2.50	2.12	2.06
31	F	103	LMT	O3B-C3B	-2.49	1.37	1.43
29	D	405	PL9	C6-C1	-2.49	1.44	1.48
31	m	101	LMT	O3'-C3'	-2.48	1.37	1.43
31	f	103	LMT	O3B-C3B	-2.48	1.37	1.43
25	C	511	CLA	C3D-C2D	2.48	1.45	1.39
25	c	511	CLA	C3D-C2D	2.48	1.45	1.39
25	C	507	CLA	C1B-NB	-2.48	1.33	1.35
25	d	401	CLA	MG-NC	2.48	2.12	2.06
31	C	522	LMT	O3'-C3'	-2.47	1.37	1.43
25	c	514	CLA	C1B-CHB	2.47	1.47	1.41
25	C	513	CLA	C1C-NC	-2.47	1.34	1.37
25	B	614	CLA	C3D-C2D	2.47	1.45	1.39
25	D	401	CLA	MG-NC	2.47	2.12	2.06
25	d	404	CLA	C1D-C2D	2.46	1.50	1.45
25	b	614	CLA	C3D-C2D	2.46	1.45	1.39
25	C	506	CLA	C4B-CHC	2.46	1.47	1.41
31	i	103	LMT	O3B-C3B	-2.46	1.37	1.43
25	A	405	CLA	C4D-CHA	2.46	1.47	1.38
25	a	405	CLA	C4D-CHA	2.46	1.47	1.38
25	B	609	CLA	C1B-CHB	2.45	1.47	1.41
25	b	609	CLA	C1B-CHB	2.45	1.47	1.41
25	D	404	CLA	C1D-C2D	2.45	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	C1B-CHB	2.45	1.47	1.41
31	I	103	LMT	O3B-C3B	-2.45	1.37	1.43
31	M	102	LMT	O2'-C2'	-2.45	1.37	1.43
31	m	102	LMT	O2'-C2'	-2.45	1.37	1.43
31	M	101	LMT	O3'-C3'	-2.45	1.37	1.43
31	M	101	LMT	O2'-C2'	-2.45	1.37	1.43
25	c	506	CLA	C4B-CHC	2.45	1.47	1.41
25	c	511	CLA	C1B-NB	-2.45	1.33	1.35
25	C	510	CLA	C1D-C2D	2.45	1.50	1.45
25	c	510	CLA	C1D-C2D	2.45	1.50	1.45
25	A	408	CLA	C4B-CHC	2.44	1.47	1.41
25	B	602	CLA	C1B-CHB	2.44	1.47	1.41
25	b	602	CLA	C1B-CHB	2.44	1.47	1.41
25	D	404	CLA	C4B-CHC	2.44	1.47	1.41
25	D	403	CLA	C3D-C2D	2.44	1.45	1.39
25	d	403	CLA	C3D-C2D	2.44	1.45	1.39
25	c	509	CLA	C4B-CHC	2.44	1.47	1.41
25	b	614	CLA	C1B-CHB	2.44	1.47	1.41
25	B	603	CLA	C1B-CHB	2.44	1.47	1.41
25	C	514	CLA	C1B-CHB	2.44	1.47	1.41
25	B	605	CLA	C4B-CHC	2.44	1.47	1.41
25	b	605	CLA	C4B-CHC	2.44	1.47	1.41
25	c	513	CLA	C1C-NC	-2.44	1.34	1.37
31	c	522	LMT	O3'-C3'	-2.43	1.37	1.43
25	B	604	CLA	C3D-C2D	2.43	1.45	1.39
25	b	604	CLA	C3D-C2D	2.43	1.45	1.39
25	B	610	CLA	C1B-CHB	2.43	1.47	1.41
25	b	610	CLA	C1B-CHB	2.43	1.47	1.41
31	X	104	LMT	O3'-C3'	-2.43	1.37	1.43
31	m	101	LMT	O3B-C3B	-2.43	1.37	1.43
25	C	504	CLA	C1B-CHB	2.43	1.47	1.41
25	c	504	CLA	C1B-CHB	2.43	1.47	1.41
31	E	103	LMT	O3'-C3'	-2.43	1.37	1.43
31	e	103	LMT	O3'-C3'	-2.43	1.37	1.43
31	x	104	LMT	O3'-C3'	-2.43	1.37	1.43
31	B	623	LMT	O2'-C2'	-2.43	1.37	1.43
31	b	623	LMT	O2'-C2'	-2.43	1.37	1.43
31	M	101	LMT	O3B-C3B	-2.43	1.37	1.43
25	B	614	CLA	C1B-CHB	2.42	1.47	1.41
25	d	404	CLA	C4B-CHC	2.42	1.47	1.41
31	D	412	LMT	O2'-C2'	-2.42	1.37	1.43
31	b	629	LMT	O3B-C3B	-2.42	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	629	LMT	O2'-C2'	-2.42	1.37	1.43
25	a	408	CLA	C4B-CHC	2.42	1.47	1.41
25	C	509	CLA	C4B-CHC	2.42	1.47	1.41
31	D	412	LMT	O2B-C2B	-2.42	1.37	1.43
31	d	412	LMT	O2B-C2B	-2.42	1.37	1.43
31	d	412	LMT	O2'-C2'	-2.41	1.37	1.43
25	C	511	CLA	C1C-NC	-2.41	1.34	1.37
25	c	511	CLA	C1C-NC	-2.41	1.34	1.37
31	m	101	LMT	O2'-C2'	-2.41	1.37	1.43
31	B	629	LMT	O3B-C3B	-2.41	1.37	1.43
25	c	507	CLA	C1B-NB	-2.41	1.33	1.35
25	b	616	CLA	C1B-CHB	2.41	1.47	1.41
25	B	605	CLA	C1B-CHB	2.41	1.47	1.41
25	b	605	CLA	C1B-CHB	2.41	1.47	1.41
31	B	625	LMT	O2B-C2B	-2.41	1.37	1.43
31	b	625	LMT	O2B-C2B	-2.41	1.37	1.43
25	B	616	CLA	C1B-CHB	2.41	1.47	1.41
25	A	405	CLA	C1B-CHB	2.41	1.47	1.41
25	a	405	CLA	C1B-CHB	2.41	1.47	1.41
25	B	614	CLA	C4B-CHC	2.40	1.47	1.41
25	C	502	CLA	C1B-CHB	2.40	1.47	1.41
25	c	502	CLA	C1B-CHB	2.40	1.47	1.41
25	B	608	CLA	C1C-NC	-2.40	1.34	1.37
25	b	608	CLA	C1C-NC	-2.40	1.34	1.37
31	E	101	LMT	O2'-C2'	-2.40	1.37	1.43
31	e	101	LMT	O2'-C2'	-2.40	1.37	1.43
31	M	101	LMT	O2B-C2B	-2.40	1.37	1.43
31	m	101	LMT	O2B-C2B	-2.40	1.37	1.43
25	B	601	CLA	C1B-CHB	2.40	1.47	1.41
25	b	601	CLA	C1B-CHB	2.40	1.47	1.41
25	b	614	CLA	C4B-CHC	2.40	1.47	1.41
31	b	629	LMT	O2'-C2'	-2.40	1.37	1.43
31	k	105	LMT	O2'-C2'	-2.40	1.37	1.43
25	C	511	CLA	C1B-NB	-2.40	1.33	1.35
25	C	503	CLA	C1B-CHB	2.39	1.47	1.41
25	c	503	CLA	C1B-CHB	2.39	1.47	1.41
31	A	415	LMT	O2B-C2B	-2.39	1.37	1.43
31	a	415	LMT	O2B-C2B	-2.39	1.37	1.43
25	B	615	CLA	C1B-CHB	2.39	1.47	1.41
25	b	615	CLA	C1B-CHB	2.39	1.47	1.41
35	V	201	HEM	C1D-ND	-2.39	1.33	1.38
35	v	201	HEM	C1D-ND	-2.39	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	524	LMT	O2'-C2'	-2.38	1.37	1.43
31	c	524	LMT	O2'-C2'	-2.38	1.37	1.43
25	B	606	CLA	C4B-CHC	2.38	1.47	1.41
25	b	606	CLA	C4B-CHC	2.38	1.47	1.41
25	B	605	CLA	MG-ND	-2.38	2.01	2.05
25	b	605	CLA	MG-ND	-2.38	2.01	2.05
31	C	524	LMT	O2B-C2B	-2.37	1.37	1.43
31	c	524	LMT	O2B-C2B	-2.37	1.37	1.43
25	C	505	CLA	C1D-C2D	2.37	1.50	1.45
25	C	506	CLA	C1B-NB	-2.37	1.33	1.35
25	c	506	CLA	C1B-NB	-2.37	1.33	1.35
31	i	103	LMT	O2B-C2B	-2.37	1.37	1.43
25	C	502	CLA	C4B-CHC	2.36	1.47	1.41
25	c	502	CLA	C4B-CHC	2.36	1.47	1.41
31	D	410	LMT	O2'-C2'	-2.36	1.37	1.43
31	K	105	LMT	O2'-C2'	-2.36	1.37	1.43
25	B	605	CLA	C4D-CHA	2.36	1.46	1.38
25	B	612	CLA	C4D-CHA	2.36	1.46	1.38
25	b	605	CLA	C4D-CHA	2.36	1.46	1.38
25	b	612	CLA	C4D-CHA	2.36	1.46	1.38
31	I	103	LMT	O2B-C2B	-2.36	1.37	1.43
25	B	602	CLA	C1D-ND	-2.35	1.34	1.37
25	b	602	CLA	C1D-ND	-2.35	1.34	1.37
25	c	505	CLA	C1D-C2D	2.35	1.50	1.45
31	A	415	LMT	O2'-C2'	-2.35	1.37	1.43
31	a	415	LMT	O2'-C2'	-2.35	1.37	1.43
26	D	402	PHO	CAC-C3C	-2.35	1.48	1.52
26	d	402	PHO	CAC-C3C	-2.35	1.48	1.52
31	I	103	LMT	O2'-C2'	-2.35	1.37	1.43
31	i	103	LMT	O2'-C2'	-2.35	1.37	1.43
25	C	507	CLA	C1B-CHB	2.34	1.47	1.41
25	c	507	CLA	C1B-CHB	2.34	1.47	1.41
31	d	410	LMT	O2'-C2'	-2.33	1.37	1.43
25	B	613	CLA	C1B-CHB	2.33	1.47	1.41
25	b	613	CLA	C1B-CHB	2.33	1.47	1.41
25	B	603	CLA	C3D-C2D	2.33	1.45	1.39
25	b	603	CLA	C3D-C2D	2.33	1.45	1.39
31	E	103	LMT	O3B-C3B	-2.33	1.37	1.43
30	c	501	SQD	O2-C2	-2.33	1.37	1.43
25	C	510	CLA	C1A-CHA	2.33	1.52	1.43
25	c	510	CLA	C1A-CHA	2.33	1.52	1.43
25	D	401	CLA	C1D-C2D	2.33	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	401	CLA	C1D-C2D	2.33	1.49	1.45
31	X	104	LMT	O2'-C2'	-2.32	1.37	1.43
31	x	104	LMT	O2'-C2'	-2.32	1.37	1.43
31	I	101	LMT	O2'-C2'	-2.32	1.37	1.43
25	c	510	CLA	C4C-C3C	2.32	1.49	1.45
31	I	104	LMT	O2'-C2'	-2.32	1.37	1.43
31	i	104	LMT	O2'-C2'	-2.32	1.37	1.43
25	B	611	CLA	C1B-CHB	2.31	1.47	1.41
25	b	611	CLA	C1B-CHB	2.31	1.47	1.41
25	D	404	CLA	MG-ND	-2.31	2.01	2.05
25	d	404	CLA	MG-ND	-2.31	2.01	2.05
25	B	613	CLA	C1A-CHA	2.31	1.52	1.43
25	b	613	CLA	C1A-CHA	2.31	1.52	1.43
31	J	101	LMT	O2'-C2'	-2.30	1.37	1.43
31	j	101	LMT	O2'-C2'	-2.30	1.37	1.43
25	B	615	CLA	C1A-CHA	2.30	1.52	1.43
25	b	615	CLA	C1A-CHA	2.30	1.52	1.43
25	C	510	CLA	C4C-C3C	2.30	1.49	1.45
30	C	501	SQD	O2-C2	-2.30	1.37	1.43
31	Y	101	LMT	O2'-C2'	-2.30	1.37	1.43
31	y	101	LMT	O2'-C2'	-2.30	1.37	1.43
31	B	624	LMT	O2'-C2'	-2.30	1.37	1.43
31	b	624	LMT	O2'-C2'	-2.30	1.37	1.43
26	D	402	PHO	CMD-C2D	-2.29	1.46	1.51
26	d	402	PHO	CMD-C2D	-2.29	1.46	1.51
31	e	103	LMT	O3B-C3B	-2.29	1.37	1.43
31	i	101	LMT	O2'-C2'	-2.29	1.37	1.43
25	A	406	CLA	C1D-C2D	2.28	1.49	1.45
25	a	406	CLA	C1D-C2D	2.28	1.49	1.45
31	D	411	LMT	O3B-C3B	-2.28	1.37	1.43
25	B	612	CLA	C1C-C2C	2.28	1.49	1.44
25	b	612	CLA	C1C-C2C	2.28	1.49	1.44
31	A	415	LMT	O3B-C3B	-2.28	1.37	1.43
31	a	415	LMT	O3B-C3B	-2.28	1.37	1.43
25	c	504	CLA	C4C-C3C	2.28	1.49	1.45
25	c	513	CLA	C4B-CHC	2.28	1.47	1.41
25	B	606	CLA	C1D-C2D	2.28	1.49	1.45
25	b	606	CLA	C1D-C2D	2.28	1.49	1.45
25	A	405	CLA	C3D-C2D	2.28	1.45	1.39
25	a	405	CLA	C3D-C2D	2.28	1.45	1.39
25	a	406	CLA	C4B-CHC	2.27	1.47	1.41
25	C	513	CLA	C4B-CHC	2.27	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	623	LMT	O3B-C3B	-2.27	1.37	1.43
31	b	623	LMT	O3B-C3B	-2.27	1.37	1.43
25	C	504	CLA	C4C-C3C	2.27	1.48	1.45
31	B	625	LMT	O4'-C4B	-2.27	1.37	1.43
31	b	625	LMT	O4'-C4B	-2.27	1.37	1.43
31	d	411	LMT	O3B-C3B	-2.27	1.37	1.43
31	f	103	LMT	O4'-C4B	-2.27	1.37	1.43
31	D	411	LMT	O4'-C4B	-2.27	1.37	1.43
25	C	502	CLA	C1D-C2D	2.26	1.49	1.45
25	c	502	CLA	C1D-C2D	2.26	1.49	1.45
25	D	401	CLA	C1B-NB	-2.26	1.33	1.35
35	v	201	HEM	FE-NB	2.25	2.08	1.96
31	D	412	LMT	O3B-C3B	-2.25	1.37	1.43
31	d	412	LMT	O3B-C3B	-2.25	1.37	1.43
36	H	101	RRX	C12-C13	-2.25	1.41	1.45
36	h	101	RRX	C12-C13	-2.25	1.41	1.45
35	V	201	HEM	FE-NB	2.25	2.08	1.96
31	d	411	LMT	O4'-C4B	-2.25	1.37	1.43
31	A	415	LMT	O4'-C4B	-2.25	1.37	1.43
31	a	415	LMT	O4'-C4B	-2.25	1.37	1.43
31	F	103	LMT	O4'-C4B	-2.25	1.37	1.43
25	A	406	CLA	C4B-CHC	2.25	1.47	1.41
25	a	408	CLA	C1B-CHB	2.25	1.47	1.41
25	B	615	CLA	C4B-CHC	2.24	1.47	1.41
31	M	101	LMT	O1'-C1'	-2.24	1.36	1.40
31	m	101	LMT	O1'-C1'	-2.24	1.36	1.40
25	b	615	CLA	C4B-CHC	2.24	1.47	1.41
31	X	105	LMT	O2'-C2'	-2.24	1.37	1.43
31	x	105	LMT	O2'-C2'	-2.24	1.37	1.43
30	A	413	SQD	O2-C2	-2.23	1.37	1.43
30	a	413	SQD	O2-C2	-2.23	1.37	1.43
31	B	629	LMT	O2B-C2B	-2.23	1.37	1.43
31	e	103	LMT	C3'-C2'	2.23	1.58	1.52
26	a	407	PHO	CMD-C2D	-2.23	1.46	1.51
25	B	602	CLA	C1D-C2D	2.23	1.49	1.45
25	b	602	CLA	C1D-C2D	2.23	1.49	1.45
25	A	408	CLA	C1B-CHB	2.23	1.47	1.41
25	B	615	CLA	MG-ND	-2.23	2.01	2.05
25	b	615	CLA	MG-ND	-2.23	2.01	2.05
25	C	513	CLA	C1A-CHA	2.22	1.52	1.43
25	c	513	CLA	C1A-CHA	2.22	1.52	1.43
31	B	625	LMT	O1'-C1'	-2.22	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	625	LMT	O1'-C1'	-2.22	1.36	1.40
25	b	610	CLA	C4C-C3C	2.22	1.48	1.45
31	E	103	LMT	C3'-C2'	2.22	1.58	1.52
30	F	102	SQD	O2-C2	-2.22	1.37	1.43
30	f	102	SQD	O2-C2	-2.22	1.37	1.43
25	b	608	CLA	C1B-CHB	2.21	1.47	1.41
26	A	407	PHO	CMD-C2D	-2.21	1.46	1.51
25	B	606	CLA	C1B-CHB	2.21	1.47	1.41
25	b	606	CLA	C1B-CHB	2.21	1.47	1.41
31	b	629	LMT	O2B-C2B	-2.21	1.37	1.43
25	C	509	CLA	C1D-C2D	2.21	1.49	1.45
25	c	509	CLA	C1D-C2D	2.21	1.49	1.45
25	B	608	CLA	C1B-CHB	2.21	1.47	1.41
36	H	101	RRX	C19-C18	-2.21	1.41	1.45
36	h	101	RRX	C19-C18	-2.21	1.41	1.45
31	K	105	LMT	O3B-C3B	-2.21	1.37	1.43
25	b	607	CLA	C1A-CHA	2.20	1.52	1.43
25	B	607	CLA	C1A-CHA	2.20	1.52	1.43
26	A	407	PHO	CMC-C2C	-2.20	1.46	1.51
26	a	407	PHO	CMC-C2C	-2.20	1.46	1.51
31	i	102	LMT	O2'-C2'	-2.20	1.37	1.43
31	k	105	LMT	O3B-C3B	-2.20	1.37	1.43
30	h	103	SQD	O2-C2	-2.20	1.37	1.43
35	V	201	HEM	CHB-C1B	2.19	1.40	1.35
35	v	201	HEM	CHB-C1B	2.19	1.40	1.35
31	C	524	LMT	O3B-C3B	-2.19	1.37	1.43
31	c	524	LMT	O3B-C3B	-2.19	1.37	1.43
31	F	103	LMT	O2'-C2'	-2.19	1.37	1.43
31	f	103	LMT	O2'-C2'	-2.19	1.37	1.43
25	B	605	CLA	C1D-C2D	2.19	1.49	1.45
25	b	605	CLA	C1D-C2D	2.19	1.49	1.45
25	B	610	CLA	C4C-C3C	2.19	1.48	1.45
30	F	102	SQD	O4-C4	-2.19	1.37	1.43
30	f	102	SQD	O4-C4	-2.19	1.37	1.43
35	V	201	HEM	O2A-CGA	-2.18	1.23	1.30
25	B	608	CLA	C4B-CHC	2.18	1.47	1.41
25	b	608	CLA	C4B-CHC	2.18	1.47	1.41
31	M	101	LMT	O4'-C4B	-2.18	1.37	1.43
31	m	101	LMT	O4'-C4B	-2.18	1.37	1.43
30	a	412	SQD	O2-C2	-2.18	1.37	1.43
25	B	609	CLA	C4B-CHC	2.18	1.47	1.41
25	b	609	CLA	C4B-CHC	2.18	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K	105	LMT	C4B-C3B	2.18	1.57	1.52
31	K	105	LMT	O2B-C2B	-2.18	1.37	1.43
31	k	105	LMT	O2B-C2B	-2.18	1.37	1.43
31	E	103	LMT	O2'-C2'	-2.17	1.37	1.43
31	e	103	LMT	O2'-C2'	-2.17	1.37	1.43
25	B	613	CLA	C1D-C2D	2.17	1.49	1.45
25	b	613	CLA	C1D-C2D	2.17	1.49	1.45
31	I	102	LMT	O2'-C2'	-2.17	1.37	1.43
31	B	629	LMT	O4'-C4B	-2.17	1.37	1.43
31	b	629	LMT	O4'-C4B	-2.17	1.37	1.43
31	k	105	LMT	C4B-C3B	2.17	1.57	1.52
35	v	201	HEM	O2A-CGA	-2.17	1.23	1.30
31	X	103	LMT	O2'-C2'	-2.17	1.37	1.43
31	x	103	LMT	O2'-C2'	-2.17	1.37	1.43
31	F	103	LMT	O2B-C2B	-2.17	1.37	1.43
31	f	103	LMT	O2B-C2B	-2.17	1.37	1.43
31	A	416	LMT	O2'-C2'	-2.17	1.37	1.43
31	a	416	LMT	O2'-C2'	-2.17	1.37	1.43
25	b	611	CLA	C4B-CHC	2.17	1.47	1.41
25	B	613	CLA	C4B-CHC	2.16	1.47	1.41
25	A	408	CLA	MG-ND	-2.16	2.01	2.05
30	H	103	SQD	O2-C2	-2.16	1.37	1.43
25	d	401	CLA	C1B-NB	-2.16	1.33	1.35
25	c	504	CLA	C1A-CHA	2.16	1.52	1.43
25	C	510	CLA	C4B-CHC	2.16	1.47	1.41
31	D	411	LMT	O2B-C2B	-2.15	1.37	1.43
31	d	411	LMT	O2B-C2B	-2.15	1.37	1.43
25	B	611	CLA	C4B-CHC	2.15	1.47	1.41
25	A	406	CLA	C1B-CHB	2.15	1.47	1.41
25	a	406	CLA	C1B-CHB	2.15	1.47	1.41
35	e	104	HEM	C1D-ND	-2.15	1.34	1.38
30	c	501	SQD	O47-C45	-2.15	1.41	1.46
25	C	511	CLA	C4B-CHC	2.15	1.47	1.41
25	c	511	CLA	C4B-CHC	2.15	1.47	1.41
25	C	508	CLA	C1B-CHB	2.15	1.47	1.41
25	c	508	CLA	C1B-CHB	2.15	1.47	1.41
25	B	603	CLA	C4B-CHC	2.15	1.47	1.41
25	b	603	CLA	C4B-CHC	2.15	1.47	1.41
25	b	613	CLA	C4B-CHC	2.15	1.47	1.41
26	A	407	PHO	CMB-C2B	-2.14	1.46	1.51
26	a	407	PHO	CMB-C2B	-2.14	1.46	1.51
30	A	412	SQD	O2-C2	-2.14	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	C4B-CHC	2.14	1.46	1.41
29	D	405	PL9	C52-C5	-2.14	1.46	1.50
29	d	405	PL9	C52-C5	-2.14	1.46	1.50
25	C	512	CLA	C1D-C2D	2.14	1.49	1.45
25	C	505	CLA	C1B-CHB	2.14	1.46	1.41
25	c	505	CLA	C1B-CHB	2.14	1.46	1.41
25	C	504	CLA	C1A-CHA	2.14	1.52	1.43
30	k	101	SQD	O2-C2	-2.13	1.38	1.43
25	A	408	CLA	C1D-C2D	2.13	1.49	1.45
31	I	103	LMT	O1'-C1'	-2.13	1.36	1.40
31	i	103	LMT	O1'-C1'	-2.13	1.36	1.40
25	c	512	CLA	C1D-C2D	2.13	1.49	1.45
30	C	501	SQD	O47-C45	-2.13	1.41	1.46
25	C	506	CLA	C1B-CHB	2.13	1.46	1.41
25	c	506	CLA	C1B-CHB	2.13	1.46	1.41
25	B	606	CLA	C4C-C3C	2.13	1.48	1.45
25	a	408	CLA	C1D-C2D	2.13	1.49	1.45
30	K	101	SQD	O2-C2	-2.13	1.38	1.43
25	d	403	CLA	C4D-CHA	2.12	1.46	1.38
25	B	614	CLA	C1C-C2C	2.12	1.48	1.44
25	b	614	CLA	C1C-C2C	2.12	1.48	1.44
25	b	607	CLA	C1B-CHB	2.12	1.46	1.41
31	E	103	LMT	O2B-C2B	-2.12	1.38	1.43
31	e	103	LMT	O2B-C2B	-2.12	1.38	1.43
35	v	201	HEM	O2D-CGD	-2.12	1.23	1.30
25	D	403	CLA	C4D-CHA	2.12	1.45	1.38
25	C	509	CLA	C1B-CHB	2.12	1.46	1.41
25	a	408	CLA	MG-ND	-2.12	2.01	2.05
25	B	607	CLA	C1B-CHB	2.12	1.46	1.41
31	K	105	LMT	O4'-C4B	-2.12	1.38	1.43
31	k	105	LMT	O4'-C4B	-2.12	1.38	1.43
35	E	104	HEM	C1D-ND	-2.11	1.34	1.38
25	B	601	CLA	C1A-CHA	2.11	1.51	1.43
25	b	601	CLA	C1A-CHA	2.11	1.51	1.43
25	c	509	CLA	C1B-CHB	2.11	1.46	1.41
31	X	104	LMT	O1'-C1'	-2.11	1.36	1.40
31	x	104	LMT	O1'-C1'	-2.11	1.36	1.40
35	V	201	HEM	O2D-CGD	-2.11	1.23	1.30
25	C	503	CLA	C4B-CHC	2.10	1.46	1.41
25	C	506	CLA	C3D-C2D	2.10	1.44	1.39
25	c	506	CLA	C3D-C2D	2.10	1.44	1.39
25	D	401	CLA	C1B-CHB	2.10	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	401	CLA	C1B-CHB	2.10	1.46	1.41
25	C	508	CLA	C4B-CHC	2.10	1.46	1.41
25	c	508	CLA	C4B-CHC	2.10	1.46	1.41
25	B	616	CLA	C1A-CHA	2.10	1.51	1.43
25	c	503	CLA	C4B-CHC	2.09	1.46	1.41
25	B	608	CLA	C4C-C3C	2.09	1.48	1.45
25	b	608	CLA	C4C-C3C	2.09	1.48	1.45
25	d	401	CLA	C1A-CHA	2.09	1.51	1.43
25	b	606	CLA	C4C-C3C	2.09	1.48	1.45
25	C	507	CLA	CMB-C2B	-2.09	1.47	1.51
25	c	507	CLA	CMB-C2B	-2.09	1.47	1.51
25	C	504	CLA	C1D-C2D	2.09	1.49	1.45
25	c	504	CLA	C1D-C2D	2.09	1.49	1.45
25	b	616	CLA	C1A-CHA	2.09	1.51	1.43
25	a	405	CLA	C1B-NB	-2.09	1.33	1.35
25	D	401	CLA	C1A-CHA	2.08	1.51	1.43
25	C	505	CLA	C4B-CHC	2.08	1.46	1.41
25	c	505	CLA	C4B-CHC	2.08	1.46	1.41
25	d	404	CLA	C1B-CHB	2.08	1.46	1.41
25	C	507	CLA	C1D-C2D	2.08	1.49	1.45
25	c	507	CLA	C1D-C2D	2.08	1.49	1.45
25	A	405	CLA	C1B-NB	-2.08	1.33	1.35
31	E	103	LMT	O4'-C4B	-2.08	1.38	1.43
31	e	103	LMT	O4'-C4B	-2.08	1.38	1.43
31	b	623	LMT	O4'-C4B	-2.08	1.38	1.43
30	F	102	SQD	O3-C3	-2.07	1.38	1.43
30	f	102	SQD	O3-C3	-2.07	1.38	1.43
25	B	607	CLA	C4B-CHC	2.07	1.46	1.41
31	D	412	LMT	O4'-C4B	-2.07	1.38	1.43
31	d	412	LMT	O4'-C4B	-2.07	1.38	1.43
25	D	401	CLA	C4B-CHC	2.07	1.46	1.41
30	H	103	SQD	O3-C3	-2.07	1.38	1.43
30	h	103	SQD	O3-C3	-2.07	1.38	1.43
25	D	404	CLA	C4C-C3C	2.07	1.48	1.45
25	d	404	CLA	C4C-C3C	2.07	1.48	1.45
25	c	508	CLA	C1A-CHA	2.07	1.51	1.43
31	C	522	LMT	C4'-C5'	2.07	1.57	1.53
31	c	522	LMT	C4'-C5'	2.07	1.57	1.53
31	B	623	LMT	O4'-C4B	-2.07	1.38	1.43
25	B	601	CLA	C4C-C3C	2.07	1.48	1.45
25	b	601	CLA	C4C-C3C	2.07	1.48	1.45
25	b	607	CLA	C4B-CHC	2.06	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	C4C-C3C	2.06	1.48	1.45
25	B	608	CLA	C1A-CHA	2.06	1.51	1.43
25	b	608	CLA	C1A-CHA	2.06	1.51	1.43
25	B	601	CLA	C1D-C2D	2.06	1.49	1.45
25	b	601	CLA	C1D-C2D	2.06	1.49	1.45
31	C	522	LMT	C3'-C2'	2.06	1.57	1.52
25	C	508	CLA	C1A-CHA	2.06	1.51	1.43
30	A	413	SQD	O4-C4	-2.06	1.38	1.43
30	a	413	SQD	O4-C4	-2.06	1.38	1.43
25	D	404	CLA	C1B-CHB	2.05	1.46	1.41
30	A	413	SQD	O3-C3	-2.05	1.38	1.43
25	C	506	CLA	C4C-C3C	2.04	1.48	1.45
31	C	522	LMT	O1'-C1'	-2.04	1.36	1.40
31	c	522	LMT	O1'-C1'	-2.04	1.36	1.40
26	D	402	PHO	C1C-NC	-2.04	1.32	1.38
30	C	501	SQD	O3-C3	-2.04	1.38	1.43
30	c	501	SQD	O3-C3	-2.04	1.38	1.43
25	C	508	CLA	C1D-C2D	2.04	1.49	1.45
25	d	401	CLA	C4B-CHC	2.04	1.46	1.41
25	B	610	CLA	C1D-C2D	2.03	1.49	1.45
30	C	501	SQD	O4-C4	-2.03	1.38	1.43
30	c	501	SQD	O4-C4	-2.03	1.38	1.43
31	C	524	LMT	O4'-C4B	-2.03	1.38	1.43
31	c	524	LMT	O4'-C4B	-2.03	1.38	1.43
31	A	416	LMT	O1'-C1'	-2.03	1.36	1.40
31	a	416	LMT	O1'-C1'	-2.03	1.36	1.40
31	I	103	LMT	O4'-C4B	-2.03	1.38	1.43
31	i	103	LMT	O4'-C4B	-2.03	1.38	1.43
26	d	402	PHO	C1C-NC	-2.03	1.32	1.38
25	C	511	CLA	C1D-C2D	2.03	1.49	1.45
25	c	511	CLA	C1D-C2D	2.03	1.49	1.45
31	c	522	LMT	C3'-C2'	2.03	1.57	1.52
25	B	604	CLA	C1B-NB	-2.03	1.33	1.35
25	b	604	CLA	C1B-NB	-2.03	1.33	1.35
28	B	621	LMG	C25-C24	-2.03	1.33	1.49
28	b	621	LMG	C25-C24	-2.03	1.33	1.49
31	E	103	LMT	C4B-C5B	2.03	1.57	1.53
28	C	519	LMG	C25-C24	-2.03	1.33	1.49
30	a	413	SQD	O3-C3	-2.03	1.38	1.43
34	c	517	DGD	CGA-CFA	-2.02	1.33	1.49
34	c	517	DGD	CGB-CFB	-2.02	1.33	1.49
28	c	519	LMG	C25-C24	-2.02	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	517	DGD	CGB-CFB	-2.02	1.33	1.49
30	H	103	SQD	O4-C4	-2.02	1.38	1.43
28	A	410	LMG	C25-C24	-2.02	1.33	1.49
28	a	410	LMG	C25-C24	-2.02	1.33	1.49
31	e	103	LMT	C4B-C5B	2.02	1.57	1.53
34	C	518	DGD	CGB-CFB	-2.02	1.33	1.49
34	c	518	DGD	CGB-CFB	-2.02	1.33	1.49
34	C	517	DGD	CGA-CFA	-2.02	1.33	1.49
25	B	601	CLA	C1C-C2C	2.02	1.48	1.44
25	b	601	CLA	C1C-C2C	2.02	1.48	1.44
25	A	406	CLA	C4C-C3C	2.02	1.48	1.45
25	a	406	CLA	C4C-C3C	2.02	1.48	1.45
31	C	525	LMT	O2'-C2'	-2.02	1.38	1.43
25	B	609	CLA	C4C-C3C	2.01	1.48	1.45
25	b	609	CLA	C4C-C3C	2.01	1.48	1.45
30	h	103	SQD	O4-C4	-2.01	1.38	1.43
28	a	410	LMG	C43-C42	-2.01	1.33	1.49
34	H	104	DGD	CGA-CFA	-2.01	1.33	1.49
34	h	104	DGD	CGA-CFA	-2.01	1.33	1.49
34	C	516	DGD	CGA-CFA	-2.01	1.33	1.49
34	c	516	DGD	CGA-CFA	-2.01	1.33	1.49
25	B	610	CLA	C1B-NB	-2.01	1.33	1.35
25	b	610	CLA	C1B-NB	-2.01	1.33	1.35
34	H	104	DGD	CGB-CFB	-2.01	1.33	1.49
34	h	104	DGD	CGB-CFB	-2.01	1.33	1.49
25	c	508	CLA	C1D-C2D	2.01	1.49	1.45
34	C	516	DGD	CGB-CFB	-2.00	1.33	1.49
34	c	516	DGD	CGB-CFB	-2.00	1.33	1.49
28	A	410	LMG	C43-C42	-2.00	1.33	1.49
25	b	610	CLA	C1D-C2D	2.00	1.49	1.45
34	C	518	DGD	CGA-CFA	-2.00	1.33	1.49

All (2574) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	k	102	BCR	C16-C17-C18	22.99	160.12	127.31
27	K	102	BCR	C16-C17-C18	22.98	160.10	127.31
27	K	102	BCR	C20-C21-C22	22.79	159.84	127.31
27	k	102	BCR	C20-C21-C22	22.77	159.81	127.31
27	C	515	BCR	C20-C21-C22	21.40	157.85	127.31
27	c	515	BCR	C20-C21-C22	21.40	157.85	127.31
27	B	617	BCR	C20-C21-C22	20.92	157.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	617	BCR	C20-C21-C22	20.92	157.17	127.31
27	F	101	BCR	C20-C21-C22	20.90	157.14	127.31
27	f	101	BCR	C20-C21-C22	20.90	157.13	127.31
27	Z	101	BCR	C20-C21-C22	20.83	157.03	127.31
27	z	101	BCR	C20-C21-C22	20.83	157.03	127.31
27	C	515	BCR	C15-C16-C17	20.68	165.84	123.47
27	c	515	BCR	C15-C16-C17	20.67	165.81	123.47
27	C	515	BCR	C16-C17-C18	20.64	156.77	127.31
27	c	515	BCR	C16-C17-C18	20.60	156.71	127.31
27	k	103	BCR	C20-C21-C22	20.55	156.64	127.31
27	K	103	BCR	C20-C21-C22	20.54	156.62	127.31
27	F	101	BCR	C15-C16-C17	20.53	165.54	123.47
27	f	101	BCR	C15-C16-C17	20.53	165.53	123.47
27	A	409	BCR	C15-C16-C17	20.53	165.53	123.47
27	a	409	BCR	C15-C16-C17	20.51	165.49	123.47
27	b	619	BCR	C15-C16-C17	20.48	165.42	123.47
27	b	619	BCR	C20-C21-C22	20.47	156.53	127.31
27	B	619	BCR	C20-C21-C22	20.47	156.52	127.31
27	B	619	BCR	C15-C16-C17	20.45	165.37	123.47
27	b	617	BCR	C15-C16-C17	20.45	165.36	123.47
27	B	617	BCR	C15-C16-C17	20.43	165.32	123.47
27	A	409	BCR	C20-C21-C22	20.24	156.19	127.31
27	a	409	BCR	C20-C21-C22	20.24	156.19	127.31
27	B	618	BCR	C15-C16-C17	20.13	164.71	123.47
27	b	618	BCR	C15-C16-C17	20.12	164.69	123.47
27	K	103	BCR	C15-C16-C17	19.98	164.40	123.47
27	k	103	BCR	C15-C16-C17	19.96	164.37	123.47
27	z	101	BCR	C16-C17-C18	19.75	155.50	127.31
27	B	619	BCR	C16-C17-C18	19.75	155.49	127.31
27	b	619	BCR	C16-C17-C18	19.75	155.49	127.31
27	Z	101	BCR	C16-C17-C18	19.74	155.49	127.31
27	B	618	BCR	C20-C21-C22	19.59	155.27	127.31
27	b	618	BCR	C20-C21-C22	19.58	155.25	127.31
27	z	101	BCR	C15-C16-C17	19.42	163.25	123.47
27	Z	101	BCR	C15-C16-C17	19.41	163.24	123.47
27	B	618	BCR	C16-C17-C18	19.38	154.97	127.31
27	b	618	BCR	C16-C17-C18	19.38	154.97	127.31
27	k	102	BCR	C15-C16-C17	18.95	162.30	123.47
27	F	101	BCR	C16-C17-C18	18.95	154.35	127.31
27	f	101	BCR	C16-C17-C18	18.95	154.35	127.31
27	K	102	BCR	C15-C16-C17	18.92	162.24	123.47
27	b	617	BCR	C16-C17-C18	18.66	153.95	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	617	BCR	C16-C17-C18	18.66	153.94	127.31
27	a	409	BCR	C16-C17-C18	18.27	153.39	127.31
27	K	103	BCR	C16-C17-C18	18.27	153.38	127.31
27	k	103	BCR	C16-C17-C18	18.27	153.38	127.31
27	A	409	BCR	C16-C17-C18	18.27	153.38	127.31
27	K	102	BCR	C10-C11-C12	17.53	177.93	123.22
27	k	102	BCR	C10-C11-C12	17.53	177.93	123.22
27	C	515	BCR	C10-C11-C12	17.52	177.88	123.22
27	c	515	BCR	C10-C11-C12	17.50	177.84	123.22
27	K	103	BCR	C10-C11-C12	17.50	177.82	123.22
27	k	103	BCR	C10-C11-C12	17.48	177.78	123.22
27	B	618	BCR	C10-C11-C12	17.30	177.19	123.22
27	b	618	BCR	C10-C11-C12	17.28	177.16	123.22
27	b	619	BCR	C10-C11-C12	17.26	177.08	123.22
27	B	619	BCR	C10-C11-C12	17.25	177.06	123.22
27	A	409	BCR	C10-C11-C12	17.02	176.33	123.22
27	a	409	BCR	C10-C11-C12	17.02	176.33	123.22
27	F	101	BCR	C10-C11-C12	16.95	176.12	123.22
27	f	101	BCR	C10-C11-C12	16.95	176.12	123.22
27	B	617	BCR	C10-C11-C12	16.77	175.56	123.22
27	b	617	BCR	C10-C11-C12	16.77	175.56	123.22
27	Z	101	BCR	C10-C11-C12	16.59	175.00	123.22
27	z	101	BCR	C10-C11-C12	16.59	175.00	123.22
27	k	102	BCR	C11-C10-C9	13.85	147.07	127.31
27	K	102	BCR	C11-C10-C9	13.84	147.06	127.31
27	b	617	BCR	C11-C10-C9	13.75	146.93	127.31
27	B	617	BCR	C11-C10-C9	13.71	146.88	127.31
27	k	102	BCR	C16-C15-C14	13.57	151.26	123.47
27	K	102	BCR	C16-C15-C14	13.55	151.23	123.47
27	F	101	BCR	C11-C10-C9	13.49	146.57	127.31
27	f	101	BCR	C11-C10-C9	13.49	146.57	127.31
27	K	103	BCR	C16-C15-C14	13.35	150.83	123.47
27	Z	101	BCR	C16-C15-C14	13.34	150.81	123.47
27	z	101	BCR	C16-C15-C14	13.34	150.81	123.47
27	k	103	BCR	C16-C15-C14	13.34	150.80	123.47
27	B	618	BCR	C21-C20-C19	13.30	164.73	123.22
27	b	618	BCR	C21-C20-C19	13.29	164.69	123.22
27	K	103	BCR	C21-C20-C19	13.28	164.67	123.22
27	k	103	BCR	C21-C20-C19	13.28	164.66	123.22
27	B	619	BCR	C21-C20-C19	13.18	164.34	123.22
27	b	619	BCR	C21-C20-C19	13.18	164.34	123.22
27	B	617	BCR	C21-C20-C19	13.13	164.18	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	617	BCR	C21-C20-C19	13.13	164.18	123.22
27	f	101	BCR	C21-C20-C19	13.12	164.16	123.22
27	F	101	BCR	C21-C20-C19	13.12	164.16	123.22
27	A	409	BCR	C11-C10-C9	13.10	146.01	127.31
27	a	409	BCR	C11-C10-C9	13.10	146.01	127.31
27	z	101	BCR	C21-C20-C19	13.09	164.06	123.22
27	Z	101	BCR	C21-C20-C19	13.08	164.05	123.22
27	A	409	BCR	C21-C20-C19	13.08	164.03	123.22
27	a	409	BCR	C21-C20-C19	13.08	164.03	123.22
27	b	618	BCR	C16-C15-C14	12.67	149.43	123.47
27	B	618	BCR	C16-C15-C14	12.67	149.42	123.47
27	A	409	BCR	C16-C15-C14	12.49	149.06	123.47
27	a	409	BCR	C16-C15-C14	12.48	149.04	123.47
27	f	101	BCR	C16-C15-C14	12.48	149.04	123.47
27	F	101	BCR	C16-C15-C14	12.48	149.04	123.47
27	b	617	BCR	C16-C15-C14	12.43	148.94	123.47
27	B	617	BCR	C16-C15-C14	12.41	148.90	123.47
27	K	103	BCR	C11-C10-C9	12.29	144.85	127.31
27	k	103	BCR	C11-C10-C9	12.29	144.85	127.31
27	B	619	BCR	C11-C10-C9	12.20	144.73	127.31
27	b	619	BCR	C11-C10-C9	12.20	144.73	127.31
27	c	515	BCR	C21-C20-C19	12.02	160.73	123.22
27	C	515	BCR	C21-C20-C19	12.02	160.72	123.22
27	B	618	BCR	C11-C10-C9	11.93	144.34	127.31
27	b	618	BCR	C11-C10-C9	11.93	144.34	127.31
27	C	515	BCR	C16-C15-C14	11.89	147.83	123.47
27	c	515	BCR	C16-C15-C14	11.89	147.83	123.47
27	K	102	BCR	C21-C20-C19	11.84	160.17	123.22
27	k	102	BCR	C21-C20-C19	11.84	160.17	123.22
27	C	515	BCR	C11-C10-C9	11.53	143.76	127.31
27	c	515	BCR	C11-C10-C9	11.50	143.73	127.31
27	b	619	BCR	C16-C15-C14	11.50	147.02	123.47
27	B	619	BCR	C16-C15-C14	11.48	146.99	123.47
27	f	101	BCR	C11-C12-C13	11.16	157.78	126.42
27	F	101	BCR	C11-C12-C13	11.16	157.77	126.42
27	b	619	BCR	C11-C12-C13	11.02	157.38	126.42
27	B	619	BCR	C11-C12-C13	11.02	157.37	126.42
27	B	617	BCR	C11-C12-C13	10.92	157.09	126.42
27	b	617	BCR	C11-C12-C13	10.92	157.09	126.42
27	a	409	BCR	C11-C12-C13	10.91	157.05	126.42
27	C	515	BCR	C11-C12-C13	10.90	157.04	126.42
27	c	515	BCR	C11-C12-C13	10.90	157.04	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	409	BCR	C11-C12-C13	10.90	157.03	126.42
27	B	618	BCR	C11-C12-C13	10.62	156.24	126.42
27	b	618	BCR	C11-C12-C13	10.61	156.22	126.42
27	z	101	BCR	C11-C10-C9	10.55	142.37	127.31
27	Z	101	BCR	C11-C10-C9	10.54	142.35	127.31
27	K	103	BCR	C11-C12-C13	10.39	155.62	126.42
27	k	103	BCR	C11-C12-C13	10.38	155.58	126.42
27	K	102	BCR	C11-C12-C13	10.19	155.04	126.42
27	k	102	BCR	C11-C12-C13	10.18	155.01	126.42
27	Z	101	BCR	C11-C12-C13	10.10	154.78	126.42
27	z	101	BCR	C11-C12-C13	10.10	154.78	126.42
25	D	403	CLA	C2D-C1D-ND	9.86	117.37	110.10
25	d	403	CLA	C2D-C1D-ND	9.86	117.37	110.10
25	A	405	CLA	CMD-C2D-C1D	9.18	140.89	124.71
25	a	405	CLA	CMD-C2D-C1D	9.17	140.87	124.71
25	C	506	CLA	CMD-C2D-C1D	8.79	140.20	124.71
25	c	506	CLA	CMD-C2D-C1D	8.78	140.19	124.71
25	c	504	CLA	CMD-C2D-C1D	8.72	140.08	124.71
25	C	504	CLA	CMD-C2D-C1D	8.70	140.04	124.71
25	c	511	CLA	CMD-C2D-C1D	8.69	140.02	124.71
25	C	511	CLA	CMD-C2D-C1D	8.67	140.00	124.71
25	B	605	CLA	CMD-C2D-C1D	8.55	139.78	124.71
25	b	605	CLA	CMD-C2D-C1D	8.55	139.78	124.71
25	a	406	CLA	CMD-C2D-C1D	8.46	139.63	124.71
25	b	605	CLA	C2D-C1D-ND	8.44	116.33	110.10
25	A	406	CLA	CMD-C2D-C1D	8.44	139.59	124.71
25	B	605	CLA	C2D-C1D-ND	8.44	116.33	110.10
25	c	513	CLA	C2D-C1D-ND	8.39	116.29	110.10
25	c	507	CLA	C2C-C1C-NC	8.38	117.83	109.97
25	C	513	CLA	C2D-C1D-ND	8.38	116.28	110.10
25	b	615	CLA	C2D-C1D-ND	8.38	116.28	110.10
25	C	507	CLA	C2C-C1C-NC	8.35	117.79	109.97
25	B	615	CLA	C2D-C1D-ND	8.32	116.23	110.10
25	c	510	CLA	CMD-C2D-C1D	8.30	139.33	124.71
25	C	508	CLA	CMD-C2D-C1D	8.29	139.32	124.71
25	C	510	CLA	CMD-C2D-C1D	8.29	139.32	124.71
25	c	508	CLA	CMD-C2D-C1D	8.28	139.31	124.71
25	B	602	CLA	CMD-C2D-C1D	8.26	139.27	124.71
25	b	602	CLA	CMD-C2D-C1D	8.26	139.27	124.71
25	b	606	CLA	CMD-C2D-C1D	8.13	139.04	124.71
25	B	606	CLA	CMD-C2D-C1D	8.11	139.01	124.71
25	C	512	CLA	CMD-C2D-C1D	8.09	138.97	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	512	CLA	CMD-C2D-C1D	8.09	138.97	124.71
25	c	502	CLA	CMD-C2D-C1D	7.99	138.80	124.71
25	C	502	CLA	CMD-C2D-C1D	7.99	138.79	124.71
25	B	613	CLA	CMD-C2D-C1D	7.97	138.76	124.71
25	b	613	CLA	CMD-C2D-C1D	7.97	138.76	124.71
35	V	201	HEM	CHC-C4B-NB	7.93	133.05	124.43
35	v	201	HEM	CHC-C4B-NB	7.93	133.05	124.43
25	c	505	CLA	CMD-C2D-C1D	7.92	138.66	124.71
25	B	607	CLA	C4A-NA-C1A	7.91	110.26	106.71
25	C	505	CLA	CMD-C2D-C1D	7.90	138.64	124.71
25	B	604	CLA	CMD-C2D-C1D	7.90	138.63	124.71
25	b	604	CLA	CMD-C2D-C1D	7.88	138.61	124.71
25	B	614	CLA	CMD-C2D-C1D	7.86	138.56	124.71
25	b	614	CLA	CMD-C2D-C1D	7.86	138.56	124.71
25	b	607	CLA	C4A-NA-C1A	7.82	110.22	106.71
25	d	404	CLA	CMD-C2D-C1D	7.70	138.29	124.71
25	B	611	CLA	C2D-C1D-ND	7.69	115.77	110.10
25	b	611	CLA	C2D-C1D-ND	7.69	115.77	110.10
25	D	404	CLA	CMD-C2D-C1D	7.69	138.27	124.71
25	b	610	CLA	CMD-C2D-C1D	7.69	138.27	124.71
25	B	613	CLA	C2D-C1D-ND	7.69	115.77	110.10
25	B	610	CLA	CMD-C2D-C1D	7.68	138.25	124.71
25	b	601	CLA	CMD-C2D-C1D	7.67	138.24	124.71
25	b	613	CLA	C2D-C1D-ND	7.67	115.76	110.10
25	B	601	CLA	CMD-C2D-C1D	7.66	138.21	124.71
25	b	612	CLA	C2D-C1D-ND	7.66	115.75	110.10
25	B	603	CLA	CMD-C2D-C1D	7.65	138.19	124.71
25	b	603	CLA	CMD-C2D-C1D	7.65	138.19	124.71
25	b	607	CLA	CMD-C2D-C1D	7.59	138.09	124.71
25	B	607	CLA	CMD-C2D-C1D	7.59	138.09	124.71
25	B	612	CLA	C2D-C1D-ND	7.59	115.69	110.10
25	d	401	CLA	CMD-C2D-C1D	7.58	138.08	124.71
25	D	401	CLA	CMD-C2D-C1D	7.58	138.07	124.71
25	b	616	CLA	C4A-NA-C1A	7.58	110.11	106.71
25	B	616	CLA	C4A-NA-C1A	7.55	110.10	106.71
25	B	610	CLA	C2C-C1C-NC	7.53	117.03	109.97
25	b	610	CLA	C2C-C1C-NC	7.51	117.00	109.97
27	c	515	BCR	C20-C19-C18	7.51	147.50	126.42
27	C	515	BCR	C20-C19-C18	7.50	147.49	126.42
25	b	615	CLA	C4A-NA-C1A	7.50	110.08	106.71
25	A	408	CLA	C2D-C1D-ND	7.46	115.60	110.10
25	c	513	CLA	C2C-C1C-NC	7.45	116.95	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	615	CLA	C4A-NA-C1A	7.44	110.05	106.71
25	c	510	CLA	C2C-C1C-NC	7.43	116.94	109.97
25	a	408	CLA	C2D-C1D-ND	7.43	115.58	110.10
25	C	513	CLA	C2C-C1C-NC	7.42	116.92	109.97
25	b	615	CLA	CMD-C2D-C1D	7.41	137.77	124.71
25	B	607	CLA	C2D-C1D-ND	7.40	115.56	110.10
25	b	607	CLA	C2D-C1D-ND	7.40	115.56	110.10
25	C	510	CLA	C2C-C1C-NC	7.40	116.91	109.97
25	B	615	CLA	CMD-C2D-C1D	7.38	137.72	124.71
25	C	507	CLA	CMD-C2D-C1D	7.38	137.71	124.71
25	c	507	CLA	CMD-C2D-C1D	7.38	137.71	124.71
25	C	506	CLA	O2D-CGD-CBD	7.36	124.35	111.27
25	c	506	CLA	O2D-CGD-CBD	7.36	124.35	111.27
25	D	403	CLA	C1D-ND-C4D	-7.35	101.11	106.33
25	d	403	CLA	C1D-ND-C4D	-7.35	101.11	106.33
25	B	609	CLA	C2C-C1C-NC	7.34	116.84	109.97
25	b	609	CLA	C2C-C1C-NC	7.34	116.84	109.97
25	C	504	CLA	C2D-C1D-ND	7.33	115.50	110.10
25	c	504	CLA	C2D-C1D-ND	7.32	115.50	110.10
25	C	512	CLA	C2D-C1D-ND	7.30	115.48	110.10
25	c	512	CLA	C2D-C1D-ND	7.29	115.47	110.10
25	C	509	CLA	C2D-C1D-ND	7.28	115.47	110.10
25	c	509	CLA	C2D-C1D-ND	7.28	115.47	110.10
25	C	514	CLA	C2D-C1D-ND	7.28	115.47	110.10
25	B	616	CLA	CMD-C2D-C1D	7.27	137.53	124.71
25	b	616	CLA	CMD-C2D-C1D	7.26	137.50	124.71
25	B	616	CLA	C2D-C1D-ND	7.24	115.44	110.10
25	b	616	CLA	C2D-C1D-ND	7.23	115.43	110.10
25	A	408	CLA	CMD-C2D-C1D	7.23	137.46	124.71
25	B	601	CLA	C2D-C1D-ND	7.22	115.43	110.10
25	b	601	CLA	C2D-C1D-ND	7.22	115.43	110.10
25	c	514	CLA	C2D-C1D-ND	7.22	115.42	110.10
25	a	408	CLA	CMD-C2D-C1D	7.22	137.43	124.71
25	D	401	CLA	C2C-C1C-NC	7.21	116.73	109.97
25	d	401	CLA	C2C-C1C-NC	7.21	116.73	109.97
25	B	601	CLA	C2C-C1C-NC	7.14	116.66	109.97
25	b	601	CLA	C2C-C1C-NC	7.14	116.66	109.97
25	B	603	CLA	C2C-C1C-NC	7.14	116.66	109.97
25	B	604	CLA	C2C-C1C-NC	7.11	116.63	109.97
25	b	604	CLA	C2C-C1C-NC	7.11	116.63	109.97
25	b	613	CLA	C4A-NA-C1A	7.10	109.90	106.71
25	A	406	CLA	C2C-C1C-NC	7.09	116.61	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	603	CLA	C2C-C1C-NC	7.08	116.61	109.97
25	C	510	CLA	C2D-C1D-ND	7.08	115.32	110.10
25	c	510	CLA	C2D-C1D-ND	7.08	115.32	110.10
25	B	608	CLA	C2C-C1C-NC	7.06	116.59	109.97
25	a	406	CLA	C2C-C1C-NC	7.06	116.59	109.97
25	b	608	CLA	C2C-C1C-NC	7.06	116.59	109.97
25	C	510	CLA	C4A-NA-C1A	7.06	109.88	106.71
25	B	613	CLA	C4A-NA-C1A	7.06	109.88	106.71
25	C	511	CLA	C2C-C1C-NC	7.05	116.58	109.97
25	c	511	CLA	C2C-C1C-NC	7.05	116.58	109.97
25	B	602	CLA	C2D-C1D-ND	7.00	115.27	110.10
25	b	602	CLA	C2D-C1D-ND	7.00	115.27	110.10
25	B	613	CLA	C2C-C1C-NC	7.00	116.53	109.97
25	b	613	CLA	C2C-C1C-NC	7.00	116.53	109.97
25	c	510	CLA	C4A-NA-C1A	6.96	109.83	106.71
25	D	403	CLA	CMD-C2D-C1D	6.93	136.94	124.71
25	d	403	CLA	CMD-C2D-C1D	6.93	136.94	124.71
25	B	609	CLA	C2D-C1D-ND	6.93	115.21	110.10
25	c	503	CLA	CMD-C2D-C1D	6.91	136.89	124.71
25	C	503	CLA	CMD-C2D-C1D	6.90	136.88	124.71
25	B	614	CLA	C2D-C1D-ND	6.87	115.17	110.10
25	b	614	CLA	C2D-C1D-ND	6.86	115.16	110.10
25	b	609	CLA	C2D-C1D-ND	6.85	115.15	110.10
25	C	503	CLA	C2C-C1C-NC	6.85	116.39	109.97
25	c	503	CLA	C2C-C1C-NC	6.85	116.39	109.97
27	f	101	BCR	C20-C19-C18	6.80	145.53	126.42
27	F	101	BCR	C20-C19-C18	6.80	145.53	126.42
25	d	404	CLA	C2D-C1D-ND	6.79	115.11	110.10
25	D	401	CLA	C2D-C1D-ND	6.79	115.11	110.10
25	d	401	CLA	C2D-C1D-ND	6.79	115.11	110.10
25	b	608	CLA	CMD-C2D-C1D	6.78	136.66	124.71
25	B	608	CLA	CMD-C2D-C1D	6.78	136.66	124.71
27	B	619	BCR	C20-C19-C18	6.78	145.45	126.42
27	b	619	BCR	C20-C19-C18	6.78	145.45	126.42
25	c	505	CLA	C2D-C1D-ND	6.77	115.09	110.10
25	C	505	CLA	C2C-C1C-NC	6.75	116.30	109.97
25	c	505	CLA	C2C-C1C-NC	6.75	116.30	109.97
25	C	504	CLA	C2C-C1C-NC	6.75	116.30	109.97
25	c	504	CLA	C2C-C1C-NC	6.75	116.30	109.97
25	D	404	CLA	C2D-C1D-ND	6.75	115.08	110.10
25	D	401	CLA	C4A-NA-C1A	6.74	109.74	106.71
25	d	401	CLA	C4A-NA-C1A	6.74	109.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	505	CLA	C2D-C1D-ND	6.74	115.07	110.10
25	C	509	CLA	CMD-C2D-C1D	6.74	136.59	124.71
25	c	509	CLA	CMD-C2D-C1D	6.73	136.57	124.71
25	B	604	CLA	C4A-NA-C1A	6.73	109.73	106.71
25	b	612	CLA	C4A-NA-C1A	6.72	109.73	106.71
25	c	508	CLA	C2C-C1C-NC	6.69	116.24	109.97
25	B	612	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	b	604	CLA	C4A-NA-C1A	6.69	109.71	106.71
25	C	508	CLA	C2C-C1C-NC	6.67	116.22	109.97
25	C	507	CLA	C2D-C1D-ND	6.64	115.00	110.10
25	c	507	CLA	C2D-C1D-ND	6.64	115.00	110.10
25	c	512	CLA	C4A-NA-C1A	6.64	109.69	106.71
25	C	512	CLA	C4A-NA-C1A	6.63	109.69	106.71
25	A	408	CLA	C2C-C1C-NC	6.61	116.17	109.97
27	z	101	BCR	C20-C19-C18	6.61	144.97	126.42
25	a	408	CLA	C2C-C1C-NC	6.60	116.16	109.97
27	Z	101	BCR	C20-C19-C18	6.60	144.96	126.42
25	C	511	CLA	C1C-C2C-C3C	-6.55	100.07	106.96
25	c	511	CLA	C1C-C2C-C3C	-6.55	100.07	106.96
25	C	513	CLA	C4A-NA-C1A	6.55	109.65	106.71
25	B	615	CLA	C2C-C1C-NC	6.53	116.09	109.97
25	C	503	CLA	C2D-C1D-ND	6.53	114.92	110.10
25	c	503	CLA	C2D-C1D-ND	6.53	114.92	110.10
25	b	615	CLA	C2C-C1C-NC	6.52	116.08	109.97
25	d	404	CLA	C2C-C1C-NC	6.51	116.07	109.97
25	C	502	CLA	C2C-C1C-NC	6.51	116.07	109.97
25	c	502	CLA	C2C-C1C-NC	6.51	116.07	109.97
27	B	617	BCR	C20-C19-C18	6.50	144.69	126.42
25	c	513	CLA	C4A-NA-C1A	6.50	109.63	106.71
27	b	617	BCR	C20-C19-C18	6.49	144.66	126.42
25	D	404	CLA	C2C-C1C-NC	6.48	116.04	109.97
25	C	502	CLA	C2D-C1D-ND	6.47	114.88	110.10
25	c	502	CLA	C2D-C1D-ND	6.47	114.88	110.10
27	K	103	BCR	C20-C19-C18	6.47	144.59	126.42
27	k	103	BCR	C20-C19-C18	6.46	144.56	126.42
25	A	405	CLA	C2D-C1D-ND	6.43	114.84	110.10
25	a	405	CLA	C2D-C1D-ND	6.43	114.84	110.10
25	B	605	CLA	C1D-ND-C4D	-6.41	101.78	106.33
25	c	503	CLA	C4A-NA-C1A	6.41	109.59	106.71
25	C	506	CLA	C2C-C1C-NC	6.41	115.98	109.97
25	c	506	CLA	C2C-C1C-NC	6.41	115.98	109.97
27	B	618	BCR	C20-C19-C18	6.40	144.40	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	512	CLA	C2C-C1C-NC	6.40	115.97	109.97
25	c	512	CLA	C2C-C1C-NC	6.40	115.97	109.97
27	b	618	BCR	C20-C19-C18	6.40	144.40	126.42
25	b	605	CLA	C1D-ND-C4D	-6.40	101.79	106.33
25	B	616	CLA	C2C-C1C-NC	6.39	115.96	109.97
25	B	610	CLA	C2D-C1D-ND	6.39	114.81	110.10
25	B	611	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	b	611	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	b	616	CLA	C2C-C1C-NC	6.39	115.96	109.97
25	b	610	CLA	C2D-C1D-ND	6.39	114.81	110.10
25	a	406	CLA	C4A-NA-C1A	6.37	109.57	106.71
25	A	406	CLA	C4A-NA-C1A	6.37	109.57	106.71
25	B	609	CLA	CMD-C2D-C1D	6.34	135.89	124.71
25	C	503	CLA	C4A-NA-C1A	6.33	109.55	106.71
25	B	613	CLA	C3D-C2D-C1D	-6.33	97.19	105.83
25	b	613	CLA	C3D-C2D-C1D	-6.33	97.19	105.83
25	b	609	CLA	CMD-C2D-C1D	6.32	135.85	124.71
25	b	606	CLA	C2C-C1C-NC	6.31	115.89	109.97
25	C	505	CLA	C4A-NA-C1A	6.31	109.54	106.71
25	c	505	CLA	C4A-NA-C1A	6.31	109.54	106.71
25	C	512	CLA	O2A-C1-C2	6.31	125.21	108.64
25	c	512	CLA	O2A-C1-C2	6.31	125.21	108.64
25	b	611	CLA	CMD-C2D-C1D	6.30	135.81	124.71
25	C	514	CLA	CMD-C2D-C1D	6.29	135.81	124.71
25	b	606	CLA	C2D-C1D-ND	6.29	114.74	110.10
25	B	611	CLA	CMD-C2D-C1D	6.29	135.79	124.71
25	B	614	CLA	C2C-C1C-NC	6.28	115.86	109.97
25	b	614	CLA	C2C-C1C-NC	6.28	115.86	109.97
25	c	514	CLA	CMD-C2D-C1D	6.28	135.78	124.71
25	B	606	CLA	C2C-C1C-NC	6.27	115.85	109.97
25	C	503	CLA	O2A-C1-C2	6.27	125.11	108.64
25	c	503	CLA	O2A-C1-C2	6.26	125.08	108.64
25	B	606	CLA	C2D-C1D-ND	6.25	114.71	110.10
27	A	409	BCR	C20-C19-C18	6.23	143.93	126.42
27	a	409	BCR	C20-C19-C18	6.23	143.93	126.42
25	A	406	CLA	C1C-C2C-C3C	-6.22	100.42	106.96
25	a	406	CLA	C1C-C2C-C3C	-6.22	100.42	106.96
30	c	501	SQD	O9-S-C6	6.18	114.29	106.94
25	C	511	CLA	C2D-C1D-ND	6.18	114.66	110.10
25	c	511	CLA	C2D-C1D-ND	6.18	114.66	110.10
35	V	201	HEM	C1B-NB-C4B	6.17	111.44	105.07
35	v	201	HEM	C1B-NB-C4B	6.17	111.44	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	501	SQD	O9-S-C6	6.15	114.25	106.94
25	B	608	CLA	C2D-C1D-ND	6.15	114.64	110.10
25	b	608	CLA	C2D-C1D-ND	6.15	114.64	110.10
25	B	607	CLA	C2C-C1C-NC	6.11	115.69	109.97
25	B	608	CLA	C1C-C2C-C3C	-6.09	100.55	106.96
25	b	608	CLA	C1C-C2C-C3C	-6.09	100.55	106.96
25	b	607	CLA	C2C-C1C-NC	6.07	115.66	109.97
25	D	401	CLA	C1C-C2C-C3C	-6.07	100.58	106.96
25	d	401	CLA	C1C-C2C-C3C	-6.07	100.58	106.96
25	B	613	CLA	C1C-C2C-C3C	-6.06	100.59	106.96
25	B	612	CLA	C2C-C1C-NC	6.04	115.63	109.97
25	b	612	CLA	C2C-C1C-NC	6.04	115.63	109.97
25	A	405	CLA	O2A-C1-C2	6.04	124.50	108.64
25	a	405	CLA	O2A-C1-C2	6.04	124.50	108.64
25	b	613	CLA	C1C-C2C-C3C	-6.04	100.61	106.96
25	A	406	CLA	C2D-C1D-ND	6.02	114.54	110.10
25	a	406	CLA	C2D-C1D-ND	6.02	114.54	110.10
25	B	609	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	B	611	CLA	C2C-C1C-NC	5.99	115.58	109.97
25	b	611	CLA	C2C-C1C-NC	5.99	115.58	109.97
25	D	403	CLA	C4A-NA-C1A	5.96	109.39	106.71
25	b	609	CLA	C4A-NA-C1A	5.95	109.38	106.71
25	d	403	CLA	C4A-NA-C1A	5.95	109.38	106.71
25	C	514	CLA	C2C-C1C-NC	5.93	115.53	109.97
25	c	514	CLA	C2C-C1C-NC	5.93	115.53	109.97
25	b	611	CLA	O2D-CGD-CBD	5.92	121.79	111.27
25	b	601	CLA	O2D-CGD-CBD	5.91	121.77	111.27
25	B	611	CLA	O2D-CGD-CBD	5.90	121.75	111.27
25	b	612	CLA	O2D-CGD-CBD	5.89	121.74	111.27
25	B	601	CLA	O2D-CGD-CBD	5.89	121.74	111.27
25	B	602	CLA	C2C-C1C-NC	5.88	115.48	109.97
25	b	602	CLA	C2C-C1C-NC	5.87	115.47	109.97
25	B	612	CLA	O2D-CGD-CBD	5.87	121.70	111.27
25	B	603	CLA	C4A-NA-C1A	5.87	109.35	106.71
25	b	603	CLA	C4A-NA-C1A	5.87	109.35	106.71
25	C	506	CLA	O2A-C1-C2	5.86	124.03	108.64
25	C	508	CLA	C2D-C1D-ND	5.86	114.42	110.10
25	c	506	CLA	O2A-C1-C2	5.86	124.03	108.64
25	b	604	CLA	O2D-CGD-CBD	5.85	121.67	111.27
25	B	604	CLA	O2D-CGD-CBD	5.85	121.67	111.27
25	c	508	CLA	C2D-C1D-ND	5.85	114.42	110.10
27	K	102	BCR	C20-C19-C18	5.85	142.84	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	k	102	BCR	C20-C19-C18	5.84	142.81	126.42
25	B	614	CLA	C4A-NA-C1A	5.84	109.33	106.71
25	C	505	CLA	O2D-CGD-CBD	5.83	121.64	111.27
25	c	513	CLA	O2D-CGD-CBD	5.83	121.63	111.27
25	C	513	CLA	O2D-CGD-CBD	5.82	121.61	111.27
25	c	505	CLA	O2D-CGD-CBD	5.82	121.61	111.27
25	b	614	CLA	C4A-NA-C1A	5.81	109.32	106.71
25	C	510	CLA	C3D-C2D-C1D	-5.80	97.91	105.83
25	c	510	CLA	C3D-C2D-C1D	-5.80	97.91	105.83
25	C	505	CLA	O2A-C1-C2	5.80	123.88	108.64
25	A	408	CLA	O2D-CGD-CBD	5.80	121.58	111.27
25	a	408	CLA	O2D-CGD-CBD	5.80	121.58	111.27
25	C	507	CLA	O2A-C1-C2	5.80	123.87	108.64
25	c	507	CLA	O2A-C1-C2	5.80	123.87	108.64
25	B	609	CLA	C1C-C2C-C3C	-5.80	100.86	106.96
25	b	609	CLA	C1C-C2C-C3C	-5.80	100.86	106.96
25	c	505	CLA	O2A-C1-C2	5.80	123.87	108.64
25	C	509	CLA	C2C-C1C-NC	5.79	115.40	109.97
25	c	509	CLA	C2C-C1C-NC	5.79	115.40	109.97
25	B	616	CLA	O2D-CGD-CBD	5.79	121.56	111.27
25	b	616	CLA	O2D-CGD-CBD	5.79	121.56	111.27
25	B	609	CLA	O2D-CGD-CBD	5.76	121.50	111.27
25	b	615	CLA	C3D-C2D-C1D	-5.76	97.97	105.83
25	b	609	CLA	O2D-CGD-CBD	5.76	121.50	111.27
25	C	513	CLA	C1C-C2C-C3C	-5.75	100.91	106.96
25	A	405	CLA	C4A-NA-C1A	5.75	109.29	106.71
25	a	405	CLA	C4A-NA-C1A	5.75	109.29	106.71
25	b	612	CLA	C1D-ND-C4D	-5.74	102.25	106.33
25	c	513	CLA	C1C-C2C-C3C	-5.74	100.92	106.96
25	C	504	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
25	c	504	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
25	B	615	CLA	C3D-C2D-C1D	-5.72	98.02	105.83
25	B	605	CLA	C4A-NA-C1A	5.72	109.28	106.71
25	b	605	CLA	C4A-NA-C1A	5.72	109.28	106.71
25	B	612	CLA	C1D-ND-C4D	-5.72	102.27	106.33
25	c	508	CLA	C4A-NA-C1A	5.72	109.28	106.71
25	c	509	CLA	O2A-C1-C2	5.70	123.63	108.64
25	C	509	CLA	O2A-C1-C2	5.70	123.62	108.64
25	c	510	CLA	O2A-CGA-O1A	-5.68	109.25	123.59
25	C	505	CLA	C1C-C2C-C3C	-5.68	100.98	106.96
25	c	505	CLA	C1C-C2C-C3C	-5.68	100.98	106.96
25	C	513	CLA	O2A-C1-C2	5.68	123.55	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	605	CLA	CHD-C1D-ND	-5.67	119.24	124.45
25	C	510	CLA	O2A-CGA-O1A	-5.67	109.28	123.59
25	b	605	CLA	CHD-C1D-ND	-5.66	119.25	124.45
25	C	503	CLA	O2D-CGD-CBD	5.66	121.33	111.27
25	c	513	CLA	O2A-C1-C2	5.66	123.51	108.64
25	c	503	CLA	O2D-CGD-CBD	5.66	121.32	111.27
25	B	602	CLA	CHD-C1D-ND	-5.65	119.26	124.45
25	b	602	CLA	CHD-C1D-ND	-5.65	119.26	124.45
25	A	408	CLA	C1D-ND-C4D	-5.63	102.33	106.33
25	C	508	CLA	C4A-NA-C1A	5.63	109.24	106.71
25	b	601	CLA	C4A-NA-C1A	5.62	109.23	106.71
25	B	605	CLA	C3D-C2D-C1D	-5.62	98.17	105.83
25	b	605	CLA	C3D-C2D-C1D	-5.62	98.17	105.83
25	C	507	CLA	C4A-NA-C1A	5.61	109.23	106.71
25	c	507	CLA	C4A-NA-C1A	5.61	109.23	106.71
25	B	603	CLA	C1C-C2C-C3C	-5.61	101.06	106.96
27	K	103	BCR	C24-C23-C22	-5.61	117.76	126.23
25	B	601	CLA	C1C-C2C-C3C	-5.61	101.06	106.96
25	b	601	CLA	C1C-C2C-C3C	-5.61	101.06	106.96
25	C	514	CLA	C4A-NA-C1A	5.61	109.23	106.71
25	B	616	CLA	C3D-C2D-C1D	-5.60	98.19	105.83
25	a	408	CLA	C4A-NA-C1A	5.60	109.22	106.71
25	b	616	CLA	C3D-C2D-C1D	-5.59	98.20	105.83
27	k	103	BCR	C24-C23-C22	-5.59	117.79	126.23
25	b	605	CLA	C2C-C1C-NC	5.58	115.20	109.97
25	B	601	CLA	C4A-NA-C1A	5.58	109.22	106.71
25	a	408	CLA	C1C-C2C-C3C	-5.58	101.09	106.96
30	f	102	SQD	C1-O5-C5	5.58	124.64	113.69
25	A	408	CLA	C4A-NA-C1A	5.57	109.21	106.71
25	B	605	CLA	C2C-C1C-NC	5.57	115.19	109.97
30	F	102	SQD	C1-O5-C5	5.57	124.62	113.69
25	A	408	CLA	C1C-C2C-C3C	-5.56	101.11	106.96
25	a	408	CLA	C1D-ND-C4D	-5.56	102.38	106.33
25	b	603	CLA	C1C-C2C-C3C	-5.56	101.11	106.96
25	c	514	CLA	C4A-NA-C1A	5.56	109.21	106.71
30	a	413	SQD	C1-O5-C5	5.56	124.61	113.69
30	A	413	SQD	C1-O5-C5	5.56	124.61	113.69
25	B	610	CLA	O2D-CGD-CBD	5.55	121.13	111.27
25	b	610	CLA	O2D-CGD-CBD	5.55	121.13	111.27
25	C	511	CLA	O2D-CGD-CBD	5.54	121.11	111.27
25	B	615	CLA	O2A-C1-C2	5.53	123.17	108.64
25	b	615	CLA	O2A-C1-C2	5.53	123.17	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	511	CLA	O2D-CGD-CBD	5.53	121.09	111.27
25	D	404	CLA	C4A-NA-C1A	5.52	109.19	106.71
32	A	417	BCT	O2-C-O1	5.52	133.86	119.55
32	a	417	BCT	O2-C-O1	5.51	133.84	119.55
25	B	610	CLA	C1C-C2C-C3C	-5.51	101.16	106.96
25	B	607	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
25	b	607	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
25	B	604	CLA	C1C-C2C-C3C	-5.51	101.17	106.96
25	b	604	CLA	C1C-C2C-C3C	-5.51	101.17	106.96
25	C	502	CLA	O2D-CGD-CBD	5.51	121.05	111.27
25	C	502	CLA	C1C-C2C-C3C	-5.50	101.17	106.96
25	B	606	CLA	O2D-CGD-CBD	5.50	121.03	111.27
25	c	507	CLA	C1C-C2C-C3C	-5.49	101.18	106.96
25	D	403	CLA	C2C-C1C-NC	5.49	115.12	109.97
25	c	502	CLA	O2D-CGD-CBD	5.49	121.02	111.27
30	A	412	SQD	O7-S-C6	5.49	113.46	106.94
30	a	412	SQD	O7-S-C6	5.49	113.46	106.94
25	d	403	CLA	C2C-C1C-NC	5.48	115.11	109.97
25	b	610	CLA	C1C-C2C-C3C	-5.48	101.19	106.96
25	C	507	CLA	C1C-C2C-C3C	-5.48	101.20	106.96
25	b	606	CLA	O2D-CGD-CBD	5.48	121.00	111.27
25	B	605	CLA	O2D-CGD-CBD	5.47	121.00	111.27
25	b	605	CLA	O2D-CGD-CBD	5.47	121.00	111.27
25	d	404	CLA	C4A-NA-C1A	5.47	109.17	106.71
25	D	403	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
25	d	403	CLA	C3D-C2D-C1D	-5.47	98.37	105.83
25	c	505	CLA	CHD-C1D-ND	-5.47	119.43	124.45
25	B	608	CLA	C4A-NA-C1A	5.47	109.16	106.71
25	c	502	CLA	C1C-C2C-C3C	-5.47	101.21	106.96
25	C	505	CLA	CHD-C1D-ND	-5.47	119.43	124.45
25	b	608	CLA	C4A-NA-C1A	5.46	109.16	106.71
25	B	603	CLA	C2D-C1D-ND	5.41	114.09	110.10
25	b	603	CLA	C2D-C1D-ND	5.41	114.09	110.10
25	D	403	CLA	CHD-C1D-ND	-5.40	119.49	124.45
25	d	403	CLA	CHD-C1D-ND	-5.40	119.49	124.45
25	C	514	CLA	O2A-CGA-O1A	-5.40	109.97	123.59
25	c	514	CLA	O2A-CGA-O1A	-5.40	109.97	123.59
25	B	602	CLA	C1D-ND-C4D	-5.40	102.50	106.33
25	b	602	CLA	C1D-ND-C4D	-5.40	102.50	106.33
25	B	612	CLA	O2A-C1-C2	5.39	122.81	108.64
25	C	510	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
25	c	510	CLA	C1C-C2C-C3C	-5.39	101.29	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	603	CLA	O2A-CGA-O1A	-5.39	109.99	123.59
25	b	603	CLA	O2A-CGA-O1A	-5.39	109.99	123.59
25	C	511	CLA	C4A-NA-C1A	5.38	109.13	106.71
25	B	604	CLA	C2D-C1D-ND	5.38	114.07	110.10
25	b	612	CLA	O2A-C1-C2	5.38	122.77	108.64
25	c	511	CLA	C4A-NA-C1A	5.38	109.12	106.71
25	b	605	CLA	C1C-C2C-C3C	-5.37	101.31	106.96
25	B	615	CLA	C1D-ND-C4D	-5.37	102.52	106.33
25	B	605	CLA	C1C-C2C-C3C	-5.36	101.32	106.96
25	b	615	CLA	C1D-ND-C4D	-5.35	102.53	106.33
25	b	604	CLA	C2D-C1D-ND	5.35	114.05	110.10
25	C	513	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
25	c	513	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
25	b	604	CLA	O2A-C1-C2	5.35	122.69	108.64
25	B	604	CLA	O2A-C1-C2	5.34	122.67	108.64
25	d	404	CLA	C1C-C2C-C3C	-5.34	101.34	106.96
35	E	104	HEM	CHC-C4B-NB	5.32	130.22	124.43
35	e	104	HEM	CHC-C4B-NB	5.32	130.21	124.43
25	B	609	CLA	O2A-CGA-O1A	-5.31	110.19	123.59
25	b	609	CLA	O2A-CGA-O1A	-5.31	110.19	123.59
25	D	404	CLA	C1C-C2C-C3C	-5.30	101.38	106.96
25	C	508	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
25	C	511	CLA	CHD-C1D-ND	-5.29	119.59	124.45
25	c	511	CLA	CHD-C1D-ND	-5.29	119.59	124.45
31	e	103	LMT	O5B-C5B-C4B	5.29	119.30	109.69
31	E	103	LMT	O5B-C5B-C4B	5.29	119.30	109.69
25	C	509	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
25	C	508	CLA	O2D-CGD-CBD	5.28	120.66	111.27
30	H	103	SQD	O9-S-C6	5.28	113.22	106.94
30	h	103	SQD	O9-S-C6	5.28	113.22	106.94
25	c	508	CLA	O2D-CGD-CBD	5.28	120.65	111.27
25	D	403	CLA	O2A-C1-C2	5.28	122.50	108.64
25	d	403	CLA	O2A-C1-C2	5.28	122.50	108.64
25	C	508	CLA	O2A-C1-C2	5.27	122.50	108.64
25	c	508	CLA	O2A-C1-C2	5.27	122.49	108.64
25	c	508	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
25	B	611	CLA	C1D-ND-C4D	-5.26	102.59	106.33
25	b	611	CLA	C1D-ND-C4D	-5.26	102.59	106.33
25	c	509	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
25	D	401	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
25	d	401	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
25	b	606	CLA	CHD-C1D-ND	-5.25	119.63	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	601	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
25	b	601	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
25	B	613	CLA	CHD-C1D-ND	-5.24	119.64	124.45
25	C	512	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
25	C	506	CLA	C2D-C1D-ND	5.23	113.96	110.10
25	c	506	CLA	C2D-C1D-ND	5.23	113.96	110.10
25	c	512	CLA	C1D-ND-C4D	-5.23	102.62	106.33
25	c	512	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
25	C	507	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
25	c	507	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
25	b	613	CLA	CHD-C1D-ND	-5.22	119.65	124.45
25	c	505	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
25	B	606	CLA	CHD-C1D-ND	-5.21	119.67	124.45
25	b	602	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
25	C	512	CLA	C1D-ND-C4D	-5.19	102.64	106.33
25	C	505	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
25	B	602	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
25	D	404	CLA	C1D-ND-C4D	-5.19	102.65	106.33
25	d	404	CLA	C1D-ND-C4D	-5.19	102.65	106.33
25	B	602	CLA	O2D-CGD-CBD	5.18	120.47	111.27
25	b	602	CLA	O2D-CGD-CBD	5.18	120.47	111.27
25	B	610	CLA	O2A-C1-C2	5.17	122.22	108.64
25	C	508	CLA	O2A-CGA-O1A	-5.17	110.55	123.59
25	c	508	CLA	O2A-CGA-O1A	-5.17	110.55	123.59
25	b	610	CLA	O2A-C1-C2	5.16	122.21	108.64
25	b	606	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
25	C	503	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
25	c	503	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
25	B	606	CLA	C1C-C2C-C3C	-5.14	101.55	106.96
25	B	614	CLA	C1C-C2C-C3C	-5.14	101.55	106.96
25	b	614	CLA	C1C-C2C-C3C	-5.14	101.55	106.96
25	D	403	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
25	d	403	CLA	C1C-C2C-C3C	-5.13	101.56	106.96
25	B	610	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
25	C	512	CLA	O2A-CGA-O1A	-5.13	110.65	123.59
25	c	512	CLA	O2A-CGA-O1A	-5.13	110.65	123.59
25	d	404	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
25	b	610	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
25	c	512	CLA	CHD-C1D-ND	-5.12	119.75	124.45
25	B	608	CLA	CMB-C2B-C3B	5.12	134.25	124.68
25	b	608	CLA	CMB-C2B-C3B	5.12	134.25	124.68
25	A	408	CLA	C3D-C2D-C1D	-5.11	98.85	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	508	CLA	C1C-C2C-C3C	-5.11	101.58	106.96
25	C	508	CLA	C1C-C2C-C3C	-5.11	101.59	106.96
25	C	513	CLA	O2A-CGA-O1A	-5.10	110.71	123.59
25	c	513	CLA	O2A-CGA-O1A	-5.10	110.72	123.59
25	a	408	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
25	D	404	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
25	C	512	CLA	CHD-C1D-ND	-5.10	119.77	124.45
25	C	507	CLA	O2D-CGD-CBD	5.09	120.32	111.27
25	B	614	CLA	C1D-ND-C4D	-5.09	102.72	106.33
25	a	406	CLA	O2A-CGA-O1A	-5.09	110.75	123.59
25	C	504	CLA	C4A-NA-C1A	5.09	108.99	106.71
25	B	611	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
25	b	611	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
25	C	502	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
25	c	502	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
25	A	406	CLA	O2A-CGA-O1A	-5.08	110.77	123.59
25	B	615	CLA	O2A-CGA-O1A	-5.08	110.77	123.59
25	b	615	CLA	O2A-CGA-O1A	-5.08	110.78	123.59
25	b	614	CLA	C1D-ND-C4D	-5.07	102.73	106.33
25	C	506	CLA	C1C-C2C-C3C	-5.07	101.63	106.96
25	c	504	CLA	C4A-NA-C1A	5.07	108.98	106.71
25	C	502	CLA	O2A-CGA-O1A	-5.07	110.81	123.59
25	c	502	CLA	O2A-CGA-O1A	-5.07	110.81	123.59
25	c	507	CLA	O2D-CGD-CBD	5.06	120.27	111.27
25	c	506	CLA	C1C-C2C-C3C	-5.06	101.64	106.96
29	A	411	PL9	C7-C3-C4	5.04	120.98	116.88
25	C	504	CLA	C1C-C2C-C3C	-5.04	101.66	106.96
25	c	504	CLA	C1C-C2C-C3C	-5.03	101.66	106.96
25	C	514	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
25	B	615	CLA	CHD-C1D-ND	-5.02	119.84	124.45
25	C	512	CLA	C1C-C2C-C3C	-5.02	101.68	106.96
25	c	512	CLA	C1C-C2C-C3C	-5.02	101.68	106.96
25	c	504	CLA	O2A-CGA-O1A	-5.02	110.93	123.59
27	B	618	BCR	C24-C23-C22	-5.02	118.65	126.23
27	b	618	BCR	C24-C23-C22	-5.02	118.65	126.23
25	a	406	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
25	C	504	CLA	O2A-CGA-O1A	-5.01	110.94	123.59
29	a	411	PL9	C7-C3-C4	5.01	120.95	116.88
25	c	514	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
25	A	406	CLA	CHD-C1D-ND	-5.01	119.85	124.45
25	b	606	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
25	C	503	CLA	C1C-C2C-C3C	-5.00	101.70	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	503	CLA	C1C-C2C-C3C	-5.00	101.70	106.96
25	D	404	CLA	O2D-CGD-CBD	5.00	120.15	111.27
25	A	406	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
25	d	404	CLA	O2D-CGD-CBD	5.00	120.15	111.27
25	c	511	CLA	O2A-CGA-O1A	-5.00	110.97	123.59
25	b	615	CLA	CHD-C1D-ND	-5.00	119.86	124.45
25	B	607	CLA	O2A-CGA-O1A	-5.00	110.98	123.59
25	B	611	CLA	O2A-CGA-O1A	-4.99	110.99	123.59
25	b	611	CLA	O2A-CGA-O1A	-4.99	110.99	123.59
25	b	607	CLA	O2A-CGA-O1A	-4.99	111.00	123.59
25	C	511	CLA	O2A-CGA-O1A	-4.99	111.01	123.59
25	A	405	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
25	a	405	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
25	B	612	CLA	C1C-C2C-C3C	-4.98	101.72	106.96
25	b	612	CLA	C1C-C2C-C3C	-4.98	101.72	106.96
25	B	606	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
25	a	406	CLA	CHD-C1D-ND	-4.98	119.88	124.45
25	C	502	CLA	C4A-NA-C1A	4.96	108.94	106.71
25	c	502	CLA	C4A-NA-C1A	4.96	108.94	106.71
25	b	608	CLA	O2A-C1-C2	4.96	121.67	108.64
25	A	405	CLA	C1D-ND-C4D	-4.96	102.81	106.33
25	a	405	CLA	C1D-ND-C4D	-4.96	102.81	106.33
25	c	509	CLA	O2A-CGA-O1A	-4.96	111.08	123.59
25	B	602	CLA	C1C-C2C-C3C	-4.95	101.75	106.96
25	b	602	CLA	C1C-C2C-C3C	-4.95	101.75	106.96
25	B	608	CLA	O2A-C1-C2	4.95	121.64	108.64
25	C	509	CLA	O2A-CGA-O1A	-4.94	111.12	123.59
25	B	609	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
30	C	501	SQD	O6-C1-C2	4.93	116.00	108.30
30	c	501	SQD	O6-C1-C2	4.92	115.98	108.30
25	C	506	CLA	C1D-ND-C4D	-4.92	102.84	106.33
25	c	506	CLA	C1D-ND-C4D	-4.92	102.84	106.33
25	C	514	CLA	O2A-C1-C2	4.91	121.55	108.64
25	c	514	CLA	O2A-C1-C2	4.91	121.55	108.64
25	B	603	CLA	O2D-CGD-CBD	4.91	120.00	111.27
25	b	603	CLA	O2D-CGD-CBD	4.91	120.00	111.27
25	B	602	CLA	C4A-NA-C1A	4.91	108.91	106.71
25	b	602	CLA	C4A-NA-C1A	4.91	108.91	106.71
25	C	514	CLA	O2D-CGD-CBD	4.91	119.99	111.27
25	c	514	CLA	O2D-CGD-CBD	4.91	119.99	111.27
25	b	606	CLA	O2A-CGA-O1A	-4.90	111.22	123.59
25	D	404	CLA	O2A-CGA-O1A	-4.90	111.23	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	401	CLA	CHD-C1D-ND	-4.90	119.95	124.45
25	B	606	CLA	O2A-CGA-O1A	-4.89	111.24	123.59
25	d	404	CLA	CHD-C1D-ND	-4.89	119.96	124.45
25	c	509	CLA	C1D-ND-C4D	-4.89	102.86	106.33
28	C	523	LMG	O7-C10-C11	4.89	122.04	111.50
28	c	523	LMG	O7-C10-C11	4.89	122.04	111.50
25	d	404	CLA	O2A-CGA-O1A	-4.89	111.26	123.59
25	d	401	CLA	CHD-C1D-ND	-4.89	119.96	124.45
25	b	609	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
25	C	502	CLA	CHD-C1D-ND	-4.86	119.99	124.45
25	c	502	CLA	CHD-C1D-ND	-4.86	119.99	124.45
27	C	515	BCR	C24-C23-C22	-4.86	118.90	126.23
25	D	404	CLA	O2A-C1-C2	4.86	121.40	108.64
25	d	404	CLA	O2A-C1-C2	4.86	121.40	108.64
25	B	611	CLA	O2A-C1-C2	4.85	121.39	108.64
25	B	607	CLA	C1D-ND-C4D	-4.85	102.89	106.33
25	b	607	CLA	C1D-ND-C4D	-4.85	102.89	106.33
25	D	404	CLA	CHD-C1D-ND	-4.85	120.00	124.45
25	c	505	CLA	O2A-CGA-O1A	-4.85	111.36	123.59
25	b	611	CLA	O2A-C1-C2	4.85	121.37	108.64
27	c	515	BCR	C24-C23-C22	-4.84	118.92	126.23
25	B	613	CLA	O2A-C1-C2	4.84	121.36	108.64
25	B	607	CLA	O2D-CGD-CBD	4.84	119.87	111.27
25	C	509	CLA	C1D-ND-C4D	-4.84	102.90	106.33
25	b	613	CLA	O2A-C1-C2	4.83	121.34	108.64
25	C	505	CLA	O2A-CGA-O1A	-4.83	111.40	123.59
25	B	610	CLA	O2A-CGA-O1A	-4.83	111.40	123.59
25	b	610	CLA	O2A-CGA-O1A	-4.83	111.40	123.59
25	b	607	CLA	O2D-CGD-CBD	4.83	119.85	111.27
25	b	608	CLA	C1D-ND-C4D	-4.81	102.92	106.33
25	B	614	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
25	B	616	CLA	O2A-CGA-O1A	-4.80	111.47	123.59
25	B	616	CLA	O2A-C1-C2	4.80	121.25	108.64
25	b	616	CLA	O2A-C1-C2	4.80	121.24	108.64
30	k	101	SQD	C4-C3-C2	4.79	119.19	110.82
25	b	614	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
30	K	101	SQD	C4-C3-C2	4.79	119.18	110.82
25	B	601	CLA	O2A-CGA-O1A	-4.78	111.38	123.30
25	b	601	CLA	O2A-CGA-O1A	-4.78	111.38	123.30
25	b	616	CLA	O2A-CGA-O1A	-4.78	111.53	123.59
25	B	609	CLA	O2A-C1-C2	4.77	121.18	108.64
30	A	413	SQD	O5-C5-C4	4.77	118.36	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	413	SQD	O5-C5-C4	4.77	118.36	109.69
25	b	609	CLA	O2A-C1-C2	4.77	121.16	108.64
27	k	102	BCR	C7-C8-C9	-4.77	119.03	126.23
25	C	506	CLA	O2A-CGA-O1A	-4.76	111.57	123.59
25	c	506	CLA	O2A-CGA-O1A	-4.76	111.57	123.59
25	C	509	CLA	CMB-C2B-C3B	4.76	133.58	124.68
25	c	509	CLA	CMB-C2B-C3B	4.76	133.58	124.68
25	C	509	CLA	CHD-C1D-ND	-4.76	120.08	124.45
25	c	509	CLA	CHD-C1D-ND	-4.76	120.08	124.45
25	A	406	CLA	O2D-CGD-CBD	4.76	119.72	111.27
25	B	608	CLA	C1D-ND-C4D	-4.76	102.96	106.33
25	C	514	CLA	C1D-ND-C4D	-4.76	102.96	106.33
25	a	406	CLA	O2D-CGD-CBD	4.75	119.71	111.27
25	B	601	CLA	C1D-ND-C4D	-4.75	102.96	106.33
27	K	102	BCR	C7-C8-C9	-4.75	119.06	126.23
30	A	412	SQD	C44-O6-C1	4.73	122.98	113.74
25	c	514	CLA	C1D-ND-C4D	-4.73	102.98	106.33
25	D	401	CLA	C1D-ND-C4D	-4.72	102.98	106.33
25	d	401	CLA	C1D-ND-C4D	-4.72	102.98	106.33
30	a	412	SQD	C44-O6-C1	4.72	122.97	113.74
25	b	601	CLA	C1D-ND-C4D	-4.72	102.98	106.33
25	C	512	CLA	O2D-CGD-CBD	4.72	119.65	111.27
25	c	512	CLA	O2D-CGD-CBD	4.72	119.65	111.27
25	C	511	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
25	c	511	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
25	B	607	CLA	CHD-C1D-ND	-4.71	120.12	124.45
25	b	607	CLA	CHD-C1D-ND	-4.71	120.12	124.45
25	C	513	CLA	CMD-C2D-C1D	4.70	133.00	124.71
25	c	513	CLA	CMD-C2D-C1D	4.70	133.00	124.71
27	B	619	BCR	C24-C23-C22	-4.70	119.14	126.23
27	A	409	BCR	C24-C23-C22	-4.70	119.14	126.23
27	a	409	BCR	C24-C23-C22	-4.70	119.14	126.23
25	C	506	CLA	C4A-NA-C1A	4.70	108.82	106.71
25	c	506	CLA	C4A-NA-C1A	4.70	108.82	106.71
25	C	510	CLA	O2D-CGD-CBD	4.69	119.60	111.27
25	c	510	CLA	O2D-CGD-CBD	4.69	119.60	111.27
25	C	514	CLA	C1C-C2C-C3C	-4.68	102.03	106.96
25	c	514	CLA	C1C-C2C-C3C	-4.68	102.03	106.96
27	b	619	BCR	C24-C23-C22	-4.66	119.19	126.23
30	f	102	SQD	O9-S-C6	4.65	112.46	106.94
25	c	514	CLA	CMB-C2B-C3B	4.64	133.37	124.68
25	B	615	CLA	C1C-C2C-C3C	-4.64	102.07	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	615	CLA	C1C-C2C-C3C	-4.64	102.08	106.96
25	b	608	CLA	O2D-CGD-CBD	4.64	119.51	111.27
25	C	504	CLA	O2A-C1-C2	4.64	120.82	108.64
25	c	504	CLA	O2A-C1-C2	4.64	120.82	108.64
25	C	514	CLA	CMB-C2B-C3B	4.64	133.35	124.68
25	A	408	CLA	O2A-CGA-O1A	-4.63	111.90	123.59
25	a	408	CLA	O2A-CGA-O1A	-4.63	111.90	123.59
33	b	627	LHG	O7-C7-C8	4.63	121.47	111.50
33	B	627	LHG	O7-C7-C8	4.63	121.47	111.50
25	C	507	CLA	O2A-CGA-O1A	-4.62	111.93	123.59
25	B	608	CLA	O2D-CGD-CBD	4.62	119.47	111.27
30	F	102	SQD	O9-S-C6	4.61	112.42	106.94
25	a	408	CLA	CHD-C1D-ND	-4.60	120.22	124.45
28	h	105	LMG	O7-C10-C11	4.60	121.41	111.50
25	B	614	CLA	O2A-CGA-O1A	-4.60	111.99	123.59
25	A	405	CLA	O2A-CGA-O1A	-4.59	112.00	123.59
25	a	405	CLA	O2A-CGA-O1A	-4.59	112.00	123.59
25	b	614	CLA	O2A-CGA-O1A	-4.59	112.00	123.59
25	c	507	CLA	O2A-CGA-O1A	-4.59	112.00	123.59
25	C	502	CLA	C1D-ND-C4D	-4.59	103.07	106.33
25	c	502	CLA	C1D-ND-C4D	-4.59	103.07	106.33
25	A	408	CLA	CHD-C1D-ND	-4.59	120.24	124.45
28	H	105	LMG	O7-C10-C11	4.58	121.38	111.50
25	C	505	CLA	C1D-ND-C4D	-4.57	103.09	106.33
25	c	505	CLA	C1D-ND-C4D	-4.57	103.09	106.33
25	c	513	CLA	C1D-ND-C4D	-4.57	103.09	106.33
25	B	611	CLA	CAC-C3C-C4C	4.57	130.74	124.81
25	C	504	CLA	CHD-C1D-ND	-4.57	120.26	124.45
25	c	504	CLA	CHD-C1D-ND	-4.57	120.26	124.45
25	b	611	CLA	CAC-C3C-C4C	4.57	130.73	124.81
27	Z	101	BCR	C7-C8-C9	-4.56	119.34	126.23
30	a	413	SQD	O7-S-C6	4.56	112.36	106.94
30	k	101	SQD	O5-C5-C4	4.56	117.70	109.52
27	Z	101	BCR	C24-C23-C22	-4.56	119.35	126.23
27	z	101	BCR	C24-C23-C22	-4.56	119.35	126.23
25	C	513	CLA	C1D-ND-C4D	-4.55	103.10	106.33
30	A	413	SQD	O7-S-C6	4.55	112.35	106.94
25	b	603	CLA	O2A-CGA-CBA	4.55	126.19	111.91
30	K	101	SQD	O5-C5-C4	4.55	117.69	109.52
27	z	101	BCR	C7-C8-C9	-4.55	119.36	126.23
25	B	603	CLA	O2A-CGA-CBA	4.55	126.18	111.91
29	d	405	PL9	C7-C3-C4	4.52	120.55	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	511	CLA	O2A-C1-C2	4.52	120.50	108.64
25	c	511	CLA	O2A-C1-C2	4.52	120.50	108.64
29	D	405	PL9	C7-C3-C4	4.51	120.55	116.88
25	B	605	CLA	O2A-CGA-O1A	-4.50	112.23	123.59
25	b	605	CLA	O2A-CGA-O1A	-4.50	112.23	123.59
25	B	613	CLA	O2A-CGA-O1A	-4.50	112.24	123.59
25	b	613	CLA	O2A-CGA-O1A	-4.50	112.24	123.59
25	B	612	CLA	O2A-CGA-O1A	-4.49	112.25	123.59
25	C	504	CLA	C1D-ND-C4D	-4.49	103.14	106.33
25	c	504	CLA	C1D-ND-C4D	-4.49	103.14	106.33
25	C	504	CLA	O2D-CGD-CBD	4.49	119.25	111.27
25	c	504	CLA	O2D-CGD-CBD	4.49	119.25	111.27
25	B	609	CLA	C1D-ND-C4D	-4.49	103.15	106.33
25	b	609	CLA	C1D-ND-C4D	-4.48	103.15	106.33
25	b	612	CLA	O2A-CGA-O1A	-4.47	112.30	123.59
25	B	615	CLA	O2D-CGD-CBD	4.46	119.20	111.27
25	b	615	CLA	O2D-CGD-CBD	4.46	119.20	111.27
25	B	614	CLA	O2A-C1-C2	4.46	120.37	108.64
25	B	608	CLA	O2A-CGA-O1A	-4.46	112.33	123.59
25	A	408	CLA	CMB-C2B-C3B	4.46	133.03	124.68
25	a	408	CLA	CMB-C2B-C3B	4.46	133.03	124.68
25	B	604	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
25	b	608	CLA	O2A-CGA-O1A	-4.46	112.34	123.59
25	b	614	CLA	O2A-C1-C2	4.45	120.34	108.64
25	b	604	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
25	A	405	CLA	C2C-C1C-NC	4.44	114.13	109.97
25	a	405	CLA	C2C-C1C-NC	4.44	114.13	109.97
25	b	604	CLA	O2A-CGA-O1A	-4.42	112.43	123.59
25	C	509	CLA	O2D-CGD-CBD	4.41	119.11	111.27
25	c	509	CLA	O2D-CGD-CBD	4.41	119.11	111.27
25	B	601	CLA	CHD-C1D-ND	-4.41	120.40	124.45
25	b	601	CLA	CHD-C1D-ND	-4.41	120.40	124.45
25	D	401	CLA	CMB-C2B-C3B	4.41	132.94	124.68
25	d	401	CLA	CMB-C2B-C3B	4.41	132.94	124.68
25	C	506	CLA	CHD-C1D-ND	-4.41	120.40	124.45
25	c	506	CLA	CHD-C1D-ND	-4.41	120.40	124.45
25	B	604	CLA	O2A-CGA-O1A	-4.41	112.47	123.59
25	B	602	CLA	O2A-CGA-O1A	-4.40	112.48	123.59
25	b	602	CLA	O2A-CGA-O1A	-4.40	112.49	123.59
34	C	517	DGD	O2G-C1B-C2B	4.40	120.98	111.50
34	c	517	DGD	O2G-C1B-C2B	4.40	120.98	111.50
25	b	612	CLA	CMD-C2D-C1D	4.39	132.45	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	607	CLA	O2A-C1-C2	4.39	120.16	108.64
25	b	607	CLA	O2A-C1-C2	4.39	120.16	108.64
25	C	511	CLA	C1D-ND-C4D	-4.37	103.23	106.33
25	c	511	CLA	C1D-ND-C4D	-4.37	103.23	106.33
30	c	501	SQD	O9-S-O7	-4.37	98.82	113.95
25	d	401	CLA	O2D-CGD-CBD	4.37	119.03	111.27
25	B	612	CLA	CMD-C2D-C1D	4.37	132.41	124.71
25	A	405	CLA	O2D-CGD-CBD	4.37	119.03	111.27
25	a	405	CLA	O2D-CGD-CBD	4.37	119.03	111.27
30	C	501	SQD	O9-S-O7	-4.36	98.85	113.95
25	D	401	CLA	O2D-CGD-CBD	4.36	119.02	111.27
25	A	405	CLA	CHD-C1D-ND	-4.35	120.45	124.45
25	a	405	CLA	CHD-C1D-ND	-4.35	120.45	124.45
25	B	607	CLA	C1C-C2C-C3C	-4.35	102.38	106.96
25	B	612	CLA	CMC-C2C-C1C	4.35	131.66	125.04
25	b	612	CLA	CMC-C2C-C1C	4.35	131.66	125.04
26	d	402	PHO	CMB-C2B-C3B	4.34	132.80	124.68
27	k	103	BCR	C3-C4-C5	-4.34	106.33	114.08
25	B	614	CLA	O2D-CGD-CBD	4.33	118.96	111.27
25	C	510	CLA	CHD-C1D-ND	-4.33	120.47	124.45
25	c	510	CLA	CHD-C1D-ND	-4.33	120.47	124.45
27	K	103	BCR	C3-C4-C5	-4.33	106.35	114.08
27	F	101	BCR	C24-C23-C22	-4.33	119.70	126.23
27	f	101	BCR	C24-C23-C22	-4.33	119.70	126.23
34	c	518	DGD	O2G-C1B-C2B	4.33	120.82	111.50
25	a	406	CLA	O2A-C1-C2	4.32	120.00	108.64
25	A	406	CLA	C1D-ND-C4D	-4.32	103.26	106.33
25	b	607	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
26	D	402	PHO	CMB-C2B-C3B	4.32	132.76	124.68
34	C	518	DGD	O2G-C1B-C2B	4.31	120.80	111.50
25	A	406	CLA	O2A-C1-C2	4.31	119.97	108.64
25	b	614	CLA	O2D-CGD-CBD	4.31	118.93	111.27
25	c	512	CLA	O2A-CGA-CBA	4.30	125.39	111.91
25	D	403	CLA	CMB-C2B-C3B	4.30	132.72	124.68
25	d	403	CLA	CMB-C2B-C3B	4.29	132.71	124.68
25	B	606	CLA	C1D-ND-C4D	-4.29	103.29	106.33
25	a	406	CLA	C1D-ND-C4D	-4.29	103.29	106.33
25	C	509	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
25	c	509	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
25	C	512	CLA	O2A-CGA-CBA	4.29	125.37	111.91
28	a	414	LMG	O7-C10-C11	4.29	120.74	111.50
25	b	606	CLA	C1D-ND-C4D	-4.28	103.29	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	414	LMG	O7-C10-C11	4.26	120.69	111.50
25	B	604	CLA	CMA-C3A-C4A	4.26	123.22	111.77
25	b	604	CLA	CMA-C3A-C4A	4.26	123.22	111.77
25	B	603	CLA	O2A-C1-C2	4.25	119.81	108.64
25	b	603	CLA	O2A-C1-C2	4.25	119.81	108.64
27	f	101	BCR	C38-C26-C25	-4.25	119.76	124.53
25	D	401	CLA	O2A-C1-C2	4.24	119.79	108.64
25	d	401	CLA	O2A-C1-C2	4.24	119.79	108.64
27	k	103	BCR	C36-C18-C17	-4.24	116.98	122.92
25	c	502	CLA	O2A-C1-C2	4.24	119.77	108.64
25	b	612	CLA	CMB-C2B-C3B	4.23	132.59	124.68
27	K	103	BCR	C36-C18-C17	-4.23	117.00	122.92
25	C	502	CLA	O2A-C1-C2	4.23	119.74	108.64
25	B	612	CLA	CMB-C2B-C3B	4.23	132.58	124.68
25	B	603	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
25	b	603	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
35	e	104	HEM	CHD-C1D-ND	4.22	129.02	124.43
25	C	503	CLA	O2A-CGA-O1A	-4.22	112.94	123.59
25	B	610	CLA	C4A-NA-C1A	4.22	108.60	106.71
25	c	507	CLA	C1D-ND-C4D	-4.21	103.34	106.33
27	F	101	BCR	C38-C26-C25	-4.21	119.80	124.53
35	E	104	HEM	CHD-C1D-ND	4.21	129.00	124.43
25	c	514	CLA	O2A-CGA-CBA	4.21	125.11	111.91
25	c	503	CLA	O2A-CGA-O1A	-4.21	112.98	123.59
27	z	101	BCR	C3-C4-C5	-4.21	106.57	114.08
25	C	514	CLA	O2A-CGA-CBA	4.20	125.10	111.91
30	A	412	SQD	O9-S-C6	4.20	111.93	106.94
30	a	412	SQD	O9-S-C6	4.20	111.93	106.94
25	C	513	CLA	O2A-CGA-CBA	4.19	125.07	111.91
27	k	102	BCR	C3-C4-C5	-4.19	106.59	114.08
25	B	610	CLA	O2A-CGA-CBA	4.19	125.06	111.91
25	b	610	CLA	O2A-CGA-CBA	4.19	125.06	111.91
27	Z	101	BCR	C3-C4-C5	-4.19	106.60	114.08
25	b	610	CLA	C4A-NA-C1A	4.19	108.59	106.71
27	B	619	BCR	C7-C8-C9	-4.19	119.91	126.23
27	b	619	BCR	C7-C8-C9	-4.19	119.91	126.23
25	c	513	CLA	O2A-CGA-CBA	4.19	125.04	111.91
27	K	102	BCR	C3-C4-C5	-4.19	106.60	114.08
25	B	608	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
25	b	616	CLA	C1D-ND-C4D	-4.17	103.37	106.33
25	A	405	CLA	CMB-C2B-C3B	4.17	132.47	124.68
25	C	507	CLA	C1D-ND-C4D	-4.17	103.38	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	V	201	HEM	CHD-C1D-ND	4.16	128.96	124.43
35	v	201	HEM	CHD-C1D-ND	4.16	128.96	124.43
25	B	609	CLA	O2A-CGA-CBA	4.16	124.95	111.91
25	b	609	CLA	O2A-CGA-CBA	4.16	124.95	111.91
25	B	616	CLA	C1D-ND-C4D	-4.16	103.38	106.33
25	b	608	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
30	K	101	SQD	C3-C4-C5	4.15	116.24	109.77
25	a	405	CLA	CMB-C2B-C3B	4.15	132.45	124.68
25	B	616	CLA	O2A-CGA-CBA	4.15	124.94	111.91
25	B	610	CLA	CHD-C1D-ND	-4.15	120.64	124.45
25	b	610	CLA	CHD-C1D-ND	-4.15	120.64	124.45
25	C	506	CLA	C4D-C3D-CAD	4.15	112.99	108.10
25	D	403	CLA	O2A-CGA-O1A	-4.15	113.12	123.59
25	d	403	CLA	O2A-CGA-O1A	-4.15	113.12	123.59
30	k	101	SQD	C3-C4-C5	4.14	116.22	109.77
25	b	616	CLA	O2A-CGA-CBA	4.14	124.89	111.91
25	C	503	CLA	CHD-C1D-ND	-4.14	120.65	124.45
25	c	506	CLA	C4D-C3D-CAD	4.12	112.95	108.10
25	B	610	CLA	C1D-ND-C4D	-4.11	103.42	106.33
25	c	510	CLA	O2A-C1-C2	4.10	119.42	108.64
25	C	510	CLA	O2A-C1-C2	4.10	119.42	108.64
25	B	611	CLA	CMB-C2B-C3B	4.10	132.35	124.68
25	c	503	CLA	CHD-C1D-ND	-4.10	120.69	124.45
25	b	611	CLA	CMB-C2B-C3B	4.09	132.33	124.68
25	a	408	CLA	CAA-C2A-C3A	-4.09	101.58	112.78
25	B	612	CLA	C3C-C4C-NC	4.09	115.15	110.57
25	b	612	CLA	C3C-C4C-NC	4.09	115.15	110.57
25	b	610	CLA	C1D-ND-C4D	-4.08	103.44	106.33
25	A	408	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
36	h	101	RRX	C34-C9-C10	-4.07	117.22	122.92
36	H	101	RRX	C34-C9-C10	-4.07	117.22	122.92
25	c	506	CLA	CMB-C2B-C3B	4.06	132.27	124.68
25	C	506	CLA	CMB-C2B-C3B	4.05	132.26	124.68
30	H	103	SQD	O9-S-O7	-4.04	99.95	113.95
30	h	103	SQD	O9-S-O7	-4.04	99.95	113.95
25	C	503	CLA	C1D-ND-C4D	-4.04	103.47	106.33
25	c	503	CLA	C1D-ND-C4D	-4.04	103.47	106.33
25	D	401	CLA	O2A-CGA-O1A	-4.03	113.41	123.59
25	d	401	CLA	O2A-CGA-O1A	-4.03	113.41	123.59
25	C	507	CLA	CHD-C1D-ND	-4.03	120.75	124.45
25	c	507	CLA	CHD-C1D-ND	-4.03	120.75	124.45
30	A	413	SQD	O9-S-C6	4.02	111.72	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	614	CLA	CMB-C2B-C3B	4.02	132.21	124.68
25	b	612	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
25	B	614	CLA	CMB-C2B-C3B	4.02	132.19	124.68
25	C	508	CLA	CHD-C1D-ND	-4.01	120.77	124.45
25	c	508	CLA	CHD-C1D-ND	-4.01	120.77	124.45
25	B	613	CLA	O2D-CGD-CBD	4.01	118.39	111.27
25	b	613	CLA	O2D-CGD-CBD	4.01	118.39	111.27
33	Z	102	LHG	O7-C7-C8	4.00	120.12	111.50
33	z	102	LHG	O7-C7-C8	4.00	120.11	111.50
30	a	413	SQD	O9-S-C6	4.00	111.69	106.94
25	a	408	CLA	O2A-C1-C2	3.99	119.13	108.64
25	B	612	CLA	C3D-C2D-C1D	-3.99	100.38	105.83
36	H	101	RRX	C37-C22-C21	-3.99	117.34	122.92
30	A	412	SQD	O9-S-O7	-3.98	100.17	113.95
30	a	412	SQD	O9-S-O7	-3.98	100.17	113.95
25	A	408	CLA	O2A-C1-C2	3.98	119.09	108.64
25	C	509	CLA	C4A-NA-C1A	3.98	108.50	106.71
25	B	614	CLA	CHD-C1D-ND	-3.98	120.80	124.45
25	c	502	CLA	CMB-C2B-C3B	3.98	132.12	124.68
36	h	101	RRX	C37-C22-C21	-3.97	117.36	122.92
30	K	101	SQD	C1-O5-C5	3.96	120.48	113.67
25	C	502	CLA	CMB-C2B-C3B	3.96	132.09	124.68
25	b	614	CLA	CHD-C1D-ND	-3.96	120.81	124.45
35	e	104	HEM	CHA-C4D-ND	3.95	129.26	124.38
30	k	101	SQD	C1-O5-C5	3.95	120.45	113.67
35	E	104	HEM	CHA-C4D-ND	3.94	129.25	124.38
28	b	621	LMG	O7-C10-C11	3.94	119.98	111.50
25	A	405	CLA	O2A-CGA-CBA	3.93	124.24	111.91
25	a	405	CLA	O2A-CGA-CBA	3.93	124.24	111.91
25	c	509	CLA	C4A-NA-C1A	3.92	108.47	106.71
30	F	102	SQD	O9-S-O7	-3.92	100.39	113.95
28	B	621	LMG	O7-C10-C11	3.92	119.95	111.50
25	B	614	CLA	CMC-C2C-C1C	3.92	131.00	125.04
25	b	614	CLA	CMC-C2C-C1C	3.92	131.00	125.04
30	A	412	SQD	C4-C3-C2	3.92	117.66	110.82
30	f	102	SQD	O9-S-O7	-3.91	100.41	113.95
25	C	514	CLA	CHD-C1D-ND	-3.91	120.86	124.45
30	a	412	SQD	C4-C3-C2	3.90	117.63	110.82
25	c	502	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
25	C	511	CLA	O2A-CGA-CBA	3.88	124.09	111.91
25	C	502	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
25	c	514	CLA	CHD-C1D-ND	-3.88	120.89	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	524	LMT	O5B-C5B-C4B	3.88	116.73	109.69
25	C	502	CLA	O2A-CGA-CBA	3.87	124.07	111.91
25	c	502	CLA	O2A-CGA-CBA	3.87	124.07	111.91
25	c	511	CLA	O2A-CGA-CBA	3.87	124.06	111.91
25	B	606	CLA	CMB-C2B-C3B	3.87	131.92	124.68
25	b	606	CLA	CMB-C2B-C3B	3.87	131.92	124.68
27	Z	101	BCR	C38-C26-C25	-3.87	120.18	124.53
27	z	101	BCR	C38-C26-C25	-3.87	120.18	124.53
31	C	524	LMT	O5B-C5B-C4B	3.86	116.71	109.69
25	a	405	CLA	CAC-C3C-C4C	3.84	129.79	124.81
25	c	511	CLA	CMB-C2B-C3B	3.84	131.86	124.68
34	H	104	DGD	O2G-C1B-C2B	3.84	119.77	111.50
35	e	104	HEM	C1B-NB-C4B	3.83	109.03	105.07
25	A	405	CLA	CAC-C3C-C4C	3.83	129.77	124.81
25	C	511	CLA	CMB-C2B-C3B	3.82	131.82	124.68
34	h	104	DGD	O2G-C1B-C2B	3.82	119.73	111.50
35	E	104	HEM	C1B-NB-C4B	3.82	109.02	105.07
25	B	607	CLA	O2A-CGA-CBA	3.82	123.88	111.91
25	b	607	CLA	O2A-CGA-CBA	3.81	123.87	111.91
25	C	505	CLA	CMB-C2B-C3B	3.81	131.81	124.68
25	b	611	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
25	c	505	CLA	CMB-C2B-C3B	3.80	131.80	124.68
36	h	101	RRX	C16-C15-C14	3.80	131.26	123.47
36	H	101	RRX	C16-C15-C14	3.79	131.25	123.47
25	b	610	CLA	CMB-C2B-C3B	3.79	131.77	124.68
25	b	603	CLA	C4-C3-C5	3.79	121.64	115.27
25	B	611	CLA	C1C-C2C-C3C	-3.79	102.98	106.96
25	C	504	CLA	O2A-CGA-CBA	3.78	123.77	111.91
25	c	504	CLA	O2A-CGA-CBA	3.77	123.75	111.91
25	B	603	CLA	C4-C3-C5	3.77	121.61	115.27
25	a	406	CLA	O2A-CGA-CBA	3.76	123.71	111.91
25	B	610	CLA	CMB-C2B-C3B	3.76	131.71	124.68
25	B	611	CLA	CHD-C1D-ND	-3.76	121.00	124.45
25	A	406	CLA	O2A-CGA-CBA	3.76	123.69	111.91
33	E	102	LHG	O7-C7-C8	3.75	119.59	111.50
33	e	102	LHG	O7-C7-C8	3.75	119.59	111.50
25	b	611	CLA	CHD-C1D-ND	-3.75	121.01	124.45
25	C	506	CLA	CMD-C2D-C3D	-3.75	118.98	127.61
25	c	506	CLA	CMD-C2D-C3D	-3.75	119.00	127.61
25	B	605	CLA	CMB-C2B-C3B	3.75	131.69	124.68
25	b	605	CLA	CMB-C2B-C3B	3.75	131.69	124.68
31	K	105	LMT	O5B-C5B-C4B	3.74	116.49	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	616	CLA	CHD-C1D-ND	-3.74	121.02	124.45
25	B	602	CLA	O2A-C1-C2	3.74	118.46	108.64
25	b	602	CLA	O2A-C1-C2	3.74	118.46	108.64
25	B	608	CLA	CHD-C1D-ND	-3.73	121.03	124.45
25	b	608	CLA	CHD-C1D-ND	-3.73	121.03	124.45
25	C	506	CLA	O2A-CGA-CBA	3.72	123.60	111.91
25	c	506	CLA	O2A-CGA-CBA	3.72	123.60	111.91
27	k	102	BCR	C24-C23-C22	-3.72	120.61	126.23
30	f	102	SQD	O7-S-C6	3.72	111.36	106.94
31	k	105	LMT	O5B-C5B-C4B	3.72	116.45	109.69
25	C	506	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
25	c	506	CLA	C3D-C2D-C1D	-3.72	100.76	105.83
30	F	102	SQD	O7-S-C6	3.71	111.35	106.94
30	H	103	SQD	O47-C7-C8	3.71	119.50	111.50
30	h	103	SQD	O47-C7-C8	3.71	119.50	111.50
30	A	413	SQD	O9-S-O7	-3.71	101.12	113.95
30	a	413	SQD	O9-S-O7	-3.71	101.12	113.95
25	B	616	CLA	CHD-C1D-ND	-3.71	121.05	124.45
27	K	102	BCR	C24-C23-C22	-3.70	120.64	126.23
30	F	102	SQD	O5-C5-C4	3.70	116.42	109.69
25	c	504	CLA	CMB-C2B-C3B	3.70	131.60	124.68
25	C	504	CLA	CMB-C2B-C3B	3.70	131.60	124.68
30	f	102	SQD	O5-C5-C4	3.70	116.41	109.69
25	c	513	CLA	CHD-C1D-ND	-3.68	121.07	124.45
25	A	405	CLA	CMC-C2C-C1C	3.68	130.64	125.04
25	a	405	CLA	CMC-C2C-C1C	3.68	130.64	125.04
28	D	409	LMG	O7-C10-C11	3.67	119.42	111.50
28	d	409	LMG	O7-C10-C11	3.67	119.42	111.50
33	D	408	LHG	O7-C7-C8	3.67	119.41	111.50
33	d	408	LHG	O7-C7-C8	3.67	119.41	111.50
25	C	513	CLA	CHD-C1D-ND	-3.67	121.08	124.45
25	c	512	CLA	CMB-C2B-C3B	3.67	131.54	124.68
25	B	604	CLA	C1D-ND-C4D	-3.66	103.73	106.33
25	b	604	CLA	C1D-ND-C4D	-3.66	103.73	106.33
27	K	103	BCR	C19-C18-C17	3.66	124.56	118.94
27	k	103	BCR	C19-C18-C17	3.66	124.56	118.94
35	E	104	HEM	CBA-CAA-C2A	-3.66	106.37	112.62
35	e	104	HEM	CBA-CAA-C2A	-3.66	106.37	112.62
25	d	404	CLA	O2A-CGA-CBA	3.66	123.39	111.91
25	B	613	CLA	C1D-ND-C4D	-3.66	103.74	106.33
25	D	404	CLA	O2A-CGA-CBA	3.65	123.38	111.91
25	C	512	CLA	CMB-C2B-C3B	3.65	131.51	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	504	CLA	CMA-C3A-C4A	3.65	121.58	111.77
25	c	504	CLA	CMA-C3A-C4A	3.64	121.57	111.77
25	b	613	CLA	C1D-ND-C4D	-3.64	103.75	106.33
28	A	410	LMG	O7-C10-C11	3.64	119.35	111.50
30	H	103	SQD	O8-S-C6	3.63	111.53	105.74
30	h	103	SQD	O8-S-C6	3.63	111.53	105.74
28	a	410	LMG	O7-C10-C11	3.62	119.31	111.50
30	K	101	SQD	O47-C7-C8	3.61	119.29	111.50
30	k	101	SQD	O47-C7-C8	3.61	119.29	111.50
25	B	605	CLA	CMC-C2C-C1C	3.61	130.53	125.04
25	b	605	CLA	CMC-C2C-C1C	3.61	130.53	125.04
25	d	403	CLA	O2D-CGD-CBD	3.60	117.67	111.27
25	C	512	CLA	C1-C2-C3	-3.59	119.83	126.04
27	Z	101	BCR	C15-C14-C13	-3.59	122.18	127.31
25	C	510	CLA	O2A-CGA-CBA	3.59	123.17	111.91
25	c	510	CLA	O2A-CGA-CBA	3.59	123.17	111.91
25	c	512	CLA	C1-C2-C3	-3.59	119.84	126.04
25	b	604	CLA	O2A-CGA-CBA	3.59	123.17	111.91
33	D	406	LHG	O7-C7-C8	3.59	119.23	111.50
25	D	403	CLA	O2D-CGD-CBD	3.58	117.64	111.27
25	B	611	CLA	O2A-CGA-CBA	3.58	123.14	111.91
25	b	611	CLA	O2A-CGA-CBA	3.58	123.14	111.91
25	C	510	CLA	C1D-ND-C4D	-3.58	103.79	106.33
25	c	510	CLA	C1D-ND-C4D	-3.58	103.79	106.33
25	B	604	CLA	O2A-CGA-CBA	3.57	123.12	111.91
33	d	406	LHG	O7-C7-C8	3.57	119.20	111.50
25	a	406	CLA	CMB-C2B-C3B	3.57	131.35	124.68
25	D	401	CLA	O2A-CGA-CBA	3.57	123.10	111.91
25	d	401	CLA	O2A-CGA-CBA	3.57	123.10	111.91
28	C	519	LMG	O7-C10-C11	3.56	119.18	111.50
25	C	507	CLA	O2A-CGA-CBA	3.56	123.09	111.91
25	B	609	CLA	CHD-C1D-ND	-3.56	121.18	124.45
27	z	101	BCR	C15-C14-C13	-3.56	122.23	127.31
25	c	507	CLA	O2A-CGA-CBA	3.55	123.06	111.91
25	B	612	CLA	O2A-CGA-CBA	3.55	123.05	111.91
25	a	405	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
25	A	405	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
36	H	101	RRX	C15-C16-C17	3.55	130.74	123.47
28	c	519	LMG	O7-C10-C11	3.55	119.14	111.50
30	f	102	SQD	O47-C7-C8	3.55	119.14	111.50
25	A	406	CLA	CMB-C2B-C3B	3.55	131.31	124.68
25	b	609	CLA	CHD-C1D-ND	-3.55	121.20	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	h	101	RRX	C15-C16-C17	3.55	130.74	123.47
25	c	513	CLA	CMB-C2B-C3B	3.54	131.31	124.68
25	b	612	CLA	O2A-CGA-CBA	3.54	123.03	111.91
30	a	412	SQD	O5-C1-C2	3.54	117.85	110.35
25	A	408	CLA	O2A-CGA-CBA	3.54	123.03	111.91
25	a	408	CLA	O2A-CGA-CBA	3.54	123.03	111.91
25	B	603	CLA	C1D-ND-C4D	-3.54	103.82	106.33
30	F	102	SQD	O47-C7-C8	3.54	119.13	111.50
30	A	412	SQD	O5-C1-C2	3.54	117.84	110.35
25	A	405	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
25	C	513	CLA	CMB-C2B-C3B	3.53	131.29	124.68
25	a	405	CLA	CAA-C2A-C3A	-3.53	103.10	112.78
33	D	407	LHG	O7-C7-C8	3.53	119.10	111.50
33	d	407	LHG	O7-C7-C8	3.52	119.09	111.50
25	d	403	CLA	C4-C3-C5	3.52	121.18	115.27
25	B	613	CLA	O2A-CGA-CBA	3.51	122.91	111.91
25	b	613	CLA	O2A-CGA-CBA	3.51	122.91	111.91
25	c	513	CLA	C3C-C4C-NC	3.50	114.50	110.57
25	D	403	CLA	C4-C3-C5	3.50	121.15	115.27
25	b	603	CLA	C1D-ND-C4D	-3.49	103.85	106.33
25	C	513	CLA	C1-C2-C3	-3.49	121.10	126.75
25	C	513	CLA	C3C-C4C-NC	3.49	114.48	110.57
25	b	606	CLA	O2A-CGA-CBA	3.49	122.86	111.91
25	B	606	CLA	O2A-CGA-CBA	3.48	122.84	111.91
25	c	509	CLA	O2A-CGA-CBA	3.48	122.81	111.91
25	c	513	CLA	C1-C2-C3	-3.47	121.13	126.75
25	B	608	CLA	O2A-CGA-CBA	3.47	122.81	111.91
25	b	608	CLA	CMC-C2C-C1C	3.47	130.32	125.04
25	B	608	CLA	CMC-C2C-C1C	3.47	130.32	125.04
25	d	404	CLA	CAA-C2A-C3A	-3.46	103.29	112.78
25	C	509	CLA	O2A-CGA-CBA	3.46	122.78	111.91
25	D	404	CLA	CAA-C2A-C3A	-3.46	103.30	112.78
25	B	603	CLA	C4D-C3D-CAD	3.46	112.17	108.10
25	b	608	CLA	O2A-CGA-CBA	3.46	122.77	111.91
25	C	511	CLA	C1-C2-C3	-3.46	120.06	126.04
25	c	511	CLA	C1-C2-C3	-3.46	120.06	126.04
27	k	103	BCR	C37-C22-C21	-3.45	118.08	122.92
25	c	503	CLA	C1-C2-C3	-3.45	120.07	126.04
27	B	617	BCR	C19-C18-C17	3.44	124.22	118.94
27	K	103	BCR	C37-C22-C21	-3.44	118.11	122.92
25	C	503	CLA	C1-C2-C3	-3.44	120.10	126.04
25	b	615	CLA	C3C-C4C-NC	3.44	114.42	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	614	CLA	C4D-C3D-CAD	3.44	112.14	108.10
25	b	614	CLA	C4D-C3D-CAD	3.44	112.14	108.10
25	b	603	CLA	C4D-C3D-CAD	3.43	112.14	108.10
27	b	617	BCR	C19-C18-C17	3.43	124.20	118.94
25	D	401	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
25	c	509	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
25	C	509	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
36	H	101	RRX	C35-C13-C14	-3.43	118.12	122.92
25	d	401	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
25	b	604	CLA	C4D-C3D-CAD	3.42	112.13	108.10
25	B	603	CLA	CMB-C2B-C3B	3.42	131.07	124.68
30	A	413	SQD	C44-O6-C1	3.42	120.41	113.74
30	a	413	SQD	C44-O6-C1	3.42	120.41	113.74
36	h	101	RRX	C35-C13-C14	-3.42	118.14	122.92
34	C	516	DGD	O2G-C1B-C2B	3.42	118.86	111.50
27	Z	101	BCR	C36-C18-C17	-3.42	118.14	122.92
27	k	102	BCR	C36-C18-C19	-3.41	112.70	118.08
34	c	516	DGD	O2G-C1B-C2B	3.41	118.86	111.50
25	b	603	CLA	CMB-C2B-C3B	3.41	131.06	124.68
28	a	410	LMG	O8-C28-C29	3.41	122.62	111.91
35	e	104	HEM	CHB-C1B-NB	3.41	128.59	124.38
27	K	102	BCR	C36-C18-C19	-3.41	112.70	118.08
25	B	615	CLA	C3C-C4C-NC	3.41	114.39	110.57
25	b	610	CLA	C3C-C4C-NC	3.40	114.39	110.57
28	A	410	LMG	O8-C28-C29	3.40	122.58	111.91
25	B	606	CLA	C4A-NA-C1A	3.40	108.23	106.71
27	z	101	BCR	C36-C18-C17	-3.40	118.17	122.92
25	B	604	CLA	C4D-C3D-CAD	3.39	112.10	108.10
27	a	409	BCR	C38-C26-C25	-3.39	120.72	124.53
35	E	104	HEM	CHB-C1B-NB	3.39	128.57	124.38
25	d	403	CLA	O2A-CGA-CBA	3.39	122.54	111.91
30	H	103	SQD	C44-O6-C1	3.39	120.36	113.74
25	b	611	CLA	O1D-CGD-CBD	-3.39	117.56	124.48
25	B	610	CLA	C3C-C4C-NC	3.38	114.36	110.57
25	D	403	CLA	O2A-CGA-CBA	3.38	122.52	111.91
25	b	606	CLA	C4A-NA-C1A	3.38	108.23	106.71
31	E	103	LMT	C3'-C4'-C5'	-3.38	103.18	110.93
25	B	611	CLA	O1D-CGD-CBD	-3.37	117.59	124.48
25	B	616	CLA	CMB-C2B-C3B	3.37	130.98	124.68
25	B	602	CLA	O2A-CGA-CBA	3.37	122.48	111.91
25	b	602	CLA	O2A-CGA-CBA	3.37	122.47	111.91
30	h	103	SQD	C44-O6-C1	3.37	120.31	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	503	CLA	O2A-CGA-CBA	3.37	122.47	111.91
25	c	503	CLA	O2A-CGA-CBA	3.37	122.47	111.91
27	A	409	BCR	C38-C26-C25	-3.36	120.75	124.53
27	B	617	BCR	C33-C5-C6	-3.36	120.75	124.53
27	b	617	BCR	C33-C5-C6	-3.36	120.75	124.53
25	b	605	CLA	C4-C3-C5	3.36	120.92	115.27
36	H	101	RRX	C36-C18-C17	-3.36	118.22	122.92
31	e	103	LMT	C3'-C4'-C5'	-3.36	103.23	110.93
27	f	101	BCR	C38-C26-C27	3.36	120.07	113.62
25	b	616	CLA	CMB-C2B-C3B	3.36	130.96	124.68
27	c	515	BCR	C7-C8-C9	-3.35	121.17	126.23
30	A	413	SQD	C45-O47-C7	3.35	126.03	117.79
27	F	101	BCR	C36-C18-C17	-3.35	118.23	122.92
27	f	101	BCR	C36-C18-C17	-3.35	118.23	122.92
25	B	602	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
25	b	602	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
30	a	413	SQD	C45-O47-C7	3.35	126.03	117.79
31	c	522	LMT	C4'-C3'-C2'	3.34	116.66	110.82
25	B	605	CLA	C4-C3-C5	3.34	120.89	115.27
27	C	515	BCR	C7-C8-C9	-3.34	121.19	126.23
36	h	101	RRX	C36-C18-C17	-3.34	118.24	122.92
25	c	505	CLA	O2A-CGA-CBA	3.34	122.39	111.91
27	F	101	BCR	C38-C26-C27	3.34	120.03	113.62
31	C	522	LMT	C4'-C3'-C2'	3.33	116.64	110.82
25	C	505	CLA	O2A-CGA-CBA	3.33	122.36	111.91
25	c	512	CLA	CMA-C3A-C4A	3.33	120.72	111.77
25	C	512	CLA	CMA-C3A-C4A	3.32	120.70	111.77
27	A	409	BCR	C7-C8-C9	-3.32	121.22	126.23
27	a	409	BCR	C7-C8-C9	-3.32	121.22	126.23
25	C	506	CLA	C1-C2-C3	-3.32	120.31	126.04
25	c	506	CLA	C1-C2-C3	-3.32	120.31	126.04
31	i	102	LMT	C3'-C4'-C5'	-3.31	104.33	110.24
25	B	605	CLA	O2A-C1-C2	3.31	117.32	108.64
25	b	605	CLA	O2A-C1-C2	3.31	117.32	108.64
30	C	501	SQD	C4-C3-C2	3.30	116.59	110.82
30	c	501	SQD	C4-C3-C2	3.30	116.59	110.82
25	B	607	CLA	CMB-C2B-C3B	3.30	130.85	124.68
25	b	607	CLA	CMB-C2B-C3B	3.30	130.85	124.68
31	I	102	LMT	C3'-C4'-C5'	-3.30	104.35	110.24
35	V	201	HEM	CHB-C1B-NB	3.30	128.46	124.38
35	v	201	HEM	CHB-C1B-NB	3.30	128.46	124.38
25	C	506	CLA	O1D-CGD-CBD	-3.30	117.73	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	506	CLA	O1D-CGD-CBD	-3.30	117.73	124.48
25	b	601	CLA	CMC-C2C-C1C	3.30	130.06	125.04
31	T	101	LMT	O1'-C1'-C2'	3.29	113.45	108.30
31	t	101	LMT	O1'-C1'-C2'	3.29	113.45	108.30
25	D	403	CLA	C3D-C4D-ND	3.29	115.56	110.24
25	d	403	CLA	C3D-C4D-ND	3.29	115.56	110.24
31	c	525	LMT	O5'-C5'-C4'	3.29	115.67	109.69
25	b	606	CLA	CAA-C2A-C3A	-3.29	103.77	112.78
25	B	601	CLA	O2A-CGA-CBA	3.29	124.59	114.03
25	b	601	CLA	O2A-CGA-CBA	3.29	124.59	114.03
25	B	601	CLA	CMC-C2C-C1C	3.29	130.04	125.04
25	B	606	CLA	CAA-C2A-C3A	-3.28	103.78	112.78
25	A	405	CLA	CMD-C2D-C3D	-3.28	120.08	127.61
29	A	411	PL9	C7-C3-C2	-3.27	119.00	123.30
29	a	411	PL9	C7-C3-C2	-3.27	119.00	123.30
25	a	405	CLA	CMD-C2D-C3D	-3.27	120.10	127.61
25	B	614	CLA	O2A-CGA-CBA	3.26	122.15	111.91
31	C	525	LMT	O5'-C5'-C4'	3.26	115.62	109.69
33	B	628	LHG	O7-C7-C8	3.26	118.53	111.50
33	d	407	LHG	C5-O7-C7	-3.26	109.76	117.79
25	B	602	CLA	CAA-C2A-C3A	-3.26	103.85	112.78
25	b	602	CLA	CAA-C2A-C3A	-3.26	103.85	112.78
27	k	103	BCR	C15-C14-C13	-3.26	122.66	127.31
25	C	504	CLA	C3C-C4C-NC	3.26	114.22	110.57
25	d	403	CLA	CMC-C2C-C1C	3.26	130.00	125.04
28	h	105	LMG	O8-C28-C29	3.25	122.12	111.91
25	c	504	CLA	C3C-C4C-NC	3.25	114.22	110.57
25	b	613	CLA	CMB-C2B-C3B	3.25	130.77	124.68
25	c	513	CLA	CMC-C2C-C1C	3.25	129.99	125.04
25	b	614	CLA	O2A-CGA-CBA	3.25	122.12	111.91
33	b	628	LHG	O7-C7-C8	3.25	118.51	111.50
28	H	105	LMG	O8-C28-C29	3.25	122.11	111.91
25	C	508	CLA	O2A-CGA-CBA	3.25	122.11	111.91
25	c	508	CLA	O2A-CGA-CBA	3.25	122.11	111.91
25	D	403	CLA	CMC-C2C-C1C	3.25	129.99	125.04
25	B	613	CLA	CMB-C2B-C3B	3.25	130.76	124.68
25	D	403	CLA	C4D-C3D-CAD	3.25	111.92	108.10
27	F	101	BCR	C19-C18-C17	3.25	123.92	118.94
27	f	101	BCR	C19-C18-C17	3.25	123.92	118.94
33	D	407	LHG	C5-O7-C7	-3.25	109.80	117.79
25	d	403	CLA	C4D-C3D-CAD	3.24	111.92	108.10
25	C	513	CLA	CMC-C2C-C1C	3.24	129.97	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	K	103	BCR	C15-C14-C13	-3.23	122.70	127.31
30	C	501	SQD	O8-S-C6	3.23	110.89	105.74
27	a	409	BCR	C36-C18-C17	-3.23	118.40	122.92
25	C	502	CLA	CMA-C3A-C4A	3.22	120.44	111.77
25	c	502	CLA	CMA-C3A-C4A	3.22	120.44	111.77
30	c	501	SQD	O8-S-C6	3.22	110.88	105.74
25	B	609	CLA	CMB-C2B-C3B	3.22	130.70	124.68
25	A	405	CLA	C4D-C3D-CAD	3.22	111.89	108.10
25	a	405	CLA	C4D-C3D-CAD	3.22	111.89	108.10
25	A	408	CLA	CMC-C2C-C1C	3.21	129.94	125.04
25	b	609	CLA	CMB-C2B-C3B	3.21	130.69	124.68
25	a	408	CLA	CMC-C2C-C1C	3.21	129.93	125.04
25	B	608	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
25	C	511	CLA	CMC-C2C-C1C	3.21	129.93	125.04
25	c	511	CLA	CMC-C2C-C1C	3.21	129.93	125.04
25	c	505	CLA	C1-O2A-CGA	3.21	124.86	116.44
25	B	604	CLA	CHD-C1D-ND	-3.21	121.51	124.45
25	C	505	CLA	C1-O2A-CGA	3.20	124.85	116.44
27	A	409	BCR	C36-C18-C17	-3.20	118.44	122.92
25	b	604	CLA	CHD-C1D-ND	-3.20	121.51	124.45
31	X	103	LMT	O5'-C5'-C4'	3.20	115.50	109.69
31	x	103	LMT	O5'-C5'-C4'	3.20	115.50	109.69
27	Z	101	BCR	C19-C18-C17	3.20	123.85	118.94
27	z	101	BCR	C19-C18-C17	3.20	123.85	118.94
25	b	608	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
27	k	102	BCR	C33-C5-C6	-3.18	120.96	124.53
30	K	101	SQD	C44-O6-C1	3.17	119.94	113.74
30	k	101	SQD	C44-O6-C1	3.17	119.94	113.74
33	E	102	LHG	C5-O7-C7	-3.17	109.98	117.79
33	e	102	LHG	C5-O7-C7	-3.17	109.98	117.79
29	d	405	PL9	C7-C3-C2	-3.17	119.14	123.30
25	B	614	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
25	B	601	CLA	C3C-C4C-NC	3.16	114.12	110.57
25	b	601	CLA	C3C-C4C-NC	3.16	114.12	110.57
25	D	404	CLA	C1-C2-C3	-3.16	120.57	126.04
25	D	404	CLA	CMB-C2B-C3B	3.16	130.59	124.68
30	F	102	SQD	O6-C1-C2	3.16	113.24	108.30
29	D	405	PL9	C7-C3-C2	-3.16	119.14	123.30
25	b	614	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
30	F	102	SQD	C44-O6-C1	3.16	119.90	113.74
25	d	404	CLA	C1-C2-C3	-3.14	120.60	126.04
25	d	404	CLA	CMB-C2B-C3B	3.14	130.56	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	616	CLA	CAC-C3C-C4C	3.14	128.89	124.81
27	F	101	BCR	C3-C4-C5	-3.14	108.47	114.08
25	B	603	CLA	CHD-C1D-ND	-3.14	121.57	124.45
25	b	603	CLA	CHD-C1D-ND	-3.14	121.57	124.45
30	f	102	SQD	O6-C1-C2	3.14	113.20	108.30
25	b	602	CLA	CMB-C2B-C3B	3.14	130.55	124.68
30	f	102	SQD	C44-O6-C1	3.14	119.87	113.74
27	K	102	BCR	C33-C5-C6	-3.13	121.01	124.53
25	b	606	CLA	C4-C3-C5	3.13	120.54	115.27
25	B	615	CLA	CMB-C2B-C3B	3.13	130.54	124.68
25	b	615	CLA	CMB-C2B-C3B	3.13	130.54	124.68
27	B	617	BCR	C34-C9-C8	3.13	123.01	118.08
25	B	616	CLA	CAC-C3C-C4C	3.13	128.87	124.81
25	B	602	CLA	CMB-C2B-C3B	3.13	130.53	124.68
25	B	606	CLA	C4-C3-C5	3.12	120.53	115.27
27	f	101	BCR	C3-C4-C5	-3.12	108.50	114.08
27	A	409	BCR	C19-C18-C17	3.12	123.73	118.94
27	a	409	BCR	C19-C18-C17	3.12	123.73	118.94
27	b	619	BCR	C40-C30-C25	3.12	115.36	110.30
25	B	616	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
25	b	616	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
27	a	409	BCR	C33-C5-C6	-3.11	121.03	124.53
25	C	511	CLA	C4D-C3D-CAD	3.11	111.77	108.10
27	B	619	BCR	C40-C30-C25	3.11	115.34	110.30
27	b	617	BCR	C34-C9-C8	3.10	122.97	118.08
25	b	604	CLA	C4-C3-C5	3.10	120.49	115.27
25	B	605	CLA	C3D-C4D-ND	3.10	115.25	110.24
25	B	604	CLA	C4-C3-C5	3.10	120.48	115.27
25	b	603	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
25	b	616	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
27	A	409	BCR	C33-C5-C6	-3.09	121.05	124.53
25	b	605	CLA	C3D-C4D-ND	3.09	115.24	110.24
25	B	616	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
26	A	407	PHO	CMB-C2B-C3B	3.09	130.45	124.68
26	a	407	PHO	CMB-C2B-C3B	3.09	130.45	124.68
25	c	511	CLA	C4D-C3D-CAD	3.08	111.73	108.10
25	D	404	CLA	C3D-C4D-ND	3.08	115.22	110.24
25	d	404	CLA	C3D-C4D-ND	3.08	115.22	110.24
25	B	614	CLA	C3C-C4C-NC	3.08	114.02	110.57
25	C	512	CLA	C3C-C4C-NC	3.08	114.02	110.57
25	b	614	CLA	C3C-C4C-NC	3.08	114.02	110.57
25	c	512	CLA	C3C-C4C-NC	3.08	114.02	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	609	CLA	CMC-C2C-C1C	3.08	129.73	125.04
25	b	609	CLA	CMC-C2C-C1C	3.08	129.73	125.04
25	B	603	CLA	CAA-C2A-C3A	-3.08	104.35	112.78
27	b	617	BCR	C36-C18-C17	-3.07	118.62	122.92
27	K	102	BCR	C15-C14-C13	-3.07	122.93	127.31
27	k	102	BCR	C15-C14-C13	-3.07	122.93	127.31
27	B	617	BCR	C36-C18-C17	-3.07	118.63	122.92
25	C	508	CLA	C4-C3-C5	3.06	120.42	115.27
25	c	508	CLA	C4-C3-C5	3.06	120.42	115.27
25	C	514	CLA	C3C-C4C-NC	3.06	114.00	110.57
25	c	514	CLA	C3C-C4C-NC	3.06	114.00	110.57
26	d	402	PHO	CMC-C2C-C3C	3.06	130.71	124.94
25	c	511	CLA	CMD-C2D-C3D	-3.06	120.57	127.61
30	K	101	SQD	O6-C1-C2	3.06	113.08	108.30
30	k	101	SQD	O6-C1-C2	3.06	113.08	108.30
25	C	511	CLA	CMD-C2D-C3D	-3.05	120.59	127.61
25	C	505	CLA	CAC-C3C-C4C	3.05	128.76	124.81
25	c	505	CLA	CAC-C3C-C4C	3.05	128.76	124.81
25	C	510	CLA	CMC-C2C-C1C	3.04	129.68	125.04
25	c	510	CLA	CMC-C2C-C1C	3.04	129.68	125.04
26	D	402	PHO	CMC-C2C-C3C	3.04	130.68	124.94
25	B	610	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
25	b	610	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
35	V	201	HEM	CBA-CAA-C2A	-3.03	107.45	112.62
35	v	201	HEM	CBA-CAA-C2A	-3.03	107.45	112.62
25	C	506	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
25	c	506	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
35	V	201	HEM	CHA-C4D-ND	3.02	128.11	124.38
35	v	201	HEM	CHA-C4D-ND	3.02	128.11	124.38
25	C	507	CLA	CAC-C3C-C4C	3.01	128.72	124.81
25	A	408	CLA	C4-C3-C5	3.01	120.34	115.27
25	a	408	CLA	C4-C3-C5	3.01	120.34	115.27
31	D	410	LMT	O5'-C5'-C4'	3.01	115.16	109.69
31	d	410	LMT	O5'-C5'-C4'	3.01	115.16	109.69
25	C	502	CLA	CMC-C2C-C1C	3.01	129.62	125.04
25	c	502	CLA	CMC-C2C-C1C	3.01	129.62	125.04
25	C	512	CLA	C4D-C3D-CAD	3.00	111.63	108.10
25	c	512	CLA	C4D-C3D-CAD	3.00	111.63	108.10
27	B	618	BCR	C36-C18-C17	-3.00	118.73	122.92
27	b	618	BCR	C36-C18-C17	-3.00	118.73	122.92
25	B	609	CLA	C3C-C4C-NC	2.99	113.93	110.57
25	C	508	CLA	C3C-C4C-NC	2.99	113.93	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	609	CLA	C3C-C4C-NC	2.99	113.93	110.57
25	c	508	CLA	C3C-C4C-NC	2.99	113.93	110.57
25	c	508	CLA	C1-O2A-CGA	2.99	124.30	116.44
27	b	617	BCR	C24-C23-C22	-2.99	121.71	126.23
25	C	508	CLA	C1-O2A-CGA	2.99	124.30	116.44
25	c	507	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
27	b	618	BCR	C7-C8-C9	-2.99	121.72	126.23
25	c	507	CLA	CAC-C3C-C4C	2.99	128.69	124.81
27	B	617	BCR	C24-C23-C22	-2.98	121.72	126.23
28	H	105	LMG	C8-O7-C10	-2.98	110.44	117.79
28	h	105	LMG	C8-O7-C10	-2.98	110.45	117.79
27	C	515	BCR	C38-C26-C25	-2.98	121.18	124.53
30	H	103	SQD	O7-S-C6	2.98	110.48	106.94
30	h	103	SQD	O7-S-C6	2.98	110.48	106.94
25	C	502	CLA	OBD-CAD-C3D	-2.98	121.35	128.52
31	x	101	LMT	C3'-C4'-C5'	-2.98	104.93	110.24
25	C	507	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
25	c	502	CLA	OBD-CAD-C3D	-2.97	121.36	128.52
25	B	603	CLA	C3C-C4C-NC	2.97	113.90	110.57
31	m	102	LMT	C3'-C4'-C5'	-2.97	104.95	110.24
25	c	510	CLA	CED-O2D-CGD	2.97	122.65	115.94
31	X	101	LMT	C3'-C4'-C5'	-2.97	104.95	110.24
25	a	406	CLA	CMA-C3A-C4A	2.96	119.74	111.77
25	A	406	CLA	CMA-C3A-C4A	2.96	119.74	111.77
25	B	613	CLA	C1-C2-C3	-2.96	120.92	126.04
27	B	618	BCR	C7-C8-C9	-2.96	121.76	126.23
25	b	603	CLA	C3C-C4C-NC	2.96	113.89	110.57
25	d	404	CLA	CMC-C2C-C1C	2.96	129.55	125.04
25	b	613	CLA	C1-C2-C3	-2.96	120.92	126.04
31	C	522	LMT	O5'-C5'-C4'	2.96	115.06	109.69
31	c	522	LMT	O5'-C5'-C4'	2.96	115.06	109.69
25	b	615	CLA	O2A-CGA-CBA	2.95	121.18	111.91
25	A	408	CLA	C3D-C4D-ND	2.95	115.02	110.24
25	B	615	CLA	O2A-CGA-CBA	2.95	121.18	111.91
25	C	510	CLA	CED-O2D-CGD	2.95	122.62	115.94
31	M	102	LMT	C3'-C4'-C5'	-2.95	104.97	110.24
25	B	615	CLA	CMC-C2C-C1C	2.95	129.53	125.04
25	b	615	CLA	CMC-C2C-C1C	2.95	129.53	125.04
25	c	507	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
27	c	515	BCR	C38-C26-C25	-2.95	121.22	124.53
25	C	507	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
25	B	615	CLA	CAC-C3C-C4C	2.95	128.63	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	615	CLA	CAC-C3C-C4C	2.95	128.63	124.81
25	b	612	CLA	C4D-C3D-CAD	2.94	111.57	108.10
27	K	103	BCR	C34-C9-C10	-2.94	118.80	122.92
27	k	103	BCR	C34-C9-C10	-2.94	118.80	122.92
25	B	613	CLA	CMC-C2C-C1C	2.94	129.52	125.04
25	b	613	CLA	CMC-C2C-C1C	2.94	129.52	125.04
25	a	408	CLA	C3D-C4D-ND	2.94	114.99	110.24
25	D	404	CLA	CMC-C2C-C1C	2.94	129.51	125.04
27	A	409	BCR	C37-C22-C21	-2.93	118.82	122.92
27	a	409	BCR	C37-C22-C21	-2.93	118.82	122.92
25	b	612	CLA	C3D-C4D-ND	2.93	114.98	110.24
25	b	612	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
35	v	201	HEM	CHD-C1D-C2D	-2.92	120.42	124.98
25	B	612	CLA	C3D-C4D-ND	2.92	114.96	110.24
35	V	201	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
31	X	103	LMT	C3'-C4'-C5'	-2.91	105.04	110.24
31	x	103	LMT	C3'-C4'-C5'	-2.91	105.04	110.24
25	B	612	CLA	C4D-C3D-CAD	2.91	111.53	108.10
25	b	614	CLA	C4-C3-C5	2.91	120.16	115.27
25	c	509	CLA	C3D-C4D-ND	2.91	114.94	110.24
27	K	102	BCR	C19-C18-C17	2.90	123.39	118.94
25	B	604	CLA	O1D-CGD-CBD	-2.90	118.55	124.48
25	B	614	CLA	C1-O2A-CGA	2.89	124.03	116.44
25	b	608	CLA	C1-C2-C3	-2.89	121.04	126.04
30	A	412	SQD	C1-C2-C3	2.89	116.02	110.00
25	b	608	CLA	C3D-C4D-ND	2.89	114.91	110.24
30	A	412	SQD	O47-C7-C8	2.89	117.73	111.50
25	a	406	CLA	CBC-CAC-C3C	-2.89	104.46	112.43
25	B	608	CLA	C1-C2-C3	-2.89	121.05	126.04
25	c	514	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
25	A	406	CLA	CBC-CAC-C3C	-2.89	104.47	112.43
25	B	612	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
30	a	412	SQD	C1-C2-C3	2.89	116.01	110.00
25	C	503	CLA	CMB-C2B-C3B	2.88	130.07	124.68
25	c	503	CLA	CMB-C2B-C3B	2.88	130.07	124.68
30	a	412	SQD	O47-C7-C8	2.88	117.72	111.50
27	k	102	BCR	C19-C18-C17	2.88	123.37	118.94
25	C	503	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
30	A	413	SQD	O6-C1-C2	2.88	112.81	108.30
30	a	413	SQD	O6-C1-C2	2.88	112.81	108.30
25	b	604	CLA	O1D-CGD-CBD	-2.88	118.59	124.48
25	B	614	CLA	C4-C3-C5	2.88	120.12	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	614	CLA	C1-O2A-CGA	2.88	124.00	116.44
25	C	509	CLA	C3D-C4D-ND	2.88	114.90	110.24
25	B	604	CLA	C1-C2-C3	-2.88	121.06	126.04
25	c	503	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
25	C	514	CLA	CAA-C2A-C3A	-2.88	104.91	112.78
25	C	506	CLA	C3D-C4D-ND	2.87	114.89	110.24
25	c	506	CLA	C3D-C4D-ND	2.87	114.89	110.24
28	A	414	LMG	O8-C28-C29	2.87	120.92	111.91
28	a	414	LMG	O8-C28-C29	2.87	120.92	111.91
25	b	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
27	k	102	BCR	C34-C9-C10	-2.87	118.90	122.92
25	b	604	CLA	C1-C2-C3	-2.87	121.08	126.04
27	b	618	BCR	C37-C22-C21	-2.87	118.91	122.92
25	B	608	CLA	C3D-C4D-ND	2.87	114.88	110.24
31	e	103	LMT	C4B-C3B-C2B	2.87	115.83	110.82
29	D	405	PL9	C7-C8-C9	-2.87	122.02	126.79
29	d	405	PL9	C7-C8-C9	-2.87	122.02	126.79
25	B	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
36	H	101	RRX	C19-C18-C17	2.86	123.33	118.94
27	B	618	BCR	C37-C22-C21	-2.86	118.92	122.92
31	E	103	LMT	C4B-C3B-C2B	2.86	115.81	110.82
25	c	510	CLA	C3C-C4C-NC	2.86	113.78	110.57
27	K	102	BCR	C34-C9-C10	-2.85	118.93	122.92
25	C	510	CLA	C3C-C4C-NC	2.85	113.77	110.57
28	H	105	LMG	C1-O6-C5	2.85	119.29	113.69
28	h	105	LMG	C1-O6-C5	2.85	119.29	113.69
25	B	616	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
25	A	408	CLA	CMA-C3A-C4A	2.85	119.44	111.77
25	C	514	CLA	CMC-C2C-C1C	2.85	129.37	125.04
25	c	514	CLA	CMC-C2C-C1C	2.85	129.37	125.04
36	h	101	RRX	C19-C18-C17	2.84	123.31	118.94
25	A	408	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	a	408	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	B	608	CLA	CMA-C3A-C4A	2.84	119.42	111.77
25	b	608	CLA	CMA-C3A-C4A	2.84	119.42	111.77
25	a	408	CLA	CMA-C3A-C4A	2.84	119.41	111.77
25	C	508	CLA	C1D-ND-C4D	-2.84	104.32	106.33
25	c	508	CLA	C1D-ND-C4D	-2.84	104.32	106.33
25	b	616	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
25	C	507	CLA	CMC-C2C-C3C	2.84	133.82	126.12
25	c	507	CLA	CMC-C2C-C3C	2.84	133.82	126.12
25	b	611	CLA	C1-C2-C3	-2.83	121.14	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	605	CLA	O2A-CGA-CBA	2.83	120.80	111.91
25	c	514	CLA	C4-C3-C5	2.82	120.02	115.27
35	V	201	HEM	CHC-C4B-C3B	-2.82	120.25	124.57
35	v	201	HEM	CHC-C4B-C3B	-2.82	120.25	124.57
25	B	605	CLA	O2A-CGA-CBA	2.82	120.75	111.91
28	C	523	LMG	O8-C28-C29	2.82	120.74	111.91
28	c	523	LMG	O8-C28-C29	2.82	120.74	111.91
25	B	611	CLA	C1-C2-C3	-2.81	121.18	126.04
30	h	103	SQD	C1-O5-C5	2.81	119.21	113.69
31	B	625	LMT	O1B-C4'-C3'	2.81	114.76	107.28
31	b	625	LMT	O1B-C4'-C3'	2.81	114.76	107.28
25	b	605	CLA	C4D-C3D-CAD	2.81	111.41	108.10
25	C	505	CLA	CMC-C2C-C1C	2.81	129.32	125.04
25	c	505	CLA	CMC-C2C-C1C	2.81	129.32	125.04
27	b	619	BCR	C37-C22-C21	-2.81	118.99	122.92
27	B	619	BCR	C37-C22-C21	-2.81	118.99	122.92
28	c	519	LMG	O8-C28-C29	2.81	120.71	111.91
27	b	618	BCR	C15-C14-C13	-2.80	123.31	127.31
28	C	519	LMG	O8-C28-C29	2.80	120.71	111.91
30	H	103	SQD	C1-O5-C5	2.80	119.19	113.69
27	B	618	BCR	C15-C14-C13	-2.80	123.31	127.31
25	B	607	CLA	CMA-C3A-C4A	2.80	119.31	111.77
25	b	607	CLA	CMA-C3A-C4A	2.80	119.31	111.77
25	B	602	CLA	C3D-C4D-ND	2.80	114.77	110.24
25	D	401	CLA	C3D-C4D-ND	2.80	114.77	110.24
25	d	401	CLA	C3D-C4D-ND	2.80	114.77	110.24
25	C	514	CLA	C4-C3-C5	2.80	119.98	115.27
25	C	503	CLA	C3C-C4C-NC	2.80	113.71	110.57
25	c	503	CLA	C3C-C4C-NC	2.80	113.71	110.57
25	b	602	CLA	C3D-C4D-ND	2.79	114.76	110.24
27	F	101	BCR	C40-C30-C25	-2.79	105.77	110.30
25	B	601	CLA	CMA-C3A-C4A	2.79	119.27	111.77
25	b	601	CLA	CMA-C3A-C4A	2.79	119.27	111.77
25	C	508	CLA	CMB-C2B-C3B	2.79	129.89	124.68
25	c	508	CLA	CMB-C2B-C3B	2.79	129.89	124.68
25	B	605	CLA	C4D-C3D-CAD	2.78	111.38	108.10
25	C	508	CLA	CBC-CAC-C3C	-2.78	104.77	112.43
25	c	508	CLA	CBC-CAC-C3C	-2.78	104.77	112.43
34	C	517	DGD	O1G-C1A-C2A	2.77	120.61	111.91
27	f	101	BCR	C40-C30-C25	-2.77	105.81	110.30
25	A	408	CLA	C3C-C4C-NC	2.77	113.67	110.57
25	a	408	CLA	C3C-C4C-NC	2.77	113.67	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	616	CLA	C1-C2-C3	-2.76	121.26	126.04
34	c	517	DGD	O1G-C1A-C2A	2.76	120.58	111.91
25	D	403	CLA	C3C-C4C-NC	2.76	113.67	110.57
31	C	524	LMT	C3'-C4'-C5'	-2.76	104.60	110.93
25	D	401	CLA	C1-C2-C3	-2.75	121.28	126.04
25	d	401	CLA	C1-C2-C3	-2.75	121.28	126.04
25	B	615	CLA	C4-C3-C5	2.75	119.90	115.27
25	b	615	CLA	C4-C3-C5	2.75	119.90	115.27
25	B	616	CLA	C1-C2-C3	-2.75	121.29	126.04
25	d	403	CLA	CAA-C2A-C3A	-2.75	105.25	112.78
31	c	524	LMT	C3'-C4'-C5'	-2.75	104.63	110.93
27	k	102	BCR	C37-C22-C21	-2.74	119.08	122.92
25	D	403	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
25	c	512	CLA	C3D-C4D-ND	2.74	114.67	110.24
25	d	403	CLA	C3C-C4C-NC	2.74	113.64	110.57
25	b	612	CLA	CHB-C4A-NA	2.73	128.29	124.51
28	C	523	LMG	C8-O7-C10	-2.73	111.07	117.79
25	B	612	CLA	CHB-C4A-NA	2.73	128.29	124.51
28	c	523	LMG	C8-O7-C10	-2.73	111.07	117.79
25	b	616	CLA	OBD-CAD-C3D	-2.73	121.95	128.52
25	B	611	CLA	C3D-C4D-ND	2.72	114.64	110.24
25	b	611	CLA	C3D-C4D-ND	2.72	114.64	110.24
27	K	102	BCR	C37-C22-C21	-2.72	119.11	122.92
25	B	601	CLA	C4D-C3D-CAD	2.72	111.31	108.10
25	b	605	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
34	H	104	DGD	O1G-C1A-C2A	2.72	120.45	111.91
34	h	104	DGD	O1G-C1A-C2A	2.72	120.45	111.91
25	c	505	CLA	C4-C3-C5	2.72	119.85	115.27
25	B	616	CLA	OBD-CAD-C3D	-2.72	121.98	128.52
30	h	103	SQD	O48-C23-C24	2.72	120.44	111.91
27	K	103	BCR	C7-C8-C9	-2.72	122.13	126.23
27	k	103	BCR	C7-C8-C9	-2.72	122.13	126.23
25	B	606	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
31	e	103	LMT	O5'-C1'-C2'	2.72	116.10	110.35
25	C	512	CLA	C3D-C4D-ND	2.72	114.63	110.24
25	b	606	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
25	A	406	CLA	C4D-C3D-CAD	2.72	111.30	108.10
25	B	605	CLA	CAA-C2A-C3A	-2.72	105.34	112.78
25	C	505	CLA	C4-C3-C5	2.71	119.84	115.27
25	a	406	CLA	CMD-C2D-C3D	-2.71	121.38	127.61
25	c	508	CLA	C4D-C3D-CAD	2.71	111.29	108.10
36	H	101	RRX	C12-C13-C14	2.71	123.10	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	F	101	BCR	C34-C9-C10	-2.71	119.13	122.92
25	c	510	CLA	C3B-C4B-NB	2.71	112.71	109.21
30	H	103	SQD	O48-C23-C24	2.71	120.40	111.91
25	b	601	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
31	E	103	LMT	O5'-C1'-C2'	2.70	116.07	110.35
25	A	406	CLA	CMD-C2D-C3D	-2.70	121.40	127.61
36	h	101	RRX	C12-C13-C14	2.70	123.09	118.94
25	C	510	CLA	C3B-C4B-NB	2.70	112.70	109.21
27	C	515	BCR	C34-C9-C10	-2.70	119.14	122.92
27	b	618	BCR	C34-C9-C10	-2.70	119.14	122.92
27	f	101	BCR	C34-C9-C10	-2.70	119.14	122.92
25	C	508	CLA	C4D-C3D-CAD	2.70	111.27	108.10
30	F	102	SQD	O8-S-C6	2.69	110.03	105.74
30	f	102	SQD	O8-S-C6	2.69	110.03	105.74
25	b	601	CLA	C4D-C3D-CAD	2.69	111.27	108.10
27	c	515	BCR	C34-C9-C10	-2.69	119.15	122.92
25	a	406	CLA	C4D-C3D-CAD	2.69	111.27	108.10
27	z	101	BCR	C34-C9-C10	-2.69	119.15	122.92
25	B	601	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	B	616	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
25	C	502	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
25	c	502	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
31	c	522	LMT	O5'-C1'-C2'	-2.69	104.66	110.35
27	Z	101	BCR	C34-C9-C10	-2.69	119.16	122.92
33	D	407	LHG	O8-C23-C24	2.68	120.32	111.91
31	e	103	LMT	C3B-C4B-C5B	2.68	115.02	110.24
27	B	618	BCR	C34-C9-C10	-2.68	119.17	122.92
25	a	408	CLA	C1-O2A-CGA	2.68	123.47	116.44
25	b	616	CLA	CAA-C2A-C3A	-2.68	105.45	112.78
33	d	407	LHG	O8-C23-C24	2.67	120.30	111.91
31	C	522	LMT	O5'-C1'-C2'	-2.67	104.69	110.35
31	E	103	LMT	C3B-C4B-C5B	2.67	115.00	110.24
30	A	413	SQD	O48-C23-C24	2.67	120.29	111.91
25	C	511	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
25	c	511	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
25	A	408	CLA	C1-O2A-CGA	2.67	123.44	116.44
31	E	101	LMT	C1'-O5'-C5'	-2.66	108.46	113.69
31	k	105	LMT	C2'-C3'-C4'	2.66	115.77	109.68
30	a	413	SQD	O48-C23-C24	2.66	120.25	111.91
25	c	514	CLA	C3D-C4D-ND	2.66	114.53	110.24
31	e	101	LMT	C1'-O5'-C5'	-2.65	108.48	113.69
25	D	403	CLA	CBC-CAC-C3C	-2.65	105.12	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	403	CLA	CBC-CAC-C3C	-2.65	105.12	112.43
31	K	105	LMT	C2'-C3'-C4'	2.65	115.74	109.68
25	b	602	CLA	C1-O2A-CGA	2.65	123.39	116.44
25	B	615	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
25	b	615	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
25	B	602	CLA	C1-O2A-CGA	2.64	123.38	116.44
25	c	502	CLA	C1-C2-C3	-2.64	121.47	126.04
27	F	101	BCR	C37-C22-C21	-2.64	119.22	122.92
25	C	514	CLA	C3D-C4D-ND	2.64	114.51	110.24
34	C	516	DGD	O1G-C1A-C2A	2.64	120.19	111.91
34	c	516	DGD	O1G-C1A-C2A	2.64	120.19	111.91
27	f	101	BCR	C37-C22-C21	-2.64	119.23	122.92
25	C	505	CLA	C3D-C4D-ND	2.64	114.50	110.24
33	B	628	LHG	O8-C23-C24	2.64	120.18	111.91
33	b	628	LHG	O8-C23-C24	2.64	120.18	111.91
25	D	401	CLA	CMC-C2C-C3C	2.64	133.27	126.12
25	B	601	CLA	CMB-C2B-C3B	2.64	129.61	124.68
25	C	502	CLA	C3D-C4D-ND	2.64	114.50	110.24
25	c	502	CLA	C3D-C4D-ND	2.64	114.50	110.24
25	C	502	CLA	C1-C2-C3	-2.63	121.49	126.04
25	B	613	CLA	C3B-C4B-NB	2.63	112.60	109.21
25	b	613	CLA	C3B-C4B-NB	2.63	112.60	109.21
25	d	401	CLA	CMC-C2C-C3C	2.62	133.24	126.12
30	C	501	SQD	O7-S-C6	2.62	110.05	106.94
30	c	501	SQD	O7-S-C6	2.62	110.05	106.94
25	b	606	CLA	O2A-C1-C2	2.61	115.51	108.64
25	B	606	CLA	O2A-C1-C2	2.61	115.50	108.64
25	b	607	CLA	CAC-C3C-C4C	2.61	128.20	124.81
25	c	505	CLA	C3D-C4D-ND	2.61	114.46	110.24
29	A	411	PL9	C22-C23-C24	-2.61	121.37	127.66
29	a	411	PL9	C22-C23-C24	-2.61	121.37	127.66
25	b	601	CLA	CMB-C2B-C3B	2.61	129.56	124.68
25	b	614	CLA	CAC-C3C-C4C	2.61	128.20	124.81
25	B	614	CLA	CAC-C3C-C4C	2.61	128.20	124.81
25	b	616	CLA	C3C-C4C-NC	2.61	113.50	110.57
30	a	412	SQD	O8-S-C6	2.61	109.89	105.74
25	B	606	CLA	C1-O2A-CGA	2.61	123.28	116.44
25	B	604	CLA	CMD-C2D-C3D	-2.60	121.62	127.61
25	b	604	CLA	CMD-C2D-C3D	-2.60	121.62	127.61
25	A	405	CLA	C3D-C4D-ND	2.60	114.45	110.24
25	a	405	CLA	C3D-C4D-ND	2.60	114.45	110.24
25	C	502	CLA	C4-C3-C5	2.60	119.65	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	606	CLA	C1-O2A-CGA	2.60	123.27	116.44
25	b	612	CLA	C1-C2-C3	-2.60	121.55	126.04
25	B	606	CLA	C3D-C4D-ND	2.59	114.43	110.24
27	Z	101	BCR	C37-C22-C21	-2.59	119.29	122.92
27	z	101	BCR	C37-C22-C21	-2.59	119.29	122.92
25	c	502	CLA	C4-C3-C5	2.59	119.63	115.27
25	C	502	CLA	C4D-C3D-CAD	2.59	111.15	108.10
25	c	502	CLA	C4D-C3D-CAD	2.59	111.15	108.10
30	A	412	SQD	O8-S-C6	2.59	109.86	105.74
25	C	504	CLA	CAC-C3C-C4C	2.59	128.17	124.81
30	A	413	SQD	C3-C4-C5	2.59	114.85	110.24
30	a	413	SQD	C3-C4-C5	2.59	114.85	110.24
25	c	504	CLA	CAC-C3C-C4C	2.59	128.16	124.81
27	B	619	BCR	C34-C9-C10	-2.59	119.30	122.92
27	b	619	BCR	C34-C9-C10	-2.59	119.30	122.92
27	b	619	BCR	C35-C13-C12	2.58	122.15	118.08
25	c	510	CLA	CMB-C2B-C3B	2.58	129.51	124.68
25	B	607	CLA	CAC-C3C-C4C	2.58	128.16	124.81
25	B	613	CLA	CBC-CAC-C3C	-2.58	105.32	112.43
25	b	613	CLA	CBC-CAC-C3C	-2.58	105.32	112.43
25	B	612	CLA	C1-C2-C3	-2.58	121.58	126.04
25	C	507	CLA	C3C-C4C-NC	2.58	113.46	110.57
25	b	611	CLA	C3C-C4C-NC	2.58	113.46	110.57
25	B	611	CLA	C3C-C4C-NC	2.58	113.46	110.57
25	B	616	CLA	C3C-C4C-NC	2.57	113.46	110.57
25	B	610	CLA	CMA-C3A-C4A	2.57	118.69	111.77
25	A	406	CLA	C3D-C4D-ND	2.57	114.40	110.24
25	B	616	CLA	C4D-C3D-CAD	2.57	111.13	108.10
25	b	606	CLA	C3D-C4D-ND	2.57	114.40	110.24
25	b	610	CLA	CMA-C3A-C4A	2.57	118.68	111.77
25	B	607	CLA	C4D-C3D-CAD	2.57	111.12	108.10
25	B	608	CLA	C1-O2A-CGA	2.57	123.18	116.44
25	B	606	CLA	CAC-C3C-C4C	2.57	128.14	124.81
27	B	619	BCR	C35-C13-C12	2.57	122.12	118.08
25	b	606	CLA	CAC-C3C-C4C	2.57	128.14	124.81
25	b	608	CLA	C1-O2A-CGA	2.57	123.17	116.44
25	C	510	CLA	CMB-C2B-C3B	2.56	129.47	124.68
25	C	505	CLA	C4D-C3D-CAD	2.56	111.11	108.10
25	C	510	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	c	510	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	C	508	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
36	H	101	RRX	C23-C22-C21	2.56	122.87	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	507	CLA	C3C-C4C-NC	2.56	113.44	110.57
25	a	406	CLA	C3D-C4D-ND	2.56	114.37	110.24
25	B	603	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
25	b	603	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
33	Z	102	LHG	O8-C23-C24	2.55	119.92	111.91
27	B	617	BCR	C37-C22-C21	-2.55	119.35	122.92
25	B	616	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
25	B	614	CLA	C3D-C4D-ND	2.55	114.36	110.24
25	b	614	CLA	C3D-C4D-ND	2.55	114.36	110.24
27	b	617	BCR	C37-C22-C21	-2.55	119.35	122.92
28	B	621	LMG	O8-C28-C29	2.55	119.91	111.91
36	h	101	RRX	C23-C22-C21	2.55	122.85	118.94
33	z	102	LHG	O8-C23-C24	2.55	119.90	111.91
25	B	608	CLA	C3C-C4C-NC	2.55	113.43	110.57
25	b	608	CLA	C3C-C4C-NC	2.55	113.43	110.57
25	B	604	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
25	b	604	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
30	K	101	SQD	C6-C5-C4	-2.55	108.37	113.07
25	c	508	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
28	b	621	LMG	O8-C28-C29	2.54	119.89	111.91
25	b	616	CLA	C4D-C3D-CAD	2.54	111.09	108.10
28	d	409	LMG	O8-C28-C29	2.54	119.88	111.91
25	B	614	CLA	C1-C2-C3	-2.54	121.65	126.04
25	b	614	CLA	C1-C2-C3	-2.54	121.65	126.04
25	C	506	CLA	C3C-C4C-NC	2.54	113.42	110.57
25	b	616	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
25	c	506	CLA	C3C-C4C-NC	2.54	113.42	110.57
27	k	103	BCR	C23-C22-C21	2.54	122.83	118.94
25	c	505	CLA	O1D-CGD-CBD	-2.54	119.30	124.48
31	K	105	LMT	C4B-C3B-C2B	2.54	115.25	110.82
31	k	105	LMT	C4B-C3B-C2B	2.54	115.25	110.82
25	B	604	CLA	C3B-C4B-NB	2.53	112.49	109.21
25	b	604	CLA	C3B-C4B-NB	2.53	112.49	109.21
31	A	415	LMT	C1-O1'-C1'	2.53	118.04	113.84
25	C	505	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
25	b	607	CLA	C4D-C3D-CAD	2.53	111.08	108.10
28	D	409	LMG	O8-C28-C29	2.53	119.84	111.91
31	a	415	LMT	C1-O1'-C1'	2.53	118.03	113.84
30	k	101	SQD	C6-C5-C4	-2.53	108.40	113.07
25	c	505	CLA	C4D-C3D-CAD	2.53	111.07	108.10
25	B	603	CLA	CMA-C3A-C4A	2.52	118.56	111.77
25	B	610	CLA	C4D-C3D-CAD	2.52	111.07	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	610	CLA	C4D-C3D-CAD	2.52	111.07	108.10
25	C	504	CLA	C4D-C3D-CAD	2.52	111.07	108.10
25	c	503	CLA	CMA-C3A-C4A	2.52	118.54	111.77
25	b	603	CLA	CMA-C3A-C4A	2.52	118.54	111.77
25	B	602	CLA	C4-C3-C5	2.52	119.50	115.27
25	b	602	CLA	C4-C3-C5	2.52	119.50	115.27
25	C	511	CLA	C3D-C4D-ND	2.52	114.31	110.24
25	c	511	CLA	C3D-C4D-ND	2.52	114.31	110.24
27	K	103	BCR	C23-C22-C21	2.52	122.80	118.94
28	A	414	LMG	C8-O7-C10	-2.52	111.59	117.79
25	C	509	CLA	C3C-C4C-NC	2.51	113.39	110.57
25	c	509	CLA	C3C-C4C-NC	2.51	113.39	110.57
25	c	504	CLA	C4D-C3D-CAD	2.51	111.06	108.10
30	a	413	SQD	C4-C3-C2	2.51	115.21	110.82
25	C	503	CLA	CMA-C3A-C4A	2.51	118.52	111.77
25	B	607	CLA	C1-O2A-CGA	2.51	123.02	116.44
25	c	513	CLA	O1D-CGD-CBD	-2.51	119.36	124.48
30	A	413	SQD	C4-C3-C2	2.50	115.19	110.82
25	C	511	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
28	a	414	LMG	C8-O7-C10	-2.50	111.64	117.79
27	B	618	BCR	C38-C26-C25	-2.50	121.72	124.53
27	b	618	BCR	C38-C26-C25	-2.50	121.72	124.53
25	A	405	CLA	C3C-C4C-NC	2.50	113.37	110.57
25	b	616	CLA	CMC-C2C-C3C	2.50	132.90	126.12
25	c	511	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
31	B	623	LMT	O5'-C1'-O1'	-2.50	104.06	109.97
31	b	623	LMT	O5'-C1'-O1'	-2.50	104.06	109.97
25	C	513	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
27	a	409	BCR	C34-C9-C10	-2.49	119.43	122.92
25	b	607	CLA	C1-O2A-CGA	2.49	122.98	116.44
30	F	102	SQD	O5-C1-C2	2.49	115.62	110.35
30	C	501	SQD	O47-C7-O49	-2.49	117.68	123.70
33	e	102	LHG	O8-C23-C24	2.49	119.72	111.91
27	C	515	BCR	C3-C4-C5	-2.49	109.63	114.08
27	c	515	BCR	C3-C4-C5	-2.49	109.63	114.08
35	E	104	HEM	CHA-C4D-C3D	-2.49	120.66	125.33
25	d	404	CLA	CAC-C3C-C4C	2.49	128.04	124.81
25	B	616	CLA	CMC-C2C-C3C	2.49	132.87	126.12
25	D	404	CLA	CAC-C3C-C4C	2.49	128.04	124.81
35	e	104	HEM	CHA-C4D-C3D	-2.48	120.67	125.33
33	E	102	LHG	O8-C23-C24	2.48	119.70	111.91
35	e	104	HEM	CHD-C1D-C2D	-2.48	121.10	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	102	SQD	O5-C1-C2	2.48	115.60	110.35
27	b	619	BCR	C3-C4-C5	-2.48	109.65	114.08
25	B	611	CLA	C4C-C3C-C2C	-2.48	103.29	106.90
27	K	102	BCR	C30-C25-C26	-2.48	119.12	122.61
27	k	102	BCR	C30-C25-C26	-2.48	119.12	122.61
25	B	605	CLA	C1-O2A-CGA	2.48	122.94	116.44
25	b	605	CLA	C1-O2A-CGA	2.48	122.94	116.44
25	C	513	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
25	c	513	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
30	c	501	SQD	O47-C7-O49	-2.48	117.72	123.70
27	K	103	BCR	C38-C26-C25	-2.48	121.75	124.53
27	k	103	BCR	C38-C26-C25	-2.48	121.75	124.53
25	b	609	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
25	c	504	CLA	CMD-C2D-C3D	-2.47	121.92	127.61
25	B	603	CLA	CMC-C2C-C1C	2.47	128.81	125.04
27	B	619	BCR	C3-C4-C5	-2.47	109.66	114.08
25	a	405	CLA	C3C-C4C-NC	2.47	113.34	110.57
25	D	401	CLA	C6-C5-C3	-2.47	106.98	113.45
25	d	401	CLA	C6-C5-C3	-2.47	106.98	113.45
25	B	607	CLA	C3D-C4D-ND	2.47	114.23	110.24
25	b	607	CLA	C3D-C4D-ND	2.47	114.23	110.24
25	D	404	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
25	d	404	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
35	E	104	HEM	CHD-C1D-C2D	-2.46	121.13	124.98
27	A	409	BCR	C34-C9-C10	-2.46	119.47	122.92
25	b	609	CLA	C3D-C4D-ND	2.46	114.22	110.24
25	B	606	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
25	B	609	CLA	CHA-C1A-NA	-2.46	120.76	126.40
25	b	609	CLA	CHA-C1A-NA	-2.46	120.76	126.40
25	B	609	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
27	b	618	BCR	C19-C18-C17	2.46	122.72	118.94
25	B	604	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
25	b	606	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
29	A	411	PL9	C7-C8-C9	-2.46	122.70	126.79
29	a	411	PL9	C7-C8-C9	-2.46	122.70	126.79
25	b	604	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
34	C	518	DGD	C2G-O2G-C1B	-2.46	111.73	117.79
25	b	603	CLA	CMC-C2C-C1C	2.46	128.78	125.04
25	b	611	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
25	C	504	CLA	CMC-C2C-C1C	2.46	128.78	125.04
25	c	504	CLA	CMC-C2C-C1C	2.46	128.78	125.04
25	B	609	CLA	O1D-CGD-CBD	-2.46	119.45	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	c	518	DGD	C2G-O2G-C1B	-2.46	111.74	117.79
25	C	504	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
25	C	507	CLA	C1-C2-C3	-2.45	121.80	126.04
31	B	623	LMT	C2'-C3'-C4'	2.45	115.28	109.68
31	b	623	LMT	C2'-C3'-C4'	2.45	115.28	109.68
27	A	409	BCR	C15-C14-C13	-2.45	123.81	127.31
25	B	606	CLA	C4D-C3D-CAD	2.45	110.98	108.10
25	b	606	CLA	C4D-C3D-CAD	2.45	110.98	108.10
25	D	401	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
25	d	401	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
27	a	409	BCR	C15-C14-C13	-2.45	123.81	127.31
27	Z	101	BCR	C2-C1-C6	2.45	114.25	110.48
25	B	602	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
25	b	602	CLA	C4D-C3D-CAD	2.45	110.98	108.10
25	C	505	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
27	B	618	BCR	C19-C18-C17	2.44	122.69	118.94
25	B	602	CLA	C4D-C3D-CAD	2.44	110.98	108.10
27	k	103	BCR	C2-C1-C6	2.44	114.24	110.48
25	b	615	CLA	C1-C2-C3	-2.44	121.82	126.04
25	b	602	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
25	b	609	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
31	j	101	LMT	O5'-C5'-C4'	2.44	114.12	109.69
25	b	615	CLA	CHD-C4C-C3C	-2.44	121.26	124.84
25	d	401	CLA	CED-O2D-CGD	2.44	121.45	115.94
29	D	405	PL9	C22-C23-C24	-2.43	121.80	127.66
29	d	405	PL9	C22-C23-C24	-2.43	121.80	127.66
25	d	404	CLA	C3C-C4C-NC	2.43	113.30	110.57
25	B	609	CLA	C3D-C4D-ND	2.43	114.17	110.24
25	C	512	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
25	c	512	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
25	c	505	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
27	z	101	BCR	C2-C1-C6	2.43	114.22	110.48
25	B	616	CLA	C3D-C4D-ND	2.42	114.16	110.24
31	J	101	LMT	O5'-C5'-C4'	2.42	114.10	109.69
25	c	507	CLA	C3D-C4D-ND	2.42	114.16	110.24
33	D	406	LHG	O8-C23-C24	2.42	119.51	111.91
33	d	406	LHG	O8-C23-C24	2.42	119.51	111.91
25	D	401	CLA	CED-O2D-CGD	2.42	121.42	115.94
25	B	615	CLA	C1-C2-C3	-2.42	121.85	126.04
25	c	507	CLA	C1-C2-C3	-2.42	121.85	126.04
25	c	508	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
25	B	605	CLA	CMD-C2D-C3D	-2.42	122.05	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	605	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
27	K	103	BCR	C2-C1-C6	2.42	114.20	110.48
29	D	405	PL9	C20-C19-C21	2.42	119.33	115.27
25	b	616	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
25	B	605	CLA	C3C-C4C-NC	2.41	113.28	110.57
25	b	605	CLA	C3C-C4C-NC	2.41	113.28	110.57
29	d	405	PL9	C20-C19-C21	2.41	119.33	115.27
25	b	616	CLA	C3D-C4D-ND	2.41	114.14	110.24
25	a	406	CLA	C4-C3-C5	2.41	119.33	115.27
25	C	507	CLA	C3D-C4D-ND	2.41	114.14	110.24
25	B	615	CLA	CHD-C4C-C3C	-2.41	121.30	124.84
25	C	508	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
25	C	510	CLA	C4-C3-C5	2.40	119.31	115.27
25	c	510	CLA	C4-C3-C5	2.40	119.31	115.27
25	B	616	CLA	O1D-CGD-CBD	-2.40	119.57	124.48
26	d	402	PHO	O2D-CGD-O1D	-2.40	119.14	123.84
25	D	404	CLA	C3C-C4C-NC	2.40	113.26	110.57
29	a	411	PL9	C20-C19-C21	2.40	119.31	115.27
25	B	610	CLA	C3D-C4D-ND	2.40	114.12	110.24
31	X	102	LMT	O5'-C5'-C4'	2.40	113.82	109.52
25	C	514	CLA	CAC-C3C-C4C	2.40	127.92	124.81
25	C	508	CLA	CMC-C2C-C1C	2.40	128.69	125.04
25	B	615	CLA	C3D-C4D-ND	2.40	114.11	110.24
35	e	104	HEM	C4D-ND-C1D	2.40	107.55	105.07
29	A	411	PL9	C20-C19-C21	2.39	119.30	115.27
25	A	406	CLA	C4-C3-C5	2.39	119.30	115.27
31	J	101	LMT	O5'-C5'-C6'	2.39	112.39	106.44
28	d	409	LMG	C7-O1-C1	-2.39	109.07	113.74
25	C	514	CLA	C1-C2-C3	-2.39	121.91	126.04
25	c	514	CLA	C1-C2-C3	-2.39	121.91	126.04
25	c	508	CLA	CMC-C2C-C1C	2.39	128.68	125.04
25	b	615	CLA	C3D-C4D-ND	2.39	114.10	110.24
35	E	104	HEM	CBD-CAD-C3D	-2.39	105.99	112.63
35	e	104	HEM	CBD-CAD-C3D	-2.39	105.99	112.63
25	B	601	CLA	C3D-C4D-ND	2.39	114.10	110.24
25	B	613	CLA	C4-C3-C5	2.39	119.29	115.27
25	c	514	CLA	CAC-C3C-C4C	2.39	127.91	124.81
25	b	610	CLA	C3D-C4D-ND	2.39	114.10	110.24
25	C	512	CLA	C4-C3-C5	2.39	119.28	115.27
25	c	512	CLA	C4-C3-C5	2.39	119.28	115.27
30	A	412	SQD	C1-O5-C5	2.38	118.37	113.69
30	a	412	SQD	C1-O5-C5	2.38	118.37	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	402	PHO	O2D-CGD-O1D	-2.38	119.18	123.84
28	D	409	LMG	C7-O1-C1	-2.38	109.09	113.74
25	b	601	CLA	C3D-C4D-ND	2.38	114.08	110.24
25	b	613	CLA	C4-C3-C5	2.38	119.27	115.27
31	j	101	LMT	O5'-C5'-C6'	2.38	112.34	106.44
25	B	609	CLA	C1-C2-C3	-2.38	121.93	126.04
25	b	609	CLA	C1-C2-C3	-2.38	121.93	126.04
31	x	102	LMT	O5'-C5'-C4'	2.38	113.78	109.52
25	b	614	CLA	CMD-C2D-C3D	-2.37	122.15	127.61
31	F	103	LMT	C2'-C3'-C4'	2.37	115.10	109.68
31	f	103	LMT	C2'-C3'-C4'	2.37	115.10	109.68
25	B	605	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
25	b	605	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
25	B	614	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
29	A	411	PL9	O2-C1-C6	2.37	124.69	120.59
35	E	104	HEM	C4D-ND-C1D	2.37	107.52	105.07
31	D	410	LMT	O1'-C1'-C2'	2.37	112.00	108.30
31	d	410	LMT	O1'-C1'-C2'	2.37	112.00	108.30
25	C	508	CLA	OBD-CAD-C3D	-2.37	122.82	128.52
25	c	508	CLA	OBD-CAD-C3D	-2.37	122.82	128.52
29	a	411	PL9	O2-C1-C6	2.37	124.69	120.59
25	C	514	CLA	CMA-C3A-C4A	2.37	118.14	111.77
25	B	610	CLA	OBD-CAD-C3D	-2.37	122.82	128.52
25	B	614	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
25	c	510	CLA	CAC-C3C-C4C	2.36	127.88	124.81
25	b	614	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
25	c	514	CLA	CMA-C3A-C4A	2.36	118.11	111.77
27	k	103	BCR	C31-C1-C6	-2.36	106.47	110.30
25	c	505	CLA	CAA-CBA-CGA	2.36	120.14	113.25
29	A	411	PL9	C42-C43-C44	-2.36	121.98	127.66
29	a	411	PL9	C42-C43-C44	-2.36	121.98	127.66
30	A	413	SQD	O5-C1-C2	2.36	115.34	110.35
30	k	101	SQD	O48-C23-C24	2.36	119.31	111.91
25	B	607	CLA	CHB-C4A-NA	2.35	127.77	124.51
25	B	606	CLA	CMC-C2C-C1C	2.35	128.62	125.04
25	b	606	CLA	CMC-C2C-C1C	2.35	128.62	125.04
30	a	413	SQD	O5-C1-C2	2.35	115.33	110.35
30	K	101	SQD	O48-C23-C24	2.35	119.29	111.91
31	B	623	LMT	C3'-C4'-C5'	-2.35	105.53	110.93
25	C	505	CLA	CAA-CBA-CGA	2.35	120.12	113.25
26	A	407	PHO	O1D-CGD-CBD	2.35	128.66	124.74
25	b	610	CLA	OBD-CAD-C3D	-2.35	122.86	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	512	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
26	a	407	PHO	O1D-CGD-CBD	2.35	128.65	124.74
30	f	102	SQD	O48-C23-C24	2.35	119.27	111.91
25	C	509	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
25	c	509	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
25	B	601	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
25	b	601	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
25	C	512	CLA	CED-O2D-CGD	2.35	121.24	115.94
25	c	512	CLA	CED-O2D-CGD	2.35	121.24	115.94
25	C	510	CLA	CAC-C3C-C4C	2.34	127.85	124.81
30	F	102	SQD	O48-C23-C24	2.34	119.26	111.91
31	c	525	LMT	C3'-C4'-C5'	-2.34	106.06	110.24
31	d	412	LMT	C3'-C4'-C5'	-2.34	105.55	110.93
31	b	623	LMT	C3'-C4'-C5'	-2.34	105.56	110.93
25	b	607	CLA	CHB-C4A-NA	2.34	127.75	124.51
27	K	103	BCR	C33-C5-C4	2.34	118.11	113.62
25	C	509	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
25	c	509	CLA	CMB-C2B-C1B	-2.34	124.87	128.46
27	K	103	BCR	C31-C1-C6	-2.34	106.51	110.30
27	B	619	BCR	C32-C1-C6	-2.34	106.51	110.30
27	b	619	BCR	C32-C1-C6	-2.34	106.51	110.30
31	C	525	LMT	C3'-C4'-C5'	-2.33	106.07	110.24
25	C	512	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
26	D	402	PHO	OBD-CAD-CBD	-2.33	122.41	125.82
26	d	402	PHO	OBD-CAD-CBD	-2.33	122.41	125.82
31	D	412	LMT	C3'-C4'-C5'	-2.33	105.59	110.93
25	c	505	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
27	C	515	BCR	C37-C22-C21	-2.33	119.67	122.92
25	C	505	CLA	CHC-C1C-C2C	-2.32	120.29	126.72
30	C	501	SQD	O47-C7-C8	2.32	116.51	111.50
25	B	613	CLA	C1-O2A-CGA	2.32	122.53	116.44
25	b	613	CLA	C1-O2A-CGA	2.32	122.53	116.44
25	C	503	CLA	C3D-C4D-ND	2.32	113.99	110.24
25	c	503	CLA	C3D-C4D-ND	2.32	113.99	110.24
30	c	501	SQD	O47-C7-C8	2.32	116.50	111.50
27	k	103	BCR	C33-C5-C4	2.32	118.07	113.62
34	C	517	DGD	O1G-C1A-O1A	-2.32	117.74	123.59
27	c	515	BCR	C37-C22-C21	-2.32	119.67	122.92
29	D	405	PL9	C27-C28-C29	-2.32	122.08	127.66
31	H	102	LMT	C1'-O5'-C5'	-2.32	109.14	113.69
31	h	102	LMT	C1'-O5'-C5'	-2.32	109.14	113.69
25	B	608	CLA	CBC-CAC-C3C	-2.32	106.04	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	608	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
25	D	401	CLA	C3B-C4B-NB	2.32	112.21	109.21
25	d	401	CLA	C3B-C4B-NB	2.32	112.21	109.21
25	b	608	CLA	C4D-C3D-CAD	2.32	110.83	108.10
25	B	608	CLA	C4D-C3D-CAD	2.32	110.83	108.10
31	Y	101	LMT	O1'-C1'-C2'	2.31	111.91	108.30
31	y	101	LMT	O1'-C1'-C2'	2.31	111.91	108.30
25	c	502	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
25	B	604	CLA	C3C-C4C-NC	2.31	113.16	110.57
25	b	604	CLA	C3C-C4C-NC	2.31	113.16	110.57
27	K	103	BCR	C34-C9-C8	2.31	121.71	118.08
27	k	103	BCR	C34-C9-C8	2.31	121.71	118.08
29	d	405	PL9	C27-C28-C29	-2.31	122.11	127.66
34	c	517	DGD	O1G-C1A-O1A	-2.31	117.77	123.59
31	E	101	LMT	C4'-C3'-C2'	2.31	114.85	110.82
31	e	101	LMT	C4'-C3'-C2'	2.31	114.85	110.82
25	b	603	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
27	B	619	BCR	C36-C18-C17	-2.30	119.70	122.92
27	b	619	BCR	C36-C18-C17	-2.30	119.70	122.92
29	a	411	PL9	C32-C33-C34	-2.30	122.11	127.66
35	V	201	HEM	CHA-C4D-C3D	-2.30	121.01	125.33
25	C	502	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
25	C	509	CLA	CED-O2D-CGD	2.30	121.14	115.94
25	c	509	CLA	CED-O2D-CGD	2.30	121.14	115.94
25	c	512	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
27	F	101	BCR	C32-C1-C6	-2.30	106.57	110.30
27	f	101	BCR	C32-C1-C6	-2.30	106.57	110.30
33	B	627	LHG	O8-C23-C24	2.30	119.12	111.91
33	b	627	LHG	O8-C23-C24	2.30	119.12	111.91
25	C	512	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
25	B	605	CLA	O1D-CGD-CBD	-2.30	119.79	124.48
25	b	605	CLA	O1D-CGD-CBD	-2.30	119.79	124.48
35	v	201	HEM	CHA-C4D-C3D	-2.29	121.02	125.33
25	b	608	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
25	b	613	CLA	C3C-C4C-NC	2.29	113.14	110.57
25	B	603	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
25	b	607	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
25	D	401	CLA	C1-O2A-CGA	2.29	122.45	116.44
25	d	401	CLA	C1-O2A-CGA	2.29	122.45	116.44
25	B	607	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
25	B	615	CLA	C1-O2A-CGA	2.28	122.44	116.44
25	C	507	CLA	C1-O2A-CGA	2.28	122.43	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	e	104	HEM	O2D-CGD-CBD	2.28	121.36	114.03
29	A	411	PL9	C32-C33-C34	-2.28	122.17	127.66
25	b	615	CLA	C1-O2A-CGA	2.28	122.43	116.44
25	B	601	CLA	CAC-C3C-C4C	2.28	127.77	124.81
25	b	601	CLA	CAC-C3C-C4C	2.28	127.77	124.81
35	E	104	HEM	O2D-CGD-CBD	2.28	121.35	114.03
25	c	514	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
25	c	507	CLA	C1-O2A-CGA	2.28	122.42	116.44
25	B	613	CLA	C3C-C4C-NC	2.28	113.12	110.57
25	C	513	CLA	C3D-C4D-ND	2.28	113.92	110.24
25	B	611	CLA	CHC-C1C-C2C	-2.28	120.43	126.72
25	b	611	CLA	CHC-C1C-C2C	-2.28	120.43	126.72
25	C	510	CLA	C4D-C3D-CAD	2.28	110.78	108.10
27	a	409	BCR	C34-C9-C8	2.27	121.66	118.08
25	b	610	CLA	C4-C3-C5	2.27	119.09	115.27
31	X	104	LMT	C1'-O5'-C5'	-2.27	109.23	113.69
31	x	104	LMT	C1'-O5'-C5'	-2.27	109.23	113.69
25	c	513	CLA	C3D-C4D-ND	2.27	113.91	110.24
33	Z	102	LHG	O4-P-O5	2.27	119.57	110.68
25	C	503	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
25	c	503	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
25	B	608	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
25	C	505	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
25	c	505	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
25	B	609	CLA	CHB-C4A-NA	2.27	127.65	124.51
34	C	517	DGD	C2G-O2G-C1B	-2.27	112.20	117.79
34	c	517	DGD	C2G-O2G-C1B	-2.27	112.20	117.79
25	B	607	CLA	C4-C3-C5	2.27	119.09	115.27
25	b	607	CLA	C4-C3-C5	2.27	119.08	115.27
25	C	514	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
33	z	102	LHG	O4-P-O5	2.27	119.55	110.68
31	t	101	LMT	C1'-O5'-C5'	-2.26	109.25	113.69
25	c	504	CLA	C4-C3-C5	2.26	119.08	115.27
25	B	612	CLA	C4-C3-C5	2.26	119.08	115.27
25	B	613	CLA	CHD-C4C-C3C	-2.26	121.52	124.84
25	b	613	CLA	CHD-C4C-C3C	-2.26	121.52	124.84
31	h	102	LMT	C4'-C3'-C2'	2.26	114.77	110.82
25	B	606	CLA	CED-O2D-CGD	2.26	121.05	115.94
25	C	503	CLA	C1-O2A-CGA	2.26	122.36	116.44
25	c	503	CLA	C1-O2A-CGA	2.26	122.36	116.44
31	H	102	LMT	C4'-C3'-C2'	2.26	114.76	110.82
25	b	609	CLA	CHB-C4A-NA	2.26	127.63	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	610	CLA	C4-C3-C5	2.26	119.07	115.27
25	b	607	CLA	C3C-C4C-NC	2.26	113.10	110.57
30	a	412	SQD	O48-C23-C24	2.25	118.98	111.91
31	T	101	LMT	C1'-O5'-C5'	-2.25	109.27	113.69
29	d	405	PL9	O1-C4-C3	-2.25	118.24	120.72
25	c	510	CLA	C4D-C3D-CAD	2.25	110.75	108.10
25	b	606	CLA	CED-O2D-CGD	2.25	121.03	115.94
25	b	612	CLA	C4-C3-C5	2.25	119.05	115.27
27	A	409	BCR	C34-C9-C8	2.25	121.62	118.08
29	D	405	PL9	O1-C4-C3	-2.25	118.25	120.72
25	C	507	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
25	c	507	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
30	A	412	SQD	O48-C23-C24	2.24	118.95	111.91
27	F	101	BCR	C7-C8-C9	-2.24	122.85	126.23
25	C	503	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
25	c	503	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
25	C	504	CLA	C4-C3-C5	2.24	119.04	115.27
30	c	501	SQD	O48-C23-C24	2.24	118.93	111.91
31	I	101	LMT	C3'-C4'-C5'	-2.24	106.25	110.24
27	C	515	BCR	C35-C13-C12	2.24	121.60	118.08
27	c	515	BCR	C35-C13-C12	2.24	121.60	118.08
25	D	401	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
30	C	501	SQD	O48-C23-C24	2.24	118.93	111.91
25	b	607	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
25	C	509	CLA	C4C-C3C-C2C	-2.24	103.64	106.90
25	c	509	CLA	C4C-C3C-C2C	-2.24	103.64	106.90
27	f	101	BCR	C7-C8-C9	-2.23	122.86	126.23
25	C	511	CLA	C4-C3-C5	2.23	119.03	115.27
26	A	407	PHO	C1B-NB-C4B	2.23	111.68	107.09
31	i	101	LMT	C3'-C4'-C5'	-2.23	106.26	110.24
25	B	607	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
25	b	615	CLA	C4C-C3C-C2C	-2.23	103.64	106.90
27	b	619	BCR	C33-C5-C6	-2.23	122.02	124.53
25	b	603	CLA	CAC-C3C-C4C	2.23	127.70	124.81
27	B	619	BCR	C39-C30-C25	-2.23	106.68	110.30
27	b	619	BCR	C39-C30-C25	-2.23	106.68	110.30
29	A	411	PL9	C41-C39-C38	-2.23	116.61	121.12
27	C	515	BCR	C36-C18-C17	-2.23	119.80	122.92
25	B	615	CLA	C4C-C3C-C2C	-2.23	103.65	106.90
25	C	509	CLA	C1-C2-C3	-2.23	122.19	126.04
25	c	509	CLA	C1-C2-C3	-2.23	122.19	126.04
25	C	511	CLA	O1D-CGD-CBD	-2.23	119.93	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	401	CLA	CBC-CAC-C3C	-2.23	106.30	112.43
25	b	607	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
33	B	628	LHG	C5-O7-C7	-2.22	112.32	117.79
33	b	628	LHG	C5-O7-C7	-2.22	112.32	117.79
25	B	607	CLA	C3C-C4C-NC	2.22	113.06	110.57
27	B	619	BCR	C33-C5-C6	-2.22	122.04	124.53
25	c	511	CLA	C4-C3-C5	2.22	119.00	115.27
25	c	511	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
25	C	512	CLA	CMC-C2C-C1C	2.22	128.41	125.04
25	c	512	CLA	CMC-C2C-C1C	2.22	128.41	125.04
25	B	604	CLA	CMB-C2B-C3B	2.21	128.82	124.68
29	a	411	PL9	C41-C39-C38	-2.21	116.64	121.12
28	h	105	LMG	O8-C28-O10	-2.21	118.01	123.59
26	a	407	PHO	C1B-NB-C4B	2.21	111.63	107.09
28	H	105	LMG	O8-C28-O10	-2.21	118.02	123.59
25	b	602	CLA	C3C-C4C-NC	2.21	113.04	110.57
25	B	603	CLA	CAC-C3C-C4C	2.21	127.67	124.81
25	d	403	CLA	C1-C2-C3	-2.20	122.23	126.04
27	c	515	BCR	C36-C18-C17	-2.20	119.83	122.92
31	j	101	LMT	C1'-O5'-C5'	2.20	118.01	113.69
25	B	613	CLA	OBD-CAD-C3D	-2.20	123.22	128.52
25	b	613	CLA	OBD-CAD-C3D	-2.20	123.22	128.52
25	b	604	CLA	C3D-C4D-ND	2.20	113.80	110.24
25	D	403	CLA	C1-C2-C3	-2.20	122.23	126.04
25	C	502	CLA	C3C-C4C-NC	2.20	113.04	110.57
27	C	515	BCR	C34-C9-C8	2.20	121.54	118.08
25	a	406	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
25	c	504	CLA	CHA-C1A-NA	-2.20	121.36	126.40
25	c	504	CLA	C4C-C3C-C2C	-2.20	103.69	106.90
25	b	604	CLA	CMB-C2B-C3B	2.20	128.79	124.68
27	K	103	BCR	C33-C5-C6	-2.20	122.06	124.53
27	k	103	BCR	C33-C5-C6	-2.20	122.06	124.53
25	B	607	CLA	C4C-C3C-C2C	-2.20	103.69	106.90
25	C	504	CLA	C4C-C3C-C2C	-2.20	103.70	106.90
25	B	602	CLA	C3C-C4C-NC	2.20	113.03	110.57
25	B	603	CLA	C3D-C4D-ND	2.19	113.79	110.24
25	C	509	CLA	CMA-C3A-C4A	2.19	117.67	111.77
25	c	509	CLA	CMA-C3A-C4A	2.19	117.67	111.77
27	c	515	BCR	C34-C9-C8	2.19	121.53	118.08
28	C	519	LMG	C8-O7-C10	-2.19	112.39	117.79
28	c	519	LMG	C8-O7-C10	-2.19	112.39	117.79
31	J	101	LMT	C1'-O5'-C5'	2.19	117.99	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	504	CLA	CHA-C1A-NA	-2.19	121.38	126.40
29	a	411	PL9	O2-C1-C2	-2.19	116.76	121.78
25	A	406	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
25	c	502	CLA	C3C-C4C-NC	2.19	113.03	110.57
25	C	509	CLA	CHA-C1A-NA	-2.19	121.39	126.40
31	A	415	LMT	C1'-O5'-C5'	-2.19	109.39	113.69
31	a	415	LMT	C1'-O5'-C5'	-2.19	109.39	113.69
31	f	103	LMT	C3B-C4B-C5B	-2.18	106.34	110.24
25	B	604	CLA	C3D-C4D-ND	2.18	113.77	110.24
27	B	618	BCR	C35-C13-C12	2.18	121.52	118.08
27	b	618	BCR	C35-C13-C12	2.18	121.52	118.08
34	C	518	DGD	O1G-C1A-C2A	2.18	118.76	111.91
25	c	509	CLA	CHA-C1A-NA	-2.18	121.40	126.40
25	C	511	CLA	C11-C10-C8	-2.18	108.87	115.92
25	c	511	CLA	C11-C10-C8	-2.18	108.87	115.92
25	b	612	CLA	CHD-C1D-C2D	-2.18	120.91	125.48
25	C	503	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
25	b	610	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
25	c	503	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
25	A	406	CLA	CMC-C2C-C1C	2.18	128.36	125.04
35	V	201	HEM	O2A-CGA-O1A	-2.18	117.87	123.30
29	d	405	PL9	C40-C39-C41	2.18	118.93	115.27
31	E	103	LMT	O1B-C4'-C3'	2.18	113.07	107.28
31	e	103	LMT	O1B-C4'-C3'	2.18	113.07	107.28
25	C	505	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
35	v	201	HEM	O2A-CGA-O1A	-2.17	117.88	123.30
25	c	505	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
25	C	507	CLA	CHA-C1A-NA	-2.17	121.42	126.40
25	c	507	CLA	CHA-C1A-NA	-2.17	121.42	126.40
25	b	603	CLA	C3D-C4D-ND	2.17	113.75	110.24
34	c	518	DGD	O1G-C1A-C2A	2.17	118.73	111.91
25	B	611	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
25	C	514	CLA	C4C-C3C-C2C	-2.17	103.73	106.90
25	c	514	CLA	C4C-C3C-C2C	-2.17	103.73	106.90
29	A	411	PL9	O2-C1-C2	-2.17	116.81	121.78
25	B	606	CLA	C6-C5-C3	-2.17	107.77	113.45
25	b	606	CLA	C6-C5-C3	-2.17	107.77	113.45
31	M	101	LMT	O1B-C4'-C3'	2.17	113.05	107.28
31	m	101	LMT	O1B-C4'-C3'	2.17	113.05	107.28
25	a	406	CLA	CMC-C2C-C1C	2.16	128.34	125.04
25	d	404	CLA	CHB-C4A-NA	2.16	127.50	124.51
25	C	511	CLA	CMB-C2B-C1B	-2.16	125.14	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	511	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
29	D	405	PL9	C40-C39-C41	2.16	118.91	115.27
25	B	612	CLA	CHD-C1D-C2D	-2.16	120.94	125.48
25	b	611	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
28	a	410	LMG	O8-C28-O10	-2.16	118.14	123.59
31	F	103	LMT	C3B-C4B-C5B	-2.16	106.39	110.24
25	b	615	CLA	C4D-C3D-CAD	2.16	110.64	108.10
25	B	603	CLA	CHC-C1C-C2C	-2.16	120.75	126.72
31	K	105	LMT	O1B-C1B-C2B	2.15	113.68	108.10
31	k	105	LMT	O1B-C1B-C2B	2.15	113.68	108.10
27	B	619	BCR	C19-C18-C17	2.15	122.24	118.94
27	b	619	BCR	C19-C18-C17	2.15	122.24	118.94
25	b	610	CLA	C1-C2-C3	-2.15	122.32	126.04
31	b	623	LMT	O6'-C6'-C5'	-2.15	103.91	111.29
25	C	509	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
25	B	616	CLA	C4-C3-C5	2.15	118.89	115.27
25	c	509	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
31	K	105	LMT	O5'-C5'-C6'	2.15	111.78	106.44
25	D	401	CLA	C4-C3-C5	2.15	118.89	115.27
25	B	615	CLA	OBD-CAD-C3D	-2.15	123.35	128.52
25	B	610	CLA	C4C-C3C-C2C	-2.15	103.77	106.90
31	k	105	LMT	O5'-C5'-C6'	2.15	111.77	106.44
28	A	410	LMG	O8-C28-O10	-2.15	118.17	123.59
31	C	524	LMT	C4B-C3B-C2B	2.15	114.57	110.82
25	b	603	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
27	B	619	BCR	C12-C13-C14	-2.14	115.65	118.94
25	B	612	CLA	C4C-C3C-C2C	-2.14	103.77	106.90
25	b	612	CLA	C4C-C3C-C2C	-2.14	103.77	106.90
25	B	611	CLA	C4D-C3D-CAD	2.14	110.62	108.10
25	b	611	CLA	C4D-C3D-CAD	2.14	110.62	108.10
25	B	612	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
25	b	615	CLA	OBD-CAD-C3D	-2.14	123.37	128.52
25	D	404	CLA	CHB-C4A-NA	2.14	127.47	124.51
25	B	610	CLA	C1-C2-C3	-2.14	122.34	126.04
25	b	616	CLA	C4-C3-C5	2.14	118.87	115.27
25	a	405	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
25	C	507	CLA	C4C-C3C-C2C	-2.14	103.78	106.90
25	C	508	CLA	CHA-C1A-NA	-2.14	121.51	126.40
25	b	610	CLA	CAC-C3C-C4C	2.14	127.58	124.81
25	B	602	CLA	C1-C2-C3	-2.14	122.35	126.04
31	D	410	LMT	C1'-O5'-C5'	2.14	117.88	113.69
31	d	410	LMT	C1'-O5'-C5'	2.14	117.88	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	505	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	c	505	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	B	615	CLA	C4D-C3D-CAD	2.13	110.61	108.10
25	C	508	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	b	602	CLA	C1-C2-C3	-2.13	122.36	126.04
25	B	602	CLA	CMC-C2C-C1C	2.13	128.29	125.04
25	b	602	CLA	CMC-C2C-C1C	2.13	128.29	125.04
34	c	517	DGD	O2G-C1B-O1B	-2.13	118.55	123.70
25	C	505	CLA	C1-C2-C3	-2.13	122.36	126.04
25	d	401	CLA	C4-C3-C5	2.13	118.86	115.27
27	b	619	BCR	C12-C13-C14	-2.13	115.67	118.94
31	B	623	LMT	O6'-C6'-C5'	-2.13	103.98	111.29
25	A	405	CLA	CAA-C2A-C1A	-2.13	105.00	111.97
25	B	607	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
25	c	507	CLA	C4C-C3C-C2C	-2.13	103.80	106.90
25	A	408	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
25	a	408	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
25	B	610	CLA	CMC-C2C-C1C	2.13	128.28	125.04
31	M	101	LMT	O5B-C5B-C4B	2.13	113.56	109.69
25	c	508	CLA	CHB-C4A-NA	2.13	127.45	124.51
31	c	524	LMT	C4B-C3B-C2B	2.13	114.53	110.82
25	b	612	CLA	O1D-CGD-CBD	-2.13	120.14	124.48
31	m	101	LMT	O5B-C5B-C4B	2.12	113.55	109.69
25	d	404	CLA	C4-C3-C5	2.12	118.84	115.27
25	b	608	CLA	C4-C3-C5	2.12	118.84	115.27
25	b	604	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
34	C	517	DGD	O2G-C1B-O1B	-2.12	118.57	123.70
25	B	611	CLA	CMC-C2C-C1C	2.12	128.27	125.04
25	b	611	CLA	CMC-C2C-C1C	2.12	128.27	125.04
25	B	608	CLA	C4-C3-C5	2.12	118.84	115.27
28	H	105	LMG	O6-C1-O1	-2.12	104.95	109.97
28	h	105	LMG	O6-C1-O1	-2.12	104.95	109.97
25	b	607	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
25	D	404	CLA	C4-C3-C5	2.12	118.84	115.27
26	D	402	PHO	C1B-NB-C4B	2.12	111.44	107.09
26	d	402	PHO	C1B-NB-C4B	2.12	111.44	107.09
27	F	101	BCR	C2-C1-C6	2.12	113.74	110.48
27	f	101	BCR	C2-C1-C6	2.12	113.74	110.48
25	B	604	CLA	CMC-C2C-C1C	2.12	128.26	125.04
25	b	604	CLA	CMC-C2C-C1C	2.12	128.26	125.04
27	k	102	BCR	C2-C1-C6	2.11	113.74	110.48
25	c	510	CLA	CMD-C2D-C3D	-2.11	122.75	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	504	CLA	C1-O2A-CGA	2.11	121.99	116.44
27	B	618	BCR	C3-C4-C5	-2.11	110.31	114.08
25	A	406	CLA	C1-C2-C3	-2.11	122.40	126.04
27	K	102	BCR	C31-C1-C6	-2.11	106.88	110.30
27	k	102	BCR	C31-C1-C6	-2.11	106.88	110.30
25	C	510	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
25	c	505	CLA	C1-C2-C3	-2.11	122.40	126.04
25	c	508	CLA	CHA-C1A-NA	-2.11	121.57	126.40
27	z	101	BCR	C31-C1-C6	-2.10	106.89	110.30
25	B	604	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
31	A	416	LMT	C1'-O5'-C5'	-2.10	109.56	113.69
25	C	504	CLA	C1-O2A-CGA	2.10	121.96	116.44
31	D	410	LMT	O5'-C5'-C6'	2.10	111.66	106.44
31	d	410	LMT	O5'-C5'-C6'	2.10	111.66	106.44
25	B	613	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
25	b	613	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
25	B	610	CLA	CAC-C3C-C4C	2.10	127.53	124.81
25	C	506	CLA	CHA-C4D-ND	2.10	136.89	132.50
25	b	610	CLA	CMC-C2C-C1C	2.10	128.24	125.04
25	B	603	CLA	C5-C3-C2	-2.10	116.87	121.12
27	F	101	BCR	C34-C9-C8	2.10	121.38	118.08
25	B	609	CLA	CHC-C1C-C2C	-2.10	120.92	126.72
33	d	406	LHG	C5-O7-C7	-2.10	112.63	117.79
31	a	416	LMT	C1'-O5'-C5'	-2.09	109.58	113.69
25	a	406	CLA	C1-C2-C3	-2.09	122.42	126.04
27	K	102	BCR	C2-C1-C6	2.09	113.70	110.48
25	C	510	CLA	C3D-C4D-ND	2.09	113.62	110.24
25	c	510	CLA	C3D-C4D-ND	2.09	113.62	110.24
27	b	618	BCR	C3-C4-C5	-2.09	110.34	114.08
25	b	609	CLA	CHC-C1C-C2C	-2.09	120.94	126.72
27	f	101	BCR	C34-C9-C8	2.09	121.37	118.08
27	Z	101	BCR	C31-C1-C6	-2.09	106.92	110.30
28	c	523	LMG	O7-C10-O9	-2.09	118.66	123.70
35	v	201	HEM	C4A-C3A-C2A	2.09	108.45	107.00
33	D	406	LHG	C5-O7-C7	-2.08	112.66	117.79
25	c	508	CLA	CHA-C4D-ND	2.08	136.86	132.50
25	b	603	CLA	C5-C3-C2	-2.08	116.90	121.12
25	B	609	CLA	C3B-C4B-NB	2.08	111.90	109.21
25	b	609	CLA	C3B-C4B-NB	2.08	111.90	109.21
25	C	511	CLA	C3B-C4B-NB	2.08	111.90	109.21
25	a	406	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
25	C	507	CLA	O1D-CGD-CBD	-2.08	120.23	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	506	CLA	CHA-C4D-ND	2.08	136.85	132.50
25	c	511	CLA	CMA-C3A-C4A	2.08	117.36	111.77
25	C	506	CLA	CAC-C3C-C4C	2.08	127.50	124.81
25	c	511	CLA	C3B-C4B-NB	2.08	111.89	109.21
25	c	506	CLA	CAC-C3C-C4C	2.07	127.50	124.81
25	c	503	CLA	C3B-C4B-NB	2.07	111.89	109.21
28	C	523	LMG	O7-C10-O9	-2.07	118.69	123.70
25	c	511	CLA	C6-C7-C8	-2.07	109.22	115.92
25	C	511	CLA	CMA-C3A-C4A	2.07	117.34	111.77
25	C	508	CLA	CHA-C4D-ND	2.07	136.83	132.50
25	D	404	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
25	C	503	CLA	C4D-C3D-CAD	2.07	110.53	108.10
25	C	511	CLA	C6-C7-C8	-2.07	109.23	115.92
29	D	405	PL9	C11-C12-C13	-2.07	105.09	111.88
29	d	405	PL9	C11-C12-C13	-2.07	105.09	111.88
25	A	406	CLA	O2D-CGD-O1D	-2.06	119.80	123.84
26	D	402	PHO	C1-C2-C3	-2.06	122.47	126.04
25	D	401	CLA	CHB-C4A-NA	2.06	127.36	124.51
25	d	401	CLA	CHB-C4A-NA	2.06	127.36	124.51
35	V	201	HEM	C4A-C3A-C2A	2.06	108.43	107.00
25	b	603	CLA	CHA-C4D-ND	2.06	136.81	132.50
25	C	502	CLA	CAC-C3C-C4C	2.06	127.48	124.81
25	d	404	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
25	a	405	CLA	CHB-C4A-NA	2.06	127.36	124.51
28	h	105	LMG	O7-C10-O9	-2.06	118.73	123.70
25	C	503	CLA	CAC-C3C-C4C	2.06	127.48	124.81
25	A	405	CLA	C4C-C3C-C2C	-2.06	103.90	106.90
31	e	101	LMT	O1'-C1'-C2'	2.06	111.51	108.30
25	B	603	CLA	CHA-C4D-ND	2.06	136.80	132.50
25	C	511	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
25	c	507	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
31	c	522	LMT	O1'-C1'-C2'	2.05	111.51	108.30
25	C	503	CLA	CMC-C2C-C3C	2.05	131.69	126.12
30	a	412	SQD	O48-C23-O10	-2.05	118.41	123.59
25	A	405	CLA	CHB-C4A-NA	2.05	127.35	124.51
25	b	610	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
25	B	610	CLA	CHA-C1A-NA	-2.05	121.70	126.40
33	D	407	LHG	O8-C23-O10	-2.05	118.42	123.59
25	c	506	CLA	C1-O2A-CGA	2.05	121.82	116.44
25	B	607	CLA	CED-O2D-CGD	2.05	120.57	115.94
25	B	602	CLA	CHB-C4A-NA	2.05	127.34	124.51
25	b	602	CLA	CHB-C4A-NA	2.05	127.34	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	105	LMG	O7-C10-O9	-2.05	118.75	123.70
25	b	610	CLA	CHA-C1A-NA	-2.05	121.71	126.40
25	C	503	CLA	C3B-C4B-NB	2.05	111.86	109.21
26	d	402	PHO	C1-C2-C3	-2.05	122.50	126.04
31	C	522	LMT	O1'-C1'-C2'	2.05	111.50	108.30
30	A	412	SQD	O48-C23-O10	-2.05	118.43	123.59
25	a	405	CLA	C4C-C3C-C2C	-2.05	103.92	106.90
25	b	611	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
25	B	611	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
25	B	610	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
30	a	412	SQD	O6-C1-C2	2.04	111.49	108.30
25	c	511	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
25	a	405	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
33	d	407	LHG	O8-C23-O10	-2.04	118.44	123.59
29	a	411	PL9	C12-C13-C14	-2.04	122.74	127.66
25	c	503	CLA	CAC-C3C-C4C	2.04	127.46	124.81
25	c	503	CLA	CMC-C2C-C3C	2.04	131.66	126.12
25	c	503	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
25	C	510	CLA	C6-C5-C3	-2.04	108.11	113.45
25	c	510	CLA	C6-C5-C3	-2.04	108.11	113.45
26	a	407	PHO	O2D-CGD-O1D	-2.04	119.85	123.84
25	C	512	CLA	C4C-C3C-C2C	-2.04	103.93	106.90
25	c	512	CLA	C4C-C3C-C2C	-2.04	103.93	106.90
25	b	607	CLA	CED-O2D-CGD	2.04	120.55	115.94
30	a	413	SQD	O8-S-C6	2.04	108.99	105.74
25	c	503	CLA	C4D-C3D-CAD	2.04	110.50	108.10
31	d	412	LMT	C3B-C4B-C5B	-2.04	106.61	110.24
30	A	412	SQD	O6-C1-C2	2.04	111.48	108.30
25	c	512	CLA	CAC-C3C-C4C	2.03	127.45	124.81
25	c	511	CLA	CHC-C1C-C2C	-2.03	121.09	126.72
25	c	510	CLA	CHC-C1C-NC	-2.03	121.12	124.20
25	C	506	CLA	C1-O2A-CGA	2.03	121.78	116.44
25	C	512	CLA	CAC-C3C-C4C	2.03	127.45	124.81
31	E	101	LMT	O1'-C1'-C2'	2.03	111.48	108.30
25	C	503	CLA	OBD-CAD-C3D	-2.03	123.63	128.52
25	B	616	CLA	C3B-C4B-NB	2.03	111.84	109.21
25	b	616	CLA	C3B-C4B-NB	2.03	111.84	109.21
34	h	104	DGD	O1G-C1A-O1A	-2.03	118.46	123.59
29	A	411	PL9	C12-C13-C14	-2.03	122.77	127.66
25	C	509	CLA	C4-C3-C5	2.03	118.69	115.27
25	c	509	CLA	C4-C3-C5	2.03	118.69	115.27
25	C	511	CLA	CHC-C1C-C2C	-2.03	121.11	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	405	CLA	CHA-C4D-ND	2.03	136.74	132.50
25	a	405	CLA	CHA-C4D-ND	2.03	136.74	132.50
33	D	408	LHG	O8-C23-C24	2.03	118.27	111.91
33	d	408	LHG	O8-C23-C24	2.03	118.27	111.91
31	D	412	LMT	C3B-C4B-C5B	-2.03	106.62	110.24
30	A	413	SQD	O8-S-C6	2.03	108.97	105.74
25	A	405	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
27	B	617	BCR	C28-C27-C26	-2.02	110.47	114.08
25	B	612	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
26	d	402	PHO	O1D-CGD-CBD	2.02	128.11	124.74
26	A	407	PHO	O2D-CGD-O1D	-2.02	119.89	123.84
30	A	412	SQD	O47-C7-O49	-2.02	118.83	123.70
30	a	412	SQD	O47-C7-O49	-2.02	118.83	123.70
25	C	506	CLA	C7-C6-C5	-2.02	107.88	113.36
25	c	506	CLA	C7-C6-C5	-2.02	107.89	113.36
25	c	506	CLA	CMC-C2C-C1C	2.02	128.11	125.04
25	C	510	CLA	CHC-C1C-NC	-2.01	121.15	124.20
25	c	502	CLA	CAC-C3C-C4C	2.01	127.42	124.81
29	d	405	PL9	O2-C1-C2	-2.01	117.17	121.78
25	C	506	CLA	CMC-C2C-C1C	2.01	128.10	125.04
34	H	104	DGD	O1G-C1A-O1A	-2.01	118.52	123.59
27	K	103	BCR	C35-C13-C12	2.01	121.25	118.08
27	k	103	BCR	C35-C13-C12	2.01	121.25	118.08
25	b	604	CLA	C1-O2A-CGA	2.01	121.72	116.44
25	d	403	CLA	CMA-C3A-C2A	-2.01	105.72	113.83
27	K	103	BCR	C4-C5-C6	-2.01	119.81	122.73
31	B	624	LMT	C3'-C4'-C5'	-2.01	106.66	110.24
31	a	415	LMT	C3'-C4'-C5'	-2.01	106.32	110.93
31	I	103	LMT	C1'-O5'-C5'	-2.01	109.75	113.69
31	i	103	LMT	C1'-O5'-C5'	-2.01	109.75	113.69
29	D	405	PL9	O2-C1-C2	-2.01	117.18	121.78
25	C	511	CLA	C3C-C4C-NC	2.01	112.82	110.57
25	c	511	CLA	C3C-C4C-NC	2.01	112.82	110.57
26	D	402	PHO	O1D-CGD-CBD	2.01	128.08	124.74
25	B	613	CLA	O2D-CGD-O1D	-2.01	119.92	123.84
25	b	613	CLA	O2D-CGD-O1D	-2.01	119.92	123.84
25	b	612	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
25	C	504	CLA	CHA-C4D-ND	2.01	136.69	132.50
25	c	504	CLA	CHA-C4D-ND	2.01	136.69	132.50
30	B	620	SQD	O8-S-C6	-2.00	102.55	105.74
25	c	514	CLA	C4D-C3D-CAD	2.00	110.46	108.10
31	X	103	LMT	O1'-C1'-C2'	2.00	111.43	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	x	103	LMT	O1'-C1'-C2'	2.00	111.43	108.30
25	D	403	CLA	CMA-C3A-C2A	-2.00	105.75	113.83
27	b	617	BCR	C28-C27-C26	-2.00	110.50	114.08
25	B	610	CLA	CHC-C1C-C2C	-2.00	121.18	126.72
25	B	604	CLA	C1-O2A-CGA	2.00	121.69	116.44

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	405	CLA	ND
25	A	406	CLA	ND
25	A	408	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	C	514	CLA	ND
25	D	401	CLA	ND

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Mol	Chain	Res	Type	Atom
25	D	403	CLA	ND
25	D	404	CLA	ND
25	a	405	CLA	ND
25	a	406	CLA	ND
25	a	408	CLA	ND
25	b	601	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	c	514	CLA	ND
25	d	401	CLA	ND
25	d	403	CLA	ND
25	d	404	CLA	ND

All (2683) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	405	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	A	406	CLA	CHA-CBD-CGD-O1D
25	A	406	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	601	CLA	C3A-C2A-CAA-CBA
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	602	CLA	CHA-CBD-CGD-O2D
25	B	603	CLA	C2-C3-C5-C6
25	B	603	CLA	C4-C3-C5-C6
25	B	604	CLA	C2-C3-C5-C6
25	B	604	CLA	C4-C3-C5-C6
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	C2-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	B	614	CLA	C11-C10-C8-C9
25	B	616	CLA	C6-C7-C8-C9
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CBD-CGD-O2D-CED
25	C	505	CLA	C2-C3-C5-C6
25	C	505	CLA	C4-C3-C5-C6
25	C	507	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	C2-C3-C5-C6
25	C	508	CLA	C4-C3-C5-C6
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	C	510	CLA	C2-C1-O2A-CGA
25	C	512	CLA	CBD-CGD-O2D-CED
25	C	513	CLA	CBA-CGA-O2A-C1
25	C	513	CLA	O1A-CGA-O2A-C1
25	C	513	CLA	CBD-CGD-O2D-CED
25	C	514	CLA	CHA-CBD-CGD-O1D
25	C	514	CLA	CHA-CBD-CGD-O2D
25	D	401	CLA	C1A-C2A-CAA-CBA
25	D	401	CLA	CHA-CBD-CGD-O1D
25	D	401	CLA	CHA-CBD-CGD-O2D
25	a	405	CLA	CBD-CGD-O2D-CED
25	a	406	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	a	406	CLA	CHA-CBD-CGD-O2D
25	b	601	CLA	C1A-C2A-CAA-CBA
25	b	601	CLA	C3A-C2A-CAA-CBA
25	b	602	CLA	CHA-CBD-CGD-O1D
25	b	602	CLA	CHA-CBD-CGD-O2D
25	b	603	CLA	C2-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
25	b	606	CLA	CHA-CBD-CGD-O1D
25	b	606	CLA	CHA-CBD-CGD-O2D
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	b	614	CLA	C2-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
25	b	614	CLA	C11-C10-C8-C9
25	b	616	CLA	C6-C7-C8-C9
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	503	CLA	CHA-CBD-CGD-O1D
25	c	503	CLA	CHA-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CBD-CGD-O2D-CED
25	c	505	CLA	C2-C3-C5-C6
25	c	505	CLA	C4-C3-C5-C6
25	c	507	CLA	CBD-CGD-O2D-CED
25	c	508	CLA	C2-C3-C5-C6
25	c	508	CLA	C4-C3-C5-C6
25	c	509	CLA	CHA-CBD-CGD-O1D
25	c	509	CLA	CHA-CBD-CGD-O2D
25	c	510	CLA	C2-C1-O2A-CGA
25	c	512	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	CBD-CGD-O2D-CED
25	c	514	CLA	CHA-CBD-CGD-O1D
25	c	514	CLA	CHA-CBD-CGD-O2D
25	d	401	CLA	C1A-C2A-CAA-CBA
25	d	401	CLA	CHA-CBD-CGD-O1D
25	d	401	CLA	CHA-CBD-CGD-O2D
27	A	409	BCR	C7-C8-C9-C10
27	A	409	BCR	C7-C8-C9-C34
27	A	409	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
27	A	409	BCR	C11-C10-C9-C34
27	B	618	BCR	C7-C8-C9-C10
27	B	618	BCR	C7-C8-C9-C34
27	B	618	BCR	C11-C10-C9-C8
27	B	618	BCR	C11-C10-C9-C34
27	B	618	BCR	C10-C11-C12-C13
27	B	619	BCR	C1-C6-C7-C8
27	B	619	BCR	C7-C8-C9-C10
27	B	619	BCR	C7-C8-C9-C34
27	B	619	BCR	C11-C10-C9-C8
27	B	619	BCR	C11-C10-C9-C34
27	C	515	BCR	C7-C8-C9-C10
27	C	515	BCR	C7-C8-C9-C34
27	C	515	BCR	C11-C10-C9-C8
27	C	515	BCR	C11-C10-C9-C34
27	C	515	BCR	C10-C11-C12-C13
27	F	101	BCR	C1-C6-C7-C8
27	F	101	BCR	C11-C10-C9-C8
27	F	101	BCR	C11-C10-C9-C34
27	K	102	BCR	C5-C6-C7-C8
27	K	102	BCR	C7-C8-C9-C10
27	K	102	BCR	C7-C8-C9-C34
27	K	102	BCR	C11-C10-C9-C8
27	K	102	BCR	C11-C10-C9-C34
27	K	102	BCR	C10-C11-C12-C13
27	K	103	BCR	C11-C10-C9-C8
27	K	103	BCR	C11-C10-C9-C34
27	K	103	BCR	C10-C11-C12-C13
27	K	103	BCR	C17-C18-C19-C20
27	K	103	BCR	C36-C18-C19-C20
27	a	409	BCR	C7-C8-C9-C10
27	a	409	BCR	C7-C8-C9-C34
27	a	409	BCR	C11-C10-C9-C8
27	a	409	BCR	C11-C10-C9-C34
27	b	618	BCR	C7-C8-C9-C10
27	b	618	BCR	C7-C8-C9-C34
27	b	618	BCR	C11-C10-C9-C8
27	b	618	BCR	C11-C10-C9-C34
27	b	618	BCR	C10-C11-C12-C13
27	b	619	BCR	C1-C6-C7-C8
27	b	619	BCR	C7-C8-C9-C10
27	b	619	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
27	b	619	BCR	C11-C10-C9-C8
27	b	619	BCR	C11-C10-C9-C34
27	c	515	BCR	C7-C8-C9-C10
27	c	515	BCR	C7-C8-C9-C34
27	c	515	BCR	C11-C10-C9-C8
27	c	515	BCR	C11-C10-C9-C34
27	c	515	BCR	C10-C11-C12-C13
27	f	101	BCR	C1-C6-C7-C8
27	f	101	BCR	C11-C10-C9-C8
27	f	101	BCR	C11-C10-C9-C34
27	k	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C7-C8-C9-C10
27	k	102	BCR	C7-C8-C9-C34
27	k	102	BCR	C11-C10-C9-C8
27	k	102	BCR	C11-C10-C9-C34
27	k	102	BCR	C10-C11-C12-C13
27	k	103	BCR	C11-C10-C9-C8
27	k	103	BCR	C11-C10-C9-C34
27	k	103	BCR	C10-C11-C12-C13
27	k	103	BCR	C17-C18-C19-C20
27	k	103	BCR	C36-C18-C19-C20
28	C	523	LMG	C2-C1-O1-C7
28	C	523	LMG	O6-C1-O1-C7
28	c	523	LMG	C2-C1-O1-C7
28	c	523	LMG	O6-C1-O1-C7
29	A	411	PL9	C24-C26-C27-C28
29	A	411	PL9	C36-C37-C38-C39
29	A	411	PL9	C37-C38-C39-C40
29	A	411	PL9	C37-C38-C39-C41
29	A	411	PL9	C39-C41-C42-C43
29	A	411	PL9	C42-C43-C44-C45
29	A	411	PL9	C42-C43-C44-C46
29	D	405	PL9	C39-C41-C42-C43
29	D	405	PL9	C42-C43-C44-C45
29	D	405	PL9	C42-C43-C44-C46
29	a	411	PL9	C24-C26-C27-C28
29	a	411	PL9	C36-C37-C38-C39
29	a	411	PL9	C37-C38-C39-C40
29	a	411	PL9	C37-C38-C39-C41
29	a	411	PL9	C39-C41-C42-C43
29	a	411	PL9	C42-C43-C44-C45
29	a	411	PL9	C42-C43-C44-C46

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Mol	Chain	Res	Type	Atoms
29	d	405	PL9	C39-C41-C42-C43
29	d	405	PL9	C42-C43-C44-C45
29	d	405	PL9	C42-C43-C44-C46
30	A	412	SQD	C44-C45-O47-C7
30	A	412	SQD	O49-C7-O47-C45
30	A	412	SQD	C8-C7-O47-C45
30	A	412	SQD	C24-C23-O48-C46
30	A	412	SQD	C5-C6-S-O8
30	A	413	SQD	C2-C1-O6-C44
30	A	413	SQD	O5-C1-O6-C44
30	A	413	SQD	O5-C5-C6-S
30	A	413	SQD	C5-C6-S-O7
30	A	413	SQD	C5-C6-S-O8
30	A	413	SQD	C5-C6-S-O9
30	B	620	SQD	O5-C1-O6-C44
30	B	620	SQD	O49-C7-O47-C45
30	B	620	SQD	O5-C5-C6-S
30	C	501	SQD	O47-C45-C46-O48
30	C	501	SQD	C5-C6-S-O7
30	C	501	SQD	C5-C6-S-O8
30	C	501	SQD	C5-C6-S-O9
30	F	102	SQD	C2-C1-O6-C44
30	F	102	SQD	O5-C1-O6-C44
30	F	102	SQD	O5-C5-C6-S
30	H	103	SQD	O5-C1-O6-C44
30	H	103	SQD	O49-C7-O47-C45
30	K	101	SQD	C2-C1-O6-C44
30	K	101	SQD	O5-C1-O6-C44
30	K	101	SQD	O47-C45-C46-O48
30	a	412	SQD	C44-C45-O47-C7
30	a	412	SQD	O49-C7-O47-C45
30	a	412	SQD	C8-C7-O47-C45
30	a	412	SQD	C24-C23-O48-C46
30	a	412	SQD	C5-C6-S-O8
30	a	413	SQD	C2-C1-O6-C44
30	a	413	SQD	O5-C1-O6-C44
30	a	413	SQD	O5-C5-C6-S
30	a	413	SQD	C5-C6-S-O7
30	a	413	SQD	C5-C6-S-O8
30	a	413	SQD	C5-C6-S-O9
30	b	620	SQD	O5-C1-O6-C44
30	b	620	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
30	b	620	SQD	O5-C5-C6-S
30	c	501	SQD	O47-C45-C46-O48
30	c	501	SQD	C5-C6-S-O7
30	c	501	SQD	C5-C6-S-O8
30	c	501	SQD	C5-C6-S-O9
30	f	102	SQD	C2-C1-O6-C44
30	f	102	SQD	O5-C1-O6-C44
30	f	102	SQD	O5-C5-C6-S
30	h	103	SQD	O5-C1-O6-C44
30	h	103	SQD	O49-C7-O47-C45
30	k	101	SQD	C2-C1-O6-C44
30	k	101	SQD	O5-C1-O6-C44
30	k	101	SQD	O47-C45-C46-O48
31	A	415	LMT	O5'-C1'-O1'-C1
31	A	416	LMT	C2-C1-O1'-C1'
31	B	626	LMT	C2-C1-O1'-C1'
31	B	629	LMT	O5'-C1'-O1'-C1
31	C	522	LMT	C2'-C1'-O1'-C1
31	C	522	LMT	O5'-C1'-O1'-C1
31	C	522	LMT	C2-C1-O1'-C1'
31	C	524	LMT	C2'-C1'-O1'-C1
31	C	524	LMT	O5'-C1'-O1'-C1
31	C	524	LMT	C2-C1-O1'-C1'
31	D	410	LMT	C2'-C1'-O1'-C1
31	D	410	LMT	O5'-C1'-O1'-C1
31	D	411	LMT	C2-C1-O1'-C1'
31	D	412	LMT	C2'-C1'-O1'-C1
31	D	412	LMT	O5'-C1'-O1'-C1
31	F	103	LMT	C2'-C1'-O1'-C1
31	F	103	LMT	O5'-C1'-O1'-C1
31	F	103	LMT	C2-C1-O1'-C1'
31	H	102	LMT	C2'-C1'-O1'-C1
31	H	102	LMT	O5'-C1'-O1'-C1
31	I	101	LMT	C2'-C1'-O1'-C1
31	I	101	LMT	O5'-C1'-O1'-C1
31	I	102	LMT	C2-C1-O1'-C1'
31	J	101	LMT	C2'-C1'-O1'-C1
31	J	101	LMT	O5'-C1'-O1'-C1
31	K	105	LMT	C2-C1-O1'-C1'
31	M	102	LMT	C2'-C1'-O1'-C1
31	M	102	LMT	O5'-C1'-O1'-C1
31	T	101	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
31	X	102	LMT	C2'-C1'-O1'-C1
31	X	102	LMT	O5'-C1'-O1'-C1
31	X	102	LMT	C2-C1-O1'-C1'
31	X	104	LMT	O5'-C1'-O1'-C1
31	X	105	LMT	C2'-C1'-O1'-C1
31	X	105	LMT	O5'-C1'-O1'-C1
31	X	105	LMT	C2-C1-O1'-C1'
31	a	415	LMT	O5'-C1'-O1'-C1
31	a	416	LMT	C2-C1-O1'-C1'
31	b	626	LMT	C2-C1-O1'-C1'
31	b	629	LMT	O5'-C1'-O1'-C1
31	c	522	LMT	C2'-C1'-O1'-C1
31	c	522	LMT	O5'-C1'-O1'-C1
31	c	522	LMT	C2-C1-O1'-C1'
31	c	524	LMT	C2'-C1'-O1'-C1
31	c	524	LMT	O5'-C1'-O1'-C1
31	c	524	LMT	C2-C1-O1'-C1'
31	d	410	LMT	C2'-C1'-O1'-C1
31	d	410	LMT	O5'-C1'-O1'-C1
31	d	411	LMT	C2-C1-O1'-C1'
31	d	412	LMT	C2'-C1'-O1'-C1
31	d	412	LMT	O5'-C1'-O1'-C1
31	f	103	LMT	C2'-C1'-O1'-C1
31	f	103	LMT	O5'-C1'-O1'-C1
31	f	103	LMT	C2-C1-O1'-C1'
31	h	102	LMT	C2'-C1'-O1'-C1
31	h	102	LMT	O5'-C1'-O1'-C1
31	i	101	LMT	C2'-C1'-O1'-C1
31	i	101	LMT	O5'-C1'-O1'-C1
31	i	102	LMT	C2-C1-O1'-C1'
31	j	101	LMT	C2'-C1'-O1'-C1
31	j	101	LMT	O5'-C1'-O1'-C1
31	k	105	LMT	C2-C1-O1'-C1'
31	m	102	LMT	C2'-C1'-O1'-C1
31	m	102	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	C2-C1-O1'-C1'
31	x	102	LMT	C2'-C1'-O1'-C1
31	x	102	LMT	O5'-C1'-O1'-C1
31	x	102	LMT	C2-C1-O1'-C1'
31	x	104	LMT	O5'-C1'-O1'-C1
31	x	105	LMT	C2'-C1'-O1'-C1
31	x	105	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	x	105	LMT	C2-C1-O1'-C1'
33	B	627	LHG	C1-C2-C3-O3
33	B	627	LHG	C8-C7-O7-C5
33	B	628	LHG	O1-C1-C2-O2
33	B	628	LHG	O1-C1-C2-C3
33	B	628	LHG	C3-O3-P-O4
33	D	406	LHG	O1-C1-C2-C3
33	D	406	LHG	C3-O3-P-O5
33	D	406	LHG	C3-O3-P-O6
33	D	407	LHG	O1-C1-C2-C3
33	D	407	LHG	C3-O3-P-O5
33	D	408	LHG	O1-C1-C2-O2
33	D	408	LHG	O6-C4-C5-O7
33	E	102	LHG	C3-O3-P-O5
33	Z	102	LHG	C4-O6-P-O3
33	Z	102	LHG	C4-O6-P-O4
33	b	627	LHG	C1-C2-C3-O3
33	b	627	LHG	C8-C7-O7-C5
33	b	628	LHG	O1-C1-C2-O2
33	b	628	LHG	O1-C1-C2-C3
33	b	628	LHG	C3-O3-P-O4
33	d	406	LHG	O1-C1-C2-C3
33	d	406	LHG	C3-O3-P-O5
33	d	406	LHG	C3-O3-P-O6
33	d	407	LHG	O1-C1-C2-C3
33	d	407	LHG	C3-O3-P-O5
33	d	408	LHG	O1-C1-C2-O2
33	d	408	LHG	O6-C4-C5-O7
33	e	102	LHG	C3-O3-P-O5
33	z	102	LHG	C4-O6-P-O3
33	z	102	LHG	C4-O6-P-O4
36	H	101	RRX	C22-C23-C24-C25
36	H	101	RRX	C37-C22-C23-C24
36	H	101	RRX	C21-C22-C23-C24
36	H	101	RRX	C20-C21-C22-C23
36	H	101	RRX	C20-C21-C22-C37
36	H	101	RRX	C18-C19-C20-C21
36	H	101	RRX	C16-C17-C18-C19
36	H	101	RRX	C16-C17-C18-C36
36	h	101	RRX	C22-C23-C24-C25
36	h	101	RRX	C37-C22-C23-C24
36	h	101	RRX	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
36	h	101	RRX	C20-C21-C22-C23
36	h	101	RRX	C20-C21-C22-C37
36	h	101	RRX	C18-C19-C20-C21
36	h	101	RRX	C16-C17-C18-C19
36	h	101	RRX	C16-C17-C18-C36
31	M	101	LMT	C3'-C4'-O1B-C1B
31	m	101	LMT	C3'-C4'-O1B-C1B
25	A	405	CLA	O1D-CGD-O2D-CED
25	C	510	CLA	O1D-CGD-O2D-CED
25	a	405	CLA	O1D-CGD-O2D-CED
25	c	510	CLA	O1D-CGD-O2D-CED
25	B	610	CLA	C15-C16-C17-C18
25	b	610	CLA	C15-C16-C17-C18
31	B	625	LMT	C3'-C4'-O1B-C1B
31	b	625	LMT	C3'-C4'-O1B-C1B
25	B	605	CLA	CBD-CGD-O2D-CED
25	B	609	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	C	514	CLA	CBD-CGD-O2D-CED
25	D	404	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CBD-CGD-O2D-CED
25	c	510	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	c	514	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	CBD-CGD-O2D-CED
28	A	410	LMG	O10-C28-O8-C9
28	C	523	LMG	O10-C28-O8-C9
28	H	105	LMG	O10-C28-O8-C9
28	a	410	LMG	O10-C28-O8-C9
28	c	523	LMG	O10-C28-O8-C9
28	h	105	LMG	O10-C28-O8-C9
30	A	412	SQD	O10-C23-O48-C46
30	H	103	SQD	O10-C23-O48-C46
30	a	412	SQD	O10-C23-O48-C46
30	h	103	SQD	O10-C23-O48-C46
34	C	516	DGD	O1A-C1A-O1G-C1G
34	c	516	DGD	O1A-C1A-O1G-C1G
25	C	504	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	C	512	CLA	O1D-CGD-O2D-CED
25	C	514	CLA	O1D-CGD-O2D-CED
25	c	504	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
25	c	514	CLA	O1D-CGD-O2D-CED
28	C	523	LMG	C29-C28-O8-C9
28	H	105	LMG	C29-C28-O8-C9
28	c	523	LMG	C29-C28-O8-C9
28	h	105	LMG	C29-C28-O8-C9
34	C	516	DGD	C2A-C1A-O1G-C1G
34	c	516	DGD	C2A-C1A-O1G-C1G
25	B	602	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	509	CLA	CBD-CGD-O2D-CED
25	b	602	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	509	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	O1A-CGA-O2A-C1
25	D	404	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
25	d	404	CLA	O1A-CGA-O2A-C1
33	B	627	LHG	O10-C23-O8-C6
33	b	627	LHG	O10-C23-O8-C6
25	C	514	CLA	C13-C15-C16-C17
25	c	514	CLA	C13-C15-C16-C17
25	C	507	CLA	O1D-CGD-O2D-CED
25	c	507	CLA	O1D-CGD-O2D-CED
25	D	403	CLA	CBD-CGD-O2D-CED
25	d	403	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	O1D-CGD-O2D-CED
30	C	501	SQD	O49-C7-O47-C45
30	c	501	SQD	O49-C7-O47-C45
33	B	627	LHG	O9-C7-O7-C5
33	b	627	LHG	O9-C7-O7-C5
25	B	604	CLA	C3-C5-C6-C7
25	B	614	CLA	C3-C5-C6-C7
25	b	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	C3-C5-C6-C7
25	D	404	CLA	CBA-CGA-O2A-C1
25	d	404	CLA	CBA-CGA-O2A-C1
28	A	410	LMG	C29-C28-O8-C9
28	a	410	LMG	C29-C28-O8-C9
30	H	103	SQD	C24-C23-O48-C46
30	h	103	SQD	C24-C23-O48-C46
33	B	627	LHG	C24-C23-O8-C6
33	b	627	LHG	C24-C23-O8-C6
31	X	101	LMT	O5'-C5'-C6'-O6'
31	x	101	LMT	O5'-C5'-C6'-O6'
30	B	620	SQD	C8-C7-O47-C45
30	H	103	SQD	C8-C7-O47-C45
30	b	620	SQD	C8-C7-O47-C45
30	h	103	SQD	C8-C7-O47-C45
29	A	411	PL9	C47-C48-C49-C50
29	a	411	PL9	C47-C48-C49-C50
25	B	609	CLA	O1D-CGD-O2D-CED
25	C	513	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	O1D-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
31	B	626	LMT	O5'-C5'-C6'-O6'
31	b	626	LMT	O5'-C5'-C6'-O6'
31	I	102	LMT	O5'-C5'-C6'-O6'
31	i	102	LMT	O5'-C5'-C6'-O6'
25	A	408	CLA	C4-C3-C5-C6
25	a	408	CLA	C4-C3-C5-C6
29	A	411	PL9	C33-C34-C36-C37
29	a	411	PL9	C33-C34-C36-C37
25	B	606	CLA	C2A-CAA-CBA-CGA
25	D	401	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	d	401	CLA	C2A-CAA-CBA-CGA
28	A	410	LMG	C17-C18-C19-C20
28	A	410	LMG	C20-C21-C22-C23
28	C	519	LMG	C17-C18-C19-C20
28	C	519	LMG	C20-C21-C22-C23
28	C	519	LMG	C38-C39-C40-C41
28	C	523	LMG	C17-C18-C19-C20
28	C	523	LMG	C38-C39-C40-C41
28	D	409	LMG	C35-C36-C37-C38
28	a	410	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
28	a	410	LMG	C20-C21-C22-C23
28	c	519	LMG	C17-C18-C19-C20
28	c	519	LMG	C20-C21-C22-C23
28	c	519	LMG	C38-C39-C40-C41
28	c	523	LMG	C17-C18-C19-C20
28	c	523	LMG	C38-C39-C40-C41
28	d	409	LMG	C35-C36-C37-C38
30	B	620	SQD	C34-C35-C36-C37
30	b	620	SQD	C34-C35-C36-C37
34	C	517	DGD	C8B-C9B-CAB-CBB
34	C	517	DGD	CBB-CCB-CDB-CEB
34	C	518	DGD	C8A-C9A-CAA-CBA
34	C	518	DGD	C8B-C9B-CAB-CBB
34	H	104	DGD	CBB-CCB-CDB-CEB
34	c	517	DGD	C8B-C9B-CAB-CBB
34	c	517	DGD	CBB-CCB-CDB-CEB
34	c	518	DGD	C8A-C9A-CAA-CBA
34	c	518	DGD	C8B-C9B-CAB-CBB
34	h	104	DGD	CBB-CCB-CDB-CEB
25	B	602	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
25	C	506	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
28	A	414	LMG	C29-C28-O8-C9
28	a	414	LMG	C29-C28-O8-C9
34	C	518	DGD	C2A-C1A-O1G-C1G
31	K	105	LMT	C3'-C4'-O1B-C1B
31	k	105	LMT	C3'-C4'-O1B-C1B
25	B	605	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
29	A	411	PL9	C47-C48-C49-C51
29	a	411	PL9	C47-C48-C49-C51
29	A	411	PL9	C12-C13-C14-C15
29	a	411	PL9	C12-C13-C14-C15
25	D	404	CLA	O1D-CGD-O2D-CED
25	d	404	CLA	O1D-CGD-O2D-CED
29	A	411	PL9	C12-C13-C14-C16
29	a	411	PL9	C12-C13-C14-C16
25	C	510	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	A	415	LMT	O5B-C5B-C6B-O6B
31	B	629	LMT	O5'-C5'-C6'-O6'
31	C	522	LMT	O5'-C5'-C6'-O6'
31	a	415	LMT	O5B-C5B-C6B-O6B
31	b	629	LMT	O5'-C5'-C6'-O6'
31	c	522	LMT	O5'-C5'-C6'-O6'
25	B	611	CLA	CBD-CGD-O2D-CED
25	B	613	CLA	CBD-CGD-O2D-CED
25	b	611	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
26	D	402	PHO	C3-C5-C6-C7
26	d	402	PHO	C3-C5-C6-C7
25	C	510	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
30	B	620	SQD	C24-C23-O48-C46
30	b	620	SQD	C24-C23-O48-C46
33	B	628	LHG	C24-C23-O8-C6
33	b	628	LHG	C24-C23-O8-C6
34	c	518	DGD	C2A-C1A-O1G-C1G
25	C	506	CLA	O1A-CGA-O2A-C1
25	c	506	CLA	O1A-CGA-O2A-C1
28	A	414	LMG	O10-C28-O8-C9
28	a	414	LMG	O10-C28-O8-C9
33	B	628	LHG	O10-C23-O8-C6
33	b	628	LHG	O10-C23-O8-C6
31	C	525	LMT	C4'-C5'-C6'-O6'
31	c	525	LMT	C4'-C5'-C6'-O6'
25	C	511	CLA	O1D-CGD-O2D-CED
33	Z	102	LHG	C8-C7-O7-C5
33	z	102	LHG	C8-C7-O7-C5
25	c	511	CLA	O1D-CGD-O2D-CED
25	B	615	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
31	B	624	LMT	C4'-C5'-C6'-O6'
31	X	101	LMT	C4'-C5'-C6'-O6'
31	b	624	LMT	C4'-C5'-C6'-O6'
31	x	101	LMT	C4'-C5'-C6'-O6'
34	C	518	DGD	O1A-C1A-O1G-C1G
34	c	518	DGD	O1A-C1A-O1G-C1G
31	B	625	LMT	C4B-C5B-C6B-O6B
31	B	626	LMT	C4'-C5'-C6'-O6'
31	E	103	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
31	I	102	LMT	C4'-C5'-C6'-O6'
31	I	104	LMT	C4'-C5'-C6'-O6'
31	b	625	LMT	C4B-C5B-C6B-O6B
31	b	626	LMT	C4'-C5'-C6'-O6'
31	e	103	LMT	C4'-C5'-C6'-O6'
31	i	102	LMT	C4'-C5'-C6'-O6'
31	i	104	LMT	C4'-C5'-C6'-O6'
28	C	523	LMG	O6-C5-C6-O5
28	c	523	LMG	O6-C5-C6-O5
31	K	105	LMT	O5B-C5B-C6B-O6B
31	k	105	LMT	O5B-C5B-C6B-O6B
31	K	105	LMT	O5'-C5'-C6'-O6'
31	k	105	LMT	O5'-C5'-C6'-O6'
31	E	103	LMT	C4B-C5B-C6B-O6B
31	K	105	LMT	C4B-C5B-C6B-O6B
31	e	103	LMT	C4B-C5B-C6B-O6B
31	k	105	LMT	C4B-C5B-C6B-O6B
25	B	607	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	C2A-CAA-CBA-CGA
31	I	103	LMT	O5'-C5'-C6'-O6'
31	i	103	LMT	O5'-C5'-C6'-O6'
30	B	620	SQD	O10-C23-O48-C46
30	b	620	SQD	O10-C23-O48-C46
31	I	104	LMT	O5'-C1'-O1'-C1
31	M	101	LMT	O5'-C1'-O1'-C1
31	i	104	LMT	O5'-C1'-O1'-C1
31	m	101	LMT	O5'-C1'-O1'-C1
26	A	407	PHO	C3-C5-C6-C7
26	a	407	PHO	C3-C5-C6-C7
31	C	524	LMT	O5B-C5B-C6B-O6B
31	c	524	LMT	O5B-C5B-C6B-O6B
31	J	101	LMT	C4'-C5'-C6'-O6'
31	j	101	LMT	C4'-C5'-C6'-O6'
25	B	610	CLA	O1D-CGD-O2D-CED
31	A	415	LMT	C4B-C5B-C6B-O6B
31	a	415	LMT	C4B-C5B-C6B-O6B
31	b	629	LMT	C4'-C5'-C6'-O6'
25	B	606	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
25	b	610	CLA	O1D-CGD-O2D-CED
31	H	102	LMT	O5'-C5'-C6'-O6'
31	h	102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
33	Z	102	LHG	O9-C7-O7-C5
33	z	102	LHG	O9-C7-O7-C5
31	B	629	LMT	C4'-C5'-C6'-O6'
25	A	406	CLA	CBA-CGA-O2A-C1
25	B	605	CLA	CBA-CGA-O2A-C1
25	B	612	CLA	CBA-CGA-O2A-C1
25	B	616	CLA	CBA-CGA-O2A-C1
25	C	509	CLA	CBA-CGA-O2A-C1
25	a	406	CLA	CBA-CGA-O2A-C1
25	b	605	CLA	CBA-CGA-O2A-C1
25	b	612	CLA	CBA-CGA-O2A-C1
25	b	616	CLA	CBA-CGA-O2A-C1
25	c	509	CLA	CBA-CGA-O2A-C1
31	I	103	LMT	C4'-C5'-C6'-O6'
31	i	103	LMT	C4'-C5'-C6'-O6'
33	D	408	LHG	C10-C11-C12-C13
33	d	408	LHG	C10-C11-C12-C13
25	C	502	CLA	C15-C16-C17-C18
25	c	502	CLA	C15-C16-C17-C18
25	A	408	CLA	C5-C6-C7-C8
25	C	507	CLA	C13-C15-C16-C17
25	a	408	CLA	C5-C6-C7-C8
25	c	507	CLA	C13-C15-C16-C17
33	E	102	LHG	O2-C2-C3-O3
33	e	102	LHG	O2-C2-C3-O3
30	A	412	SQD	C2-C1-O6-C44
30	a	412	SQD	C2-C1-O6-C44
31	B	624	LMT	C2'-C1'-O1'-C1
31	D	411	LMT	C2'-C1'-O1'-C1
31	X	104	LMT	C2'-C1'-O1'-C1
31	b	624	LMT	C2'-C1'-O1'-C1
31	d	411	LMT	C2'-C1'-O1'-C1
31	x	104	LMT	C2'-C1'-O1'-C1
33	E	102	LHG	O7-C5-C6-O8
33	e	102	LHG	O7-C5-C6-O8
31	B	624	LMT	O5'-C5'-C6'-O6'
31	B	625	LMT	O5B-C5B-C6B-O6B
31	E	103	LMT	O5'-C5'-C6'-O6'
31	b	624	LMT	O5'-C5'-C6'-O6'
31	b	625	LMT	O5B-C5B-C6B-O6B
31	e	103	LMT	O5'-C5'-C6'-O6'
31	K	105	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
31	k	105	LMT	C4'-C5'-C6'-O6'
25	C	505	CLA	C11-C12-C13-C14
25	C	510	CLA	C6-C7-C8-C9
25	C	510	CLA	C11-C12-C13-C14
25	C	514	CLA	C6-C7-C8-C9
25	c	505	CLA	C11-C12-C13-C14
25	c	510	CLA	C6-C7-C8-C9
25	c	510	CLA	C11-C12-C13-C14
25	c	514	CLA	C6-C7-C8-C9
25	C	503	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
28	A	410	LMG	C8-C9-O8-C28
27	B	617	BCR	C37-C22-C23-C24
27	Z	101	BCR	C37-C22-C23-C24
27	b	617	BCR	C37-C22-C23-C24
27	z	101	BCR	C37-C22-C23-C24
36	H	101	RRX	C36-C18-C19-C20
36	h	101	RRX	C36-C18-C19-C20
36	H	101	RRX	C17-C18-C19-C20
36	h	101	RRX	C17-C18-C19-C20
31	F	103	LMT	O5'-C5'-C6'-O6'
31	I	104	LMT	O5'-C5'-C6'-O6'
31	f	103	LMT	O5'-C5'-C6'-O6'
31	i	104	LMT	O5'-C5'-C6'-O6'
30	F	102	SQD	O49-C7-O47-C45
30	f	102	SQD	O49-C7-O47-C45
31	C	522	LMT	C4'-C5'-C6'-O6'
31	c	522	LMT	C4'-C5'-C6'-O6'
33	D	408	LHG	C7-C8-C9-C10
33	Z	102	LHG	C7-C8-C9-C10
33	d	408	LHG	C7-C8-C9-C10
33	z	102	LHG	C7-C8-C9-C10
25	B	612	CLA	O1A-CGA-O2A-C1
25	B	616	CLA	O1A-CGA-O2A-C1
25	C	509	CLA	O1A-CGA-O2A-C1
25	b	612	CLA	O1A-CGA-O2A-C1
25	b	616	CLA	O1A-CGA-O2A-C1
25	c	509	CLA	O1A-CGA-O2A-C1
31	I	101	LMT	O5'-C5'-C6'-O6'
31	i	101	LMT	O5'-C5'-C6'-O6'
25	b	602	CLA	O1D-CGD-O2D-CED
25	d	403	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	609	CLA	CBA-CGA-O2A-C1
25	b	609	CLA	CBA-CGA-O2A-C1
25	A	406	CLA	C15-C16-C17-C18
25	B	611	CLA	C15-C16-C17-C18
25	C	507	CLA	C15-C16-C17-C18
25	C	508	CLA	C15-C16-C17-C18
25	D	403	CLA	C15-C16-C17-C18
25	D	404	CLA	C13-C15-C16-C17
25	a	406	CLA	C15-C16-C17-C18
25	b	611	CLA	C15-C16-C17-C18
25	c	507	CLA	C15-C16-C17-C18
25	c	508	CLA	C15-C16-C17-C18
25	d	403	CLA	C15-C16-C17-C18
25	d	404	CLA	C13-C15-C16-C17
30	K	101	SQD	C7-C8-C9-C10
30	k	101	SQD	C7-C8-C9-C10
25	B	602	CLA	O1D-CGD-O2D-CED
25	D	403	CLA	O1D-CGD-O2D-CED
25	B	602	CLA	C15-C16-C17-C18
25	B	611	CLA	C13-C15-C16-C17
25	B	614	CLA	C8-C10-C11-C12
25	C	514	CLA	C15-C16-C17-C18
25	b	602	CLA	C15-C16-C17-C18
25	b	611	CLA	C13-C15-C16-C17
25	b	614	CLA	C8-C10-C11-C12
25	c	514	CLA	C15-C16-C17-C18
33	D	406	LHG	O1-C1-C2-O2
33	d	406	LHG	O1-C1-C2-O2
33	D	406	LHG	C23-C24-C25-C26
33	E	102	LHG	C7-C8-C9-C10
33	d	406	LHG	C23-C24-C25-C26
33	e	102	LHG	C7-C8-C9-C10
28	D	409	LMG	O6-C5-C6-O5
28	d	409	LMG	O6-C5-C6-O5
25	C	509	CLA	O1D-CGD-O2D-CED
25	c	509	CLA	O1D-CGD-O2D-CED
25	C	514	CLA	C10-C11-C12-C13
25	D	401	CLA	C15-C16-C17-C18
25	c	514	CLA	C10-C11-C12-C13
25	d	401	CLA	C15-C16-C17-C18
25	B	607	CLA	CBA-CGA-O2A-C1
25	b	607	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	a	410	LMG	C8-C9-O8-C28
31	Y	101	LMT	O1'-C1-C2-C3
31	y	101	LMT	O1'-C1-C2-C3
33	E	102	LHG	C25-C26-C27-C28
33	e	102	LHG	C25-C26-C27-C28
25	A	406	CLA	C2-C1-O2A-CGA
25	B	612	CLA	C2-C1-O2A-CGA
25	a	406	CLA	C2-C1-O2A-CGA
25	b	612	CLA	C2-C1-O2A-CGA
25	B	608	CLA	C15-C16-C17-C18
25	C	511	CLA	C13-C15-C16-C17
25	b	608	CLA	C15-C16-C17-C18
25	c	511	CLA	C13-C15-C16-C17
28	H	105	LMG	C28-C29-C30-C31
28	h	105	LMG	C28-C29-C30-C31
30	A	412	SQD	C23-C24-C25-C26
30	a	412	SQD	C23-C24-C25-C26
33	D	408	LHG	C23-C24-C25-C26
33	Z	102	LHG	C23-C24-C25-C26
33	d	408	LHG	C23-C24-C25-C26
33	z	102	LHG	C23-C24-C25-C26
31	D	412	LMT	O5'-C5'-C6'-O6'
31	d	412	LMT	O5'-C5'-C6'-O6'
25	C	505	CLA	C15-C16-C17-C18
25	c	505	CLA	C15-C16-C17-C18
25	B	605	CLA	O1A-CGA-O2A-C1
25	B	609	CLA	O1A-CGA-O2A-C1
25	b	605	CLA	O1A-CGA-O2A-C1
25	b	609	CLA	O1A-CGA-O2A-C1
31	X	105	LMT	O1'-C1-C2-C3
31	x	105	LMT	O1'-C1-C2-C3
33	B	627	LHG	C7-C8-C9-C10
33	b	627	LHG	C7-C8-C9-C10
25	B	609	CLA	C13-C15-C16-C17
25	B	613	CLA	C10-C11-C12-C13
25	C	512	CLA	C15-C16-C17-C18
25	b	609	CLA	C13-C15-C16-C17
25	b	613	CLA	C10-C11-C12-C13
25	c	512	CLA	C15-C16-C17-C18
31	C	525	LMT	O5'-C5'-C6'-O6'
31	H	102	LMT	O1'-C1-C2-C3
31	h	102	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	D	410	LMT	C4'-C5'-C6'-O6'
31	d	410	LMT	C4'-C5'-C6'-O6'
31	c	525	LMT	O5'-C5'-C6'-O6'
29	A	411	PL9	C9-C11-C12-C13
29	a	411	PL9	C9-C11-C12-C13
31	T	101	LMT	O1'-C1-C2-C3
31	t	101	LMT	O1'-C1-C2-C3
27	A	409	BCR	C10-C11-C12-C13
27	B	619	BCR	C10-C11-C12-C13
27	F	101	BCR	C10-C11-C12-C13
27	Z	101	BCR	C10-C11-C12-C13
27	a	409	BCR	C10-C11-C12-C13
27	b	619	BCR	C10-C11-C12-C13
27	f	101	BCR	C10-C11-C12-C13
27	z	101	BCR	C10-C11-C12-C13
36	H	101	RRX	C10-C11-C12-C13
36	h	101	RRX	C10-C11-C12-C13
31	A	416	LMT	O1'-C1-C2-C3
31	a	416	LMT	O1'-C1-C2-C3
31	F	103	LMT	O5B-C5B-C6B-O6B
31	I	103	LMT	O5B-C5B-C6B-O6B
31	f	103	LMT	O5B-C5B-C6B-O6B
31	i	103	LMT	O5B-C5B-C6B-O6B
33	B	627	LHG	O2-C2-C3-O3
33	b	627	LHG	O2-C2-C3-O3
25	A	408	CLA	C3-C5-C6-C7
25	a	408	CLA	C3-C5-C6-C7
25	A	405	CLA	C15-C16-C17-C18
25	C	504	CLA	C15-C16-C17-C18
25	D	404	CLA	C15-C16-C17-C18
25	a	405	CLA	C15-C16-C17-C18
25	a	406	CLA	C13-C15-C16-C17
25	c	504	CLA	C15-C16-C17-C18
25	d	404	CLA	C15-C16-C17-C18
25	C	505	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
25	A	406	CLA	O1A-CGA-O2A-C1
25	B	607	CLA	O1A-CGA-O2A-C1
25	a	406	CLA	O1A-CGA-O2A-C1
25	b	607	CLA	O1A-CGA-O2A-C1
31	D	412	LMT	C4'-C5'-C6'-O6'
31	d	412	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
25	A	406	CLA	C13-C15-C16-C17
25	B	611	CLA	C8-C10-C11-C12
25	C	503	CLA	C13-C15-C16-C17
25	b	611	CLA	C8-C10-C11-C12
25	c	503	CLA	C13-C15-C16-C17
33	D	406	LHG	C8-C7-O7-C5
33	d	406	LHG	C8-C7-O7-C5
25	B	604	CLA	C8-C10-C11-C12
25	C	508	CLA	C13-C15-C16-C17
25	C	512	CLA	C10-C11-C12-C13
25	C	514	CLA	C5-C6-C7-C8
25	b	604	CLA	C8-C10-C11-C12
25	c	512	CLA	C10-C11-C12-C13
25	c	514	CLA	C5-C6-C7-C8
33	B	627	LHG	C3-O3-P-O6
33	B	627	LHG	C4-O6-P-O3
33	B	628	LHG	C4-O6-P-O3
33	D	407	LHG	C4-O6-P-O3
33	E	102	LHG	C4-O6-P-O3
33	b	627	LHG	C3-O3-P-O6
33	b	627	LHG	C4-O6-P-O3
33	b	628	LHG	C4-O6-P-O3
33	d	407	LHG	C4-O6-P-O3
33	e	102	LHG	C4-O6-P-O3
25	c	508	CLA	C13-C15-C16-C17
31	D	410	LMT	O5'-C5'-C6'-O6'
31	d	410	LMT	O5'-C5'-C6'-O6'
33	D	406	LHG	O9-C7-O7-C5
33	d	406	LHG	O9-C7-O7-C5
31	B	629	LMT	O1'-C1-C2-C3
31	b	629	LMT	O1'-C1-C2-C3
25	A	405	CLA	C16-C17-C18-C20
25	a	405	CLA	C16-C17-C18-C20
25	B	616	CLA	C3-C5-C6-C7
25	b	616	CLA	C3-C5-C6-C7
25	C	514	CLA	CBA-CGA-O2A-C1
25	c	514	CLA	CBA-CGA-O2A-C1
30	C	501	SQD	C8-C7-O47-C45
30	c	501	SQD	C8-C7-O47-C45
28	C	519	LMG	C34-C35-C36-C37
28	c	519	LMG	C34-C35-C36-C37
28	h	105	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	A	412	SQD	C11-C10-C9-C8
30	H	103	SQD	C15-C16-C17-C18
30	a	412	SQD	C11-C10-C9-C8
30	h	103	SQD	C15-C16-C17-C18
31	B	623	LMT	C5-C6-C7-C8
31	M	101	LMT	C11-C10-C9-C8
31	b	623	LMT	C5-C6-C7-C8
31	m	101	LMT	C11-C10-C9-C8
33	E	102	LHG	C14-C15-C16-C17
33	e	102	LHG	C14-C15-C16-C17
25	A	406	CLA	C16-C17-C18-C20
25	A	408	CLA	C11-C12-C13-C15
25	B	616	CLA	C11-C12-C13-C15
25	C	505	CLA	C16-C17-C18-C20
25	a	406	CLA	C16-C17-C18-C20
25	a	408	CLA	C11-C12-C13-C15
25	b	616	CLA	C11-C12-C13-C15
25	c	505	CLA	C16-C17-C18-C20
28	C	519	LMG	C39-C40-C41-C42
28	H	105	LMG	C11-C12-C13-C14
28	c	519	LMG	C39-C40-C41-C42
30	K	101	SQD	C26-C27-C28-C29
30	k	101	SQD	C26-C27-C28-C29
31	I	102	LMT	C7-C8-C9-C10
31	T	101	LMT	C11-C10-C9-C8
31	X	103	LMT	C5-C6-C7-C8
31	i	102	LMT	C7-C8-C9-C10
31	t	101	LMT	C11-C10-C9-C8
31	x	103	LMT	C5-C6-C7-C8
33	Z	102	LHG	C29-C30-C31-C32
33	z	102	LHG	C29-C30-C31-C32
34	C	516	DGD	CAA-CBA-CCA-CDA
34	c	516	DGD	CAA-CBA-CCA-CDA
25	B	616	CLA	C10-C11-C12-C13
25	C	506	CLA	C5-C6-C7-C8
25	b	616	CLA	C10-C11-C12-C13
30	A	413	SQD	C9-C10-C11-C12
30	C	501	SQD	C25-C26-C27-C28
30	a	413	SQD	C9-C10-C11-C12
30	c	501	SQD	C25-C26-C27-C28
31	I	104	LMT	C2-C3-C4-C5
31	J	101	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	K	105	LMT	C3-C4-C5-C6
31	i	104	LMT	C2-C3-C4-C5
31	j	101	LMT	C4-C5-C6-C7
31	k	105	LMT	C3-C4-C5-C6
28	C	519	LMG	C33-C34-C35-C36
28	H	105	LMG	C13-C14-C15-C16
28	c	519	LMG	C33-C34-C35-C36
28	h	105	LMG	C13-C14-C15-C16
33	B	627	LHG	C18-C19-C20-C21
33	D	407	LHG	C13-C14-C15-C16
33	D	408	LHG	C9-C10-C11-C12
33	b	627	LHG	C18-C19-C20-C21
33	d	407	LHG	C13-C14-C15-C16
33	d	408	LHG	C9-C10-C11-C12
34	C	518	DGD	C9B-CAB-CBB-CCB
34	c	518	DGD	C9B-CAB-CBB-CCB
25	B	611	CLA	O1D-CGD-O2D-CED
25	b	611	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	C5-C6-C7-C8
35	E	104	HEM	C3D-CAD-CBD-CGD
35	e	104	HEM	C3D-CAD-CBD-CGD
31	I	102	LMT	O1'-C1-C2-C3
31	i	102	LMT	O1'-C1-C2-C3
34	H	104	DGD	C4A-C5A-C6A-C7A
34	h	104	DGD	C4A-C5A-C6A-C7A
30	F	102	SQD	C7-C8-C9-C10
30	f	102	SQD	C7-C8-C9-C10
31	B	623	LMT	C2'-C1'-O1'-C1
31	C	525	LMT	C2'-C1'-O1'-C1
31	M	101	LMT	C2'-C1'-O1'-C1
31	b	623	LMT	C2'-C1'-O1'-C1
31	c	525	LMT	C2'-C1'-O1'-C1
31	m	101	LMT	C2'-C1'-O1'-C1
25	C	507	CLA	CBA-CGA-O2A-C1
25	c	507	CLA	CBA-CGA-O2A-C1
28	A	410	LMG	C32-C33-C34-C35
28	a	410	LMG	C32-C33-C34-C35
31	C	525	LMT	C5-C6-C7-C8
31	J	101	LMT	C7-C8-C9-C10
31	c	525	LMT	C5-C6-C7-C8
31	j	101	LMT	C7-C8-C9-C10
33	B	628	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
33	b	628	LHG	C27-C28-C29-C30
25	A	406	CLA	C16-C17-C18-C19
25	B	610	CLA	C16-C17-C18-C20
25	a	406	CLA	C16-C17-C18-C19
25	b	610	CLA	C16-C17-C18-C20
31	A	416	LMT	O5'-C5'-C6'-O6'
31	a	416	LMT	O5'-C5'-C6'-O6'
31	H	102	LMT	C6-C7-C8-C9
31	X	102	LMT	C5-C6-C7-C8
31	h	102	LMT	C6-C7-C8-C9
31	x	102	LMT	C5-C6-C7-C8
33	B	628	LHG	C13-C14-C15-C16
33	D	406	LHG	C28-C29-C30-C31
33	D	407	LHG	C24-C25-C26-C27
33	b	628	LHG	C13-C14-C15-C16
33	d	406	LHG	C28-C29-C30-C31
33	d	407	LHG	C24-C25-C26-C27
25	B	613	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
30	B	620	SQD	C31-C32-C33-C34
30	b	620	SQD	C31-C32-C33-C34
31	X	102	LMT	C4-C5-C6-C7
31	x	102	LMT	C4-C5-C6-C7
25	C	509	CLA	C8-C10-C11-C12
25	C	511	CLA	C8-C10-C11-C12
25	c	509	CLA	C8-C10-C11-C12
25	c	511	CLA	C8-C10-C11-C12
25	C	508	CLA	C2A-CAA-CBA-CGA
25	c	508	CLA	C2A-CAA-CBA-CGA
31	I	104	LMT	C5-C6-C7-C8
31	J	101	LMT	C6-C7-C8-C9
31	i	104	LMT	C5-C6-C7-C8
31	i	104	LMT	C6-C7-C8-C9
31	j	101	LMT	C6-C7-C8-C9
34	H	104	DGD	CCB-CDB-CEB-CFB
34	h	104	DGD	CCB-CDB-CEB-CFB
33	D	408	LHG	O1-C1-C2-C3
33	E	102	LHG	O1-C1-C2-C3
33	d	408	LHG	O1-C1-C2-C3
33	e	102	LHG	O1-C1-C2-C3
31	K	105	LMT	C1-C2-C3-C4
31	k	105	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
30	B	620	SQD	C32-C33-C34-C35
30	K	101	SQD	C12-C13-C14-C15
30	b	620	SQD	C32-C33-C34-C35
31	I	104	LMT	C6-C7-C8-C9
33	D	407	LHG	C26-C27-C28-C29
33	d	407	LHG	C26-C27-C28-C29
28	A	414	LMG	C28-C29-C30-C31
28	a	414	LMG	C28-C29-C30-C31
30	k	101	SQD	C12-C13-C14-C15
31	C	522	LMT	C4-C5-C6-C7
31	F	103	LMT	C11-C10-C9-C8
31	I	101	LMT	C11-C10-C9-C8
31	Y	101	LMT	C5-C6-C7-C8
31	c	522	LMT	C4-C5-C6-C7
31	f	103	LMT	C11-C10-C9-C8
31	i	101	LMT	C11-C10-C9-C8
31	y	101	LMT	C5-C6-C7-C8
33	B	627	LHG	C15-C16-C17-C18
33	D	406	LHG	C13-C14-C15-C16
33	b	627	LHG	C15-C16-C17-C18
33	d	406	LHG	C13-C14-C15-C16
34	H	104	DGD	C7B-C8B-C9B-CAB
34	h	104	DGD	C7B-C8B-C9B-CAB
31	M	102	LMT	O5'-C5'-C6'-O6'
31	m	102	LMT	O5'-C5'-C6'-O6'
25	A	408	CLA	C11-C12-C13-C14
25	a	408	CLA	C11-C12-C13-C14
33	B	628	LHG	C5-C6-O8-C23
33	b	628	LHG	C5-C6-O8-C23
31	B	623	LMT	O5'-C1'-O1'-C1
31	b	623	LMT	O5'-C1'-O1'-C1
28	B	621	LMG	C33-C34-C35-C36
28	b	621	LMG	C33-C34-C35-C36
33	D	408	LHG	C33-C34-C35-C36
33	Z	102	LHG	C30-C31-C32-C33
33	d	408	LHG	C33-C34-C35-C36
33	z	102	LHG	C30-C31-C32-C33
31	D	411	LMT	C1-C2-C3-C4
31	E	103	LMT	C1-C2-C3-C4
31	d	411	LMT	C1-C2-C3-C4
31	e	103	LMT	C1-C2-C3-C4
31	x	101	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
28	A	410	LMG	C12-C13-C14-C15
28	D	409	LMG	C32-C33-C34-C35
28	D	409	LMG	C34-C35-C36-C37
28	D	409	LMG	C37-C38-C39-C40
28	a	410	LMG	C12-C13-C14-C15
28	d	409	LMG	C32-C33-C34-C35
28	d	409	LMG	C34-C35-C36-C37
28	d	409	LMG	C36-C37-C38-C39
28	d	409	LMG	C37-C38-C39-C40
31	M	101	LMT	C4-C5-C6-C7
31	X	103	LMT	C4-C5-C6-C7
31	m	101	LMT	C4-C5-C6-C7
31	x	103	LMT	C4-C5-C6-C7
34	C	518	DGD	C7A-C8A-C9A-CAA
34	c	518	DGD	C7A-C8A-C9A-CAA
28	D	409	LMG	C36-C37-C38-C39
31	B	626	LMT	C2-C3-C4-C5
31	b	626	LMT	C2-C3-C4-C5
31	X	101	LMT	C1-C2-C3-C4
31	M	101	LMT	O5'-C5'-C6'-O6'
31	m	101	LMT	O5'-C5'-C6'-O6'
30	A	413	SQD	C26-C27-C28-C29
30	C	501	SQD	C17-C18-C19-C20
30	a	413	SQD	C26-C27-C28-C29
30	c	501	SQD	C17-C18-C19-C20
33	D	408	LHG	C32-C33-C34-C35
33	d	408	LHG	C32-C33-C34-C35
25	B	615	CLA	O1D-CGD-O2D-CED
25	b	615	CLA	O1D-CGD-O2D-CED
25	B	603	CLA	C5-C6-C7-C8
25	b	603	CLA	C5-C6-C7-C8
31	B	623	LMT	C2-C1-O1'-C1'
31	B	624	LMT	C2-C1-O1'-C1'
31	J	101	LMT	C2-C1-O1'-C1'
31	b	623	LMT	C2-C1-O1'-C1'
31	b	624	LMT	C2-C1-O1'-C1'
31	j	101	LMT	C2-C1-O1'-C1'
28	H	105	LMG	C30-C31-C32-C33
28	h	105	LMG	C30-C31-C32-C33
30	A	413	SQD	C12-C13-C14-C15
30	F	102	SQD	C9-C10-C11-C12
30	a	413	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	f	102	SQD	C9-C10-C11-C12
31	B	629	LMT	C4-C5-C6-C7
31	K	105	LMT	C2-C3-C4-C5
31	b	629	LMT	C4-C5-C6-C7
31	k	105	LMT	C2-C3-C4-C5
33	D	408	LHG	C28-C29-C30-C31
33	d	408	LHG	C28-C29-C30-C31
34	C	516	DGD	C4B-C5B-C6B-C7B
34	c	516	DGD	C4B-C5B-C6B-C7B
30	F	102	SQD	O10-C23-O48-C46
30	f	102	SQD	O10-C23-O48-C46
25	B	610	CLA	C16-C17-C18-C19
25	B	616	CLA	C11-C12-C13-C14
25	C	505	CLA	C16-C17-C18-C19
25	b	610	CLA	C16-C17-C18-C19
25	b	616	CLA	C11-C12-C13-C14
25	c	505	CLA	C16-C17-C18-C19
30	C	501	SQD	C14-C15-C16-C17
30	C	501	SQD	C29-C30-C31-C32
30	c	501	SQD	C29-C30-C31-C32
31	B	625	LMT	C2-C3-C4-C5
31	B	629	LMT	C6-C7-C8-C9
31	E	103	LMT	C2-C3-C4-C5
31	F	103	LMT	C3-C4-C5-C6
31	Y	101	LMT	C4-C5-C6-C7
31	e	103	LMT	C2-C3-C4-C5
31	f	103	LMT	C3-C4-C5-C6
31	x	102	LMT	C6-C7-C8-C9
31	y	101	LMT	C4-C5-C6-C7
30	c	501	SQD	C14-C15-C16-C17
31	B	626	LMT	C11-C10-C9-C8
31	X	102	LMT	C6-C7-C8-C9
31	b	625	LMT	C2-C3-C4-C5
31	b	626	LMT	C11-C10-C9-C8
31	b	629	LMT	C6-C7-C8-C9
36	H	101	RRX	C14-C15-C16-C17
36	h	101	RRX	C14-C15-C16-C17
25	C	506	CLA	C4-C3-C5-C6
25	c	506	CLA	C4-C3-C5-C6
25	C	511	CLA	CBA-CGA-O2A-C1
25	c	511	CLA	CBA-CGA-O2A-C1
25	a	408	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	D	405	PL9	C13-C14-C16-C17
29	d	405	PL9	C13-C14-C16-C17
31	X	104	LMT	C1-C2-C3-C4
28	C	523	LMG	C4-C5-C6-O5
28	c	523	LMG	C4-C5-C6-O5
33	D	407	LHG	O1-C1-C2-O2
33	d	407	LHG	O1-C1-C2-O2
31	D	411	LMT	C2-C3-C4-C5
31	d	411	LMT	C2-C3-C4-C5
33	D	407	LHG	C11-C12-C13-C14
33	d	407	LHG	C11-C12-C13-C14
25	C	505	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
31	B	623	LMT	C3-C4-C5-C6
31	b	623	LMT	C3-C4-C5-C6
34	C	517	DGD	CAA-CBA-CCA-CDA
31	x	104	LMT	C1-C2-C3-C4
28	C	523	LMG	C13-C14-C15-C16
28	c	523	LMG	C13-C14-C15-C16
30	H	103	SQD	C14-C15-C16-C17
30	h	103	SQD	C14-C15-C16-C17
34	c	517	DGD	CAA-CBA-CCA-CDA
31	M	101	LMT	C1-C2-C3-C4
31	m	101	LMT	C1-C2-C3-C4
30	K	101	SQD	C24-C23-O48-C46
30	k	101	SQD	C24-C23-O48-C46
33	b	628	LHG	C11-C10-C9-C8
25	C	514	CLA	O1A-CGA-O2A-C1
25	c	514	CLA	O1A-CGA-O2A-C1
28	A	410	LMG	C28-C29-C30-C31
28	a	410	LMG	C28-C29-C30-C31
30	A	412	SQD	C12-C13-C14-C15
30	A	413	SQD	C28-C29-C30-C31
30	a	412	SQD	C12-C13-C14-C15
30	a	413	SQD	C28-C29-C30-C31
31	B	623	LMT	C6-C7-C8-C9
31	B	623	LMT	C7-C8-C9-C10
31	b	623	LMT	C6-C7-C8-C9
33	B	628	LHG	C11-C10-C9-C8
30	A	413	SQD	O49-C7-O47-C45
30	a	413	SQD	O49-C7-O47-C45
25	C	503	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	C	508	CLA	C2-C1-O2A-CGA
25	c	503	CLA	C2-C1-O2A-CGA
25	c	508	CLA	C2-C1-O2A-CGA
28	D	409	LMG	C31-C32-C33-C34
28	d	409	LMG	C31-C32-C33-C34
30	A	413	SQD	C11-C10-C9-C8
30	A	413	SQD	C14-C15-C16-C17
30	a	413	SQD	C11-C10-C9-C8
30	a	413	SQD	C14-C15-C16-C17
31	b	623	LMT	C7-C8-C9-C10
33	Z	102	LHG	C10-C11-C12-C13
33	z	102	LHG	C10-C11-C12-C13
34	C	518	DGD	C3A-C4A-C5A-C6A
34	c	518	DGD	C3A-C4A-C5A-C6A
25	C	507	CLA	O1A-CGA-O2A-C1
25	c	507	CLA	O1A-CGA-O2A-C1
31	C	524	LMT	C1-C2-C3-C4
31	Y	101	LMT	C1-C2-C3-C4
31	c	524	LMT	C1-C2-C3-C4
31	y	101	LMT	C1-C2-C3-C4
30	B	620	SQD	C9-C10-C11-C12
33	D	407	LHG	C33-C34-C35-C36
33	D	407	LHG	C34-C35-C36-C37
33	d	407	LHG	C33-C34-C35-C36
33	d	407	LHG	C34-C35-C36-C37
28	B	621	LMG	C10-C11-C12-C13
28	b	621	LMG	C10-C11-C12-C13
30	C	501	SQD	C7-C8-C9-C10
30	c	501	SQD	C7-C8-C9-C10
27	B	617	BCR	C1-C6-C7-C8
27	B	617	BCR	C5-C6-C7-C8
27	B	619	BCR	C5-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C26
27	B	619	BCR	C23-C24-C25-C30
27	C	515	BCR	C23-C24-C25-C26
27	C	515	BCR	C23-C24-C25-C30
27	F	101	BCR	C5-C6-C7-C8
27	K	102	BCR	C1-C6-C7-C8
27	K	102	BCR	C23-C24-C25-C26
27	Z	101	BCR	C23-C24-C25-C26
27	Z	101	BCR	C23-C24-C25-C30
27	b	617	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	b	617	BCR	C5-C6-C7-C8
27	b	619	BCR	C5-C6-C7-C8
27	b	619	BCR	C23-C24-C25-C26
27	b	619	BCR	C23-C24-C25-C30
27	c	515	BCR	C23-C24-C25-C26
27	c	515	BCR	C23-C24-C25-C30
27	f	101	BCR	C5-C6-C7-C8
27	k	102	BCR	C1-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C26
27	z	101	BCR	C23-C24-C25-C26
27	z	101	BCR	C23-C24-C25-C30
30	b	620	SQD	C9-C10-C11-C12
31	C	524	LMT	C4-C5-C6-C7
33	Z	102	LHG	C26-C27-C28-C29
33	z	102	LHG	C26-C27-C28-C29
28	H	105	LMG	C11-C10-O7-C8
28	h	105	LMG	C11-C10-O7-C8
31	D	410	LMT	C3-C4-C5-C6
31	c	524	LMT	C4-C5-C6-C7
31	d	410	LMT	C3-C4-C5-C6
30	B	620	SQD	C26-C27-C28-C29
30	F	102	SQD	C11-C10-C9-C8
30	b	620	SQD	C26-C27-C28-C29
30	f	102	SQD	C11-C10-C9-C8
33	D	406	LHG	C16-C17-C18-C19
33	d	406	LHG	C16-C17-C18-C19
25	C	509	CLA	C13-C15-C16-C17
25	C	510	CLA	C10-C11-C12-C13
25	c	510	CLA	C10-C11-C12-C13
28	B	621	LMG	C16-C17-C18-C19
28	b	621	LMG	C16-C17-C18-C19
31	a	415	LMT	C4-C5-C6-C7
25	A	408	CLA	C2-C3-C5-C6
25	B	615	CLA	C11-C12-C13-C15
25	C	503	CLA	C11-C12-C13-C15
25	C	505	CLA	C11-C12-C13-C15
25	C	506	CLA	C2-C3-C5-C6
25	C	507	CLA	C12-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C15
25	c	503	CLA	C11-C12-C13-C15
25	c	505	CLA	C11-C12-C13-C15
25	c	506	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	c	507	CLA	C12-C13-C15-C16
29	D	405	PL9	C28-C29-C31-C32
29	d	405	PL9	C28-C29-C31-C32
25	C	511	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
31	A	415	LMT	C4-C5-C6-C7
31	C	525	LMT	O1'-C1-C2-C3
31	c	525	LMT	O1'-C1-C2-C3
25	c	509	CLA	C13-C15-C16-C17
28	C	523	LMG	O9-C10-O7-C8
28	c	523	LMG	O9-C10-O7-C8
25	B	601	CLA	C2A-CAA-CBA-CGA
25	C	502	CLA	C2A-CAA-CBA-CGA
25	b	601	CLA	C2A-CAA-CBA-CGA
25	c	502	CLA	C2A-CAA-CBA-CGA
31	C	524	LMT	O1'-C1-C2-C3
31	I	104	LMT	C3-C4-C5-C6
31	c	524	LMT	O1'-C1-C2-C3
31	i	104	LMT	C3-C4-C5-C6
30	A	412	SQD	C7-C8-C9-C10
30	a	412	SQD	C7-C8-C9-C10
25	B	604	CLA	C5-C6-C7-C8
25	b	604	CLA	C5-C6-C7-C8
31	D	411	LMT	C11-C10-C9-C8
31	I	102	LMT	C2-C3-C4-C5
31	X	102	LMT	O1'-C1-C2-C3
31	d	411	LMT	C11-C10-C9-C8
31	i	102	LMT	C2-C3-C4-C5
31	x	102	LMT	O1'-C1-C2-C3
31	B	625	LMT	O1'-C1-C2-C3
31	b	625	LMT	O1'-C1-C2-C3
31	C	525	LMT	O5'-C1'-O1'-C1
31	c	525	LMT	O5'-C1'-O1'-C1
34	C	516	DGD	O6E-C1E-O5D-C6D
34	C	517	DGD	O6E-C1E-O5D-C6D
34	c	516	DGD	O6E-C1E-O5D-C6D
34	c	517	DGD	O6E-C1E-O5D-C6D
28	A	410	LMG	C21-C22-C23-C24
28	a	410	LMG	C21-C22-C23-C24
30	C	501	SQD	C11-C10-C9-C8
30	c	501	SQD	C11-C10-C9-C8
33	D	408	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	b	627	LHG	C13-C14-C15-C16
33	d	408	LHG	C11-C12-C13-C14
28	C	523	LMG	C11-C10-O7-C8
28	c	523	LMG	C11-C10-O7-C8
30	F	102	SQD	C8-C7-O47-C45
30	f	102	SQD	C8-C7-O47-C45
33	E	102	LHG	C8-C7-O7-C5
33	e	102	LHG	C8-C7-O7-C5
31	K	105	LMT	C6-C7-C8-C9
31	k	105	LMT	C6-C7-C8-C9
33	B	627	LHG	C13-C14-C15-C16
34	C	518	DGD	C5B-C6B-C7B-C8B
34	c	518	DGD	C5B-C6B-C7B-C8B
25	B	603	CLA	C15-C16-C17-C18
25	B	609	CLA	C15-C16-C17-C18
25	b	603	CLA	C15-C16-C17-C18
25	b	609	CLA	C15-C16-C17-C18
30	B	620	SQD	C24-C25-C26-C27
30	b	620	SQD	C24-C25-C26-C27
31	B	624	LMT	C7-C8-C9-C10
31	b	624	LMT	C7-C8-C9-C10
31	A	416	LMT	C4'-C5'-C6'-O6'
31	a	416	LMT	C4'-C5'-C6'-O6'
31	E	101	LMT	O1'-C1-C2-C3
31	e	101	LMT	O1'-C1-C2-C3
31	A	415	LMT	C2'-C1'-O1'-C1
31	a	415	LMT	C2'-C1'-O1'-C1
34	C	517	DGD	C2E-C1E-O5D-C6D
34	c	517	DGD	C2E-C1E-O5D-C6D
30	A	412	SQD	C27-C28-C29-C30
30	a	412	SQD	C27-C28-C29-C30
33	Z	102	LHG	C11-C10-C9-C8
28	B	621	LMG	C28-C29-C30-C31
28	b	621	LMG	C28-C29-C30-C31
31	X	104	LMT	O1'-C1-C2-C3
31	x	104	LMT	O1'-C1-C2-C3
33	z	102	LHG	C11-C10-C9-C8
25	B	608	CLA	C11-C12-C13-C14
25	B	615	CLA	C11-C12-C13-C14
25	C	503	CLA	C11-C12-C13-C14
25	C	507	CLA	C14-C13-C15-C16
25	b	608	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	b	615	CLA	C11-C12-C13-C14
25	c	503	CLA	C11-C12-C13-C14
25	c	507	CLA	C14-C13-C15-C16
25	B	610	CLA	C2A-CAA-CBA-CGA
25	b	610	CLA	C2A-CAA-CBA-CGA
27	Z	101	BCR	C7-C8-C9-C10
27	z	101	BCR	C7-C8-C9-C10
25	A	408	CLA	C1A-C2A-CAA-CBA
25	B	603	CLA	C1A-C2A-CAA-CBA
25	B	605	CLA	C1A-C2A-CAA-CBA
25	B	606	CLA	C1A-C2A-CAA-CBA
25	B	609	CLA	C1A-C2A-CAA-CBA
25	C	502	CLA	C1A-C2A-CAA-CBA
25	C	507	CLA	C1A-C2A-CAA-CBA
25	C	509	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	C	514	CLA	C1A-C2A-CAA-CBA
25	D	404	CLA	C1A-C2A-CAA-CBA
25	a	408	CLA	C1A-C2A-CAA-CBA
25	b	603	CLA	C1A-C2A-CAA-CBA
25	b	605	CLA	C1A-C2A-CAA-CBA
25	b	606	CLA	C1A-C2A-CAA-CBA
25	b	609	CLA	C1A-C2A-CAA-CBA
25	c	502	CLA	C1A-C2A-CAA-CBA
25	c	507	CLA	C1A-C2A-CAA-CBA
25	c	509	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	514	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	C1A-C2A-CAA-CBA
34	C	516	DGD	O6E-C5E-C6E-O5E
34	c	516	DGD	O6E-C5E-C6E-O5E
26	A	407	PHO	C16-C17-C18-C20
26	a	407	PHO	C16-C17-C18-C20
28	H	105	LMG	O9-C10-O7-C8
28	h	105	LMG	O9-C10-O7-C8
33	E	102	LHG	O9-C7-O7-C5
33	e	102	LHG	O9-C7-O7-C5
31	Y	101	LMT	C2-C3-C4-C5
31	y	101	LMT	C2-C3-C4-C5
33	Z	102	LHG	C31-C32-C33-C34
33	z	102	LHG	C31-C32-C33-C34
27	K	102	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	k	102	BCR	C9-C10-C11-C12
25	B	607	CLA	C13-C15-C16-C17
25	B	612	CLA	C10-C11-C12-C13
25	B	616	CLA	C8-C10-C11-C12
25	b	607	CLA	C13-C15-C16-C17
25	b	612	CLA	C10-C11-C12-C13
25	b	616	CLA	C8-C10-C11-C12
31	A	416	LMT	C7-C8-C9-C10
31	a	416	LMT	C7-C8-C9-C10
31	D	411	LMT	O1'-C1-C2-C3
31	T	101	LMT	C3-C4-C5-C6
31	d	411	LMT	O1'-C1-C2-C3
31	t	101	LMT	C3-C4-C5-C6
31	C	525	LMT	C1-C2-C3-C4
31	c	525	LMT	C1-C2-C3-C4
25	C	512	CLA	C13-C15-C16-C17
25	c	512	CLA	C13-C15-C16-C17
33	B	627	LHG	O6-C4-C5-C6
33	b	627	LHG	O6-C4-C5-C6
31	D	412	LMT	C6-C7-C8-C9
31	K	105	LMT	C5'-C4'-O1B-C1B
31	d	412	LMT	C6-C7-C8-C9
31	k	105	LMT	C5'-C4'-O1B-C1B
33	E	102	LHG	C15-C16-C17-C18
33	e	102	LHG	C15-C16-C17-C18
30	K	101	SQD	C10-C11-C12-C13
30	k	101	SQD	C10-C11-C12-C13
34	C	518	DGD	C4A-C5A-C6A-C7A
34	c	518	DGD	C4A-C5A-C6A-C7A
33	b	627	LHG	C26-C27-C28-C29
33	B	627	LHG	C26-C27-C28-C29
26	D	402	PHO	CBD-CGD-O2D-CED
29	D	405	PL9	C15-C14-C16-C17
29	d	405	PL9	C15-C14-C16-C17
25	C	511	CLA	C15-C16-C17-C18
25	c	511	CLA	C15-C16-C17-C18
26	d	402	PHO	CBD-CGD-O2D-CED
30	H	103	SQD	C11-C12-C13-C14
30	h	103	SQD	C11-C12-C13-C14
30	h	103	SQD	C25-C26-C27-C28
33	E	102	LHG	C16-C17-C18-C19
33	e	102	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	A	410	LMG	C37-C38-C39-C40
28	a	410	LMG	C37-C38-C39-C40
30	H	103	SQD	C25-C26-C27-C28
33	D	406	LHG	C25-C26-C27-C28
33	d	406	LHG	C25-C26-C27-C28
30	A	412	SQD	O6-C44-C45-C46
30	C	501	SQD	C44-C45-C46-O48
30	a	412	SQD	O6-C44-C45-C46
30	c	501	SQD	C44-C45-C46-O48
31	I	101	LMT	C7-C8-C9-C10
31	Y	101	LMT	C6-C7-C8-C9
31	y	101	LMT	C6-C7-C8-C9
33	D	407	LHG	C4-C5-C6-O8
33	E	102	LHG	C4-C5-C6-O8
33	d	407	LHG	C4-C5-C6-O8
33	e	102	LHG	C4-C5-C6-O8
25	C	502	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	CBA-CGA-O2A-C1
31	i	101	LMT	C7-C8-C9-C10
33	Z	102	LHG	C11-C12-C13-C14
33	z	102	LHG	C11-C12-C13-C14
30	F	102	SQD	C45-C44-O6-C1
30	f	102	SQD	C45-C44-O6-C1
34	C	517	DGD	C5D-C6D-O5D-C1E
34	c	517	DGD	C5D-C6D-O5D-C1E
28	H	105	LMG	C8-C9-O8-C28
28	h	105	LMG	C8-C9-O8-C28
31	E	103	LMT	O5B-C5B-C6B-O6B
31	M	101	LMT	C9-C10-C11-C12
31	m	101	LMT	C9-C10-C11-C12
33	d	407	LHG	C35-C36-C37-C38
34	H	104	DGD	O2G-C1B-C2B-C3B
34	h	104	DGD	O2G-C1B-C2B-C3B
31	e	103	LMT	O5B-C5B-C6B-O6B
31	D	411	LMT	C6-C7-C8-C9
31	d	411	LMT	C6-C7-C8-C9
33	D	407	LHG	C35-C36-C37-C38
30	K	101	SQD	C27-C28-C29-C30
30	k	101	SQD	C27-C28-C29-C30
31	C	524	LMT	C3-C4-C5-C6
31	Y	101	LMT	C3-C4-C5-C6
31	c	524	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
31	y	101	LMT	C3-C4-C5-C6
34	h	104	DGD	CDA-CEA-CFA-CGA
30	H	103	SQD	C35-C36-C37-C38
30	h	103	SQD	C35-C36-C37-C38
33	D	406	LHG	C26-C27-C28-C29
34	C	518	DGD	CDA-CEA-CFA-CGA
34	H	104	DGD	CDA-CEA-CFA-CGA
34	c	518	DGD	CDA-CEA-CFA-CGA
31	T	101	LMT	O5'-C5'-C6'-O6'
31	t	101	LMT	O5'-C5'-C6'-O6'
33	d	406	LHG	C26-C27-C28-C29
34	C	517	DGD	C2B-C1B-O2G-C2G
34	c	517	DGD	C2B-C1B-O2G-C2G
31	A	415	LMT	O1'-C1-C2-C3
31	a	415	LMT	O1'-C1-C2-C3
33	E	102	LHG	C13-C14-C15-C16
33	e	102	LHG	C13-C14-C15-C16
28	A	414	LMG	O6-C5-C6-O5
28	a	414	LMG	O6-C5-C6-O5
31	B	623	LMT	O5B-C5B-C6B-O6B
31	b	623	LMT	O5B-C5B-C6B-O6B
25	B	609	CLA	C4-C3-C5-C6
25	b	609	CLA	C4-C3-C5-C6
30	F	102	SQD	C24-C23-O48-C46
30	f	102	SQD	C24-C23-O48-C46
30	B	620	SQD	C35-C36-C37-C38
30	b	620	SQD	C35-C36-C37-C38
25	B	615	CLA	C10-C11-C12-C13
25	b	615	CLA	C10-C11-C12-C13
30	K	101	SQD	C24-C25-C26-C27
30	k	101	SQD	C24-C25-C26-C27
31	C	524	LMT	C9-C10-C11-C12
31	c	524	LMT	C9-C10-C11-C12
30	A	413	SQD	C44-C45-O47-C7
30	C	501	SQD	C44-C45-O47-C7
30	a	413	SQD	C44-C45-O47-C7
30	c	501	SQD	C44-C45-O47-C7
25	B	610	CLA	C2-C1-O2A-CGA
25	B	615	CLA	C2-C1-O2A-CGA
25	C	502	CLA	C2-C1-O2A-CGA
25	C	513	CLA	C2-C1-O2A-CGA
25	C	514	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	b	610	CLA	C2-C1-O2A-CGA
25	b	615	CLA	C2-C1-O2A-CGA
25	c	502	CLA	C2-C1-O2A-CGA
25	c	513	CLA	C2-C1-O2A-CGA
25	c	514	CLA	C2-C1-O2A-CGA
33	B	627	LHG	C35-C36-C37-C38
33	b	627	LHG	C35-C36-C37-C38
31	X	104	LMT	O5'-C5'-C6'-O6'
31	x	104	LMT	O5'-C5'-C6'-O6'
33	Z	102	LHG	C4-O6-P-O5
33	z	102	LHG	C4-O6-P-O5
30	K	101	SQD	C14-C15-C16-C17
30	k	101	SQD	C14-C15-C16-C17
33	E	102	LHG	C9-C10-C11-C12
33	e	102	LHG	C9-C10-C11-C12
33	d	406	LHG	C24-C23-O8-C6
33	D	407	LHG	O6-C4-C5-O7
33	d	407	LHG	O6-C4-C5-O7
28	C	519	LMG	C22-C23-C24-C25
28	c	519	LMG	C22-C23-C24-C25
31	D	412	LMT	C11-C10-C9-C8
31	I	104	LMT	C7-C8-C9-C10
31	d	412	LMT	C11-C10-C9-C8
31	i	104	LMT	C7-C8-C9-C10
31	D	411	LMT	C4'-C5'-C6'-O6'
31	d	411	LMT	C4'-C5'-C6'-O6'
25	C	502	CLA	O1A-CGA-O2A-C1
25	c	502	CLA	O1A-CGA-O2A-C1
33	B	627	LHG	C23-C24-C25-C26
33	D	407	LHG	C7-C8-C9-C10
33	b	627	LHG	C23-C24-C25-C26
33	d	407	LHG	C7-C8-C9-C10
33	E	102	LHG	C12-C13-C14-C15
33	e	102	LHG	C12-C13-C14-C15
30	A	413	SQD	O47-C45-C46-O48
30	F	102	SQD	O6-C44-C45-O47
30	a	413	SQD	O47-C45-C46-O48
30	f	102	SQD	O6-C44-C45-O47
33	B	628	LHG	O7-C5-C6-O8
33	b	628	LHG	O7-C5-C6-O8
33	D	406	LHG	C24-C23-O8-C6
31	I	104	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	i	104	LMT	O1'-C1-C2-C3
33	B	627	LHG	C25-C26-C27-C28
33	b	627	LHG	C25-C26-C27-C28
34	C	516	DGD	O6D-C5D-C6D-O5D
34	c	516	DGD	O6D-C5D-C6D-O5D
25	A	408	CLA	C10-C11-C12-C13
25	B	604	CLA	C13-C15-C16-C17
25	a	408	CLA	C10-C11-C12-C13
25	b	604	CLA	C13-C15-C16-C17
33	B	627	LHG	C11-C12-C13-C14
33	b	627	LHG	C11-C12-C13-C14
25	B	616	CLA	C4-C3-C5-C6
25	b	616	CLA	C4-C3-C5-C6
26	A	407	PHO	C4-C3-C5-C6
26	a	407	PHO	C4-C3-C5-C6
33	B	627	LHG	C34-C35-C36-C37
25	B	602	CLA	C6-C7-C8-C10
25	B	608	CLA	C11-C12-C13-C15
25	B	609	CLA	C2-C3-C5-C6
25	B	616	CLA	C6-C7-C8-C10
25	B	616	CLA	C11-C10-C8-C7
25	C	510	CLA	C6-C7-C8-C10
25	b	602	CLA	C6-C7-C8-C10
25	b	608	CLA	C11-C12-C13-C15
25	b	609	CLA	C2-C3-C5-C6
25	b	616	CLA	C6-C7-C8-C10
25	b	616	CLA	C11-C10-C8-C7
25	c	510	CLA	C6-C7-C8-C10
26	A	407	PHO	C2-C3-C5-C6
26	a	407	PHO	C2-C3-C5-C6
30	A	413	SQD	C11-C12-C13-C14
30	a	413	SQD	C11-C12-C13-C14
33	b	627	LHG	C34-C35-C36-C37
25	A	408	CLA	C6-C7-C8-C9
25	B	602	CLA	C6-C7-C8-C9
25	B	603	CLA	C6-C7-C8-C9
25	B	616	CLA	C11-C10-C8-C9
25	C	514	CLA	C14-C13-C15-C16
25	a	408	CLA	C6-C7-C8-C9
25	b	602	CLA	C6-C7-C8-C9
25	b	603	CLA	C6-C7-C8-C9
25	b	616	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	514	CLA	C14-C13-C15-C16
25	B	611	CLA	CBA-CGA-O2A-C1
25	b	611	CLA	CBA-CGA-O2A-C1
25	B	602	CLA	C2A-CAA-CBA-CGA
25	C	504	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
25	c	504	CLA	C2A-CAA-CBA-CGA
33	D	408	LHG	C13-C14-C15-C16
33	d	408	LHG	C13-C14-C15-C16
27	B	619	BCR	C37-C22-C23-C24
27	Z	101	BCR	C7-C8-C9-C34
27	b	619	BCR	C37-C22-C23-C24
27	z	101	BCR	C7-C8-C9-C34
31	X	104	LMT	C2-C3-C4-C5
33	E	102	LHG	C18-C19-C20-C21
33	e	102	LHG	C18-C19-C20-C21
31	x	104	LMT	C2-C3-C4-C5
33	D	406	LHG	C11-C12-C13-C14
33	d	406	LHG	C11-C12-C13-C14
33	d	407	LHG	C11-C10-C9-C8
30	B	620	SQD	C10-C11-C12-C13
30	b	620	SQD	C10-C11-C12-C13
33	D	407	LHG	C11-C10-C9-C8
33	b	627	LHG	C30-C31-C32-C33
28	C	519	LMG	O6-C5-C6-O5
28	c	519	LMG	O6-C5-C6-O5
30	A	412	SQD	C14-C15-C16-C17
30	a	412	SQD	C14-C15-C16-C17
33	B	627	LHG	C30-C31-C32-C33
25	B	615	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19
31	H	102	LMT	C4'-C5'-C6'-O6'
31	h	102	LMT	C4'-C5'-C6'-O6'
25	C	514	CLA	C8-C10-C11-C12
25	c	514	CLA	C8-C10-C11-C12
33	B	628	LHG	O6-C4-C5-C6
33	D	407	LHG	O6-C4-C5-C6
33	b	628	LHG	O6-C4-C5-C6
33	d	407	LHG	O6-C4-C5-C6
25	A	405	CLA	C3-C5-C6-C7
25	a	405	CLA	C3-C5-C6-C7
30	b	620	SQD	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
31	B	625	LMT	C7-C8-C9-C10
31	b	625	LMT	C7-C8-C9-C10
25	D	403	CLA	C13-C15-C16-C17
25	d	403	CLA	C13-C15-C16-C17
30	B	620	SQD	C19-C20-C21-C22
25	C	514	CLA	C4-C3-C5-C6
25	c	514	CLA	C4-C3-C5-C6
25	B	616	CLA	C2-C3-C5-C6
25	b	616	CLA	C2-C3-C5-C6
30	h	103	SQD	C34-C35-C36-C37
30	H	103	SQD	C34-C35-C36-C37
30	A	413	SQD	C23-C24-C25-C26
30	a	413	SQD	C23-C24-C25-C26
33	B	627	LHG	C5-C4-O6-P
33	b	627	LHG	C5-C4-O6-P
25	A	406	CLA	C3A-C2A-CAA-CBA
25	B	607	CLA	C3A-C2A-CAA-CBA
25	B	608	CLA	C3A-C2A-CAA-CBA
25	B	609	CLA	C3A-C2A-CAA-CBA
25	a	406	CLA	C3A-C2A-CAA-CBA
25	b	607	CLA	C3A-C2A-CAA-CBA
25	b	608	CLA	C3A-C2A-CAA-CBA
25	b	609	CLA	C3A-C2A-CAA-CBA
31	B	625	LMT	C2-C1-O1'-C1'
31	B	629	LMT	C2-C1-O1'-C1'
31	C	525	LMT	C2-C1-O1'-C1'
31	D	410	LMT	C2-C1-O1'-C1'
31	E	101	LMT	C2-C1-O1'-C1'
31	X	104	LMT	C2-C1-O1'-C1'
31	b	625	LMT	C2-C1-O1'-C1'
31	b	629	LMT	C2-C1-O1'-C1'
31	c	525	LMT	C2-C1-O1'-C1'
31	d	410	LMT	C2-C1-O1'-C1'
31	e	101	LMT	C2-C1-O1'-C1'
31	x	104	LMT	C2-C1-O1'-C1'
30	B	620	SQD	C27-C28-C29-C30
30	b	620	SQD	C27-C28-C29-C30
31	I	103	LMT	C11-C10-C9-C8
31	i	103	LMT	C11-C10-C9-C8
28	B	621	LMG	C13-C14-C15-C16
30	H	103	SQD	C16-C17-C18-C19
30	h	103	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
34	C	518	DGD	C9A-CAA-CBA-CCA
34	c	518	DGD	C9A-CAA-CBA-CCA
28	b	621	LMG	C13-C14-C15-C16
33	D	408	LHG	C34-C35-C36-C37
25	C	510	CLA	C13-C15-C16-C17
25	c	510	CLA	C13-C15-C16-C17
33	B	627	LHG	C4-C5-C6-O8
33	B	628	LHG	C4-C5-C6-O8
33	b	627	LHG	C4-C5-C6-O8
33	b	628	LHG	C4-C5-C6-O8
34	C	517	DGD	O1B-C1B-O2G-C2G
34	c	517	DGD	O1B-C1B-O2G-C2G
31	X	105	LMT	C4-C5-C6-C7
31	x	105	LMT	C4-C5-C6-C7
33	d	408	LHG	C34-C35-C36-C37
31	a	415	LMT	C4'-C5'-C6'-O6'
28	A	414	LMG	C29-C30-C31-C32
28	a	414	LMG	C29-C30-C31-C32
31	A	415	LMT	O5'-C5'-C6'-O6'
31	a	415	LMT	O5'-C5'-C6'-O6'
28	C	519	LMG	C40-C41-C42-C43
31	A	415	LMT	C4'-C5'-C6'-O6'
25	B	603	CLA	O1D-CGD-O2D-CED
25	b	603	CLA	O1D-CGD-O2D-CED
28	A	410	LMG	C33-C34-C35-C36
28	a	410	LMG	C33-C34-C35-C36
28	c	519	LMG	C40-C41-C42-C43
30	A	412	SQD	C30-C31-C32-C33
30	a	412	SQD	C30-C31-C32-C33
31	M	101	LMT	C3-C4-C5-C6
31	m	101	LMT	C3-C4-C5-C6
30	H	103	SQD	C17-C18-C19-C20
30	h	103	SQD	C17-C18-C19-C20
33	Z	102	LHG	C34-C35-C36-C37
33	z	102	LHG	C34-C35-C36-C37
31	J	101	LMT	C1-C2-C3-C4
31	j	101	LMT	C1-C2-C3-C4
33	B	627	LHG	O6-C4-C5-O7
33	b	627	LHG	O6-C4-C5-O7
34	C	516	DGD	C4D-C5D-C6D-O5D
34	c	516	DGD	C4D-C5D-C6D-O5D
31	i	103	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	K	101	SQD	C23-C24-C25-C26
30	k	101	SQD	C23-C24-C25-C26
25	A	405	CLA	C16-C17-C18-C19
25	a	405	CLA	C16-C17-C18-C19
31	I	103	LMT	C6-C7-C8-C9
31	B	623	LMT	C2-C3-C4-C5
31	b	623	LMT	C2-C3-C4-C5
33	D	408	LHG	C29-C30-C31-C32
33	d	408	LHG	C29-C30-C31-C32
31	D	411	LMT	C9-C10-C11-C12
31	d	411	LMT	C9-C10-C11-C12
30	F	102	SQD	O47-C45-C46-O48
30	f	102	SQD	O47-C45-C46-O48
33	B	627	LHG	O7-C5-C6-O8
33	D	406	LHG	O7-C5-C6-O8
33	b	627	LHG	O7-C5-C6-O8
33	d	406	LHG	O7-C5-C6-O8
28	D	409	LMG	C14-C15-C16-C17
28	d	409	LMG	C14-C15-C16-C17
33	Z	102	LHG	C35-C36-C37-C38
33	z	102	LHG	C35-C36-C37-C38
26	A	407	PHO	C16-C17-C18-C19
26	a	407	PHO	C16-C17-C18-C19
31	B	624	LMT	O5'-C1'-O1'-C1
31	b	624	LMT	O5'-C1'-O1'-C1
28	H	105	LMG	C29-C30-C31-C32
28	h	105	LMG	C29-C30-C31-C32
25	b	613	CLA	C3-C5-C6-C7
28	D	409	LMG	C29-C30-C31-C32
28	d	409	LMG	C29-C30-C31-C32
31	X	101	LMT	O1'-C1-C2-C3
31	x	101	LMT	O1'-C1-C2-C3
33	d	407	LHG	C25-C26-C27-C28
33	d	408	LHG	C26-C27-C28-C29
31	J	101	LMT	O5'-C5'-C6'-O6'
31	j	101	LMT	O5'-C5'-C6'-O6'
25	A	406	CLA	C6-C7-C8-C9
25	B	611	CLA	C11-C12-C13-C14
25	C	512	CLA	C11-C10-C8-C9
25	a	406	CLA	C6-C7-C8-C9
25	b	611	CLA	C11-C12-C13-C14
25	c	512	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	C	501	SQD	C9-C10-C11-C12
30	c	501	SQD	C9-C10-C11-C12
33	D	407	LHG	C25-C26-C27-C28
33	D	408	LHG	C26-C27-C28-C29
25	B	602	CLA	C8-C10-C11-C12
25	B	605	CLA	C5-C6-C7-C8
25	b	602	CLA	C8-C10-C11-C12
25	B	611	CLA	O1A-CGA-O2A-C1
25	b	611	CLA	O1A-CGA-O2A-C1
31	B	623	LMT	C1-C2-C3-C4
31	b	623	LMT	C1-C2-C3-C4
30	H	103	SQD	C12-C13-C14-C15
30	K	101	SQD	C11-C10-C9-C8
30	h	103	SQD	C12-C13-C14-C15
30	k	101	SQD	C11-C10-C9-C8
31	H	102	LMT	C5-C6-C7-C8
31	T	101	LMT	C9-C10-C11-C12
31	h	102	LMT	C5-C6-C7-C8
31	t	101	LMT	C9-C10-C11-C12
33	B	628	LHG	C31-C32-C33-C34
33	b	628	LHG	C31-C32-C33-C34
25	B	613	CLA	C3-C5-C6-C7
27	A	409	BCR	C1-C6-C7-C8
27	A	409	BCR	C5-C6-C7-C8
27	A	409	BCR	C23-C24-C25-C26
27	A	409	BCR	C23-C24-C25-C30
27	B	617	BCR	C23-C24-C25-C26
27	B	617	BCR	C23-C24-C25-C30
27	F	101	BCR	C23-C24-C25-C26
27	F	101	BCR	C23-C24-C25-C30
27	K	102	BCR	C23-C24-C25-C30
27	K	103	BCR	C23-C24-C25-C26
27	a	409	BCR	C1-C6-C7-C8
27	a	409	BCR	C5-C6-C7-C8
27	a	409	BCR	C23-C24-C25-C26
27	a	409	BCR	C23-C24-C25-C30
27	b	617	BCR	C23-C24-C25-C26
27	b	617	BCR	C23-C24-C25-C30
27	f	101	BCR	C23-C24-C25-C26
27	f	101	BCR	C23-C24-C25-C30
27	k	102	BCR	C23-C24-C25-C30
27	k	103	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	B	605	CLA	C8-C10-C11-C12
25	b	605	CLA	C5-C6-C7-C8
25	b	605	CLA	C8-C10-C11-C12
33	B	627	LHG	C24-C25-C26-C27
33	b	627	LHG	C24-C25-C26-C27
34	c	518	DGD	CCA-CDA-CEA-CFA
30	K	101	SQD	O47-C7-C8-C9
30	k	101	SQD	O47-C7-C8-C9
34	C	518	DGD	CCA-CDA-CEA-CFA
27	B	617	BCR	C21-C22-C23-C24
27	Z	101	BCR	C21-C22-C23-C24
27	b	617	BCR	C21-C22-C23-C24
27	z	101	BCR	C21-C22-C23-C24
28	a	414	LMG	C14-C15-C16-C17
28	c	519	LMG	C37-C38-C39-C40
30	A	413	SQD	C31-C32-C33-C34
30	a	413	SQD	C31-C32-C33-C34
33	D	407	LHG	C27-C28-C29-C30
33	d	407	LHG	C27-C28-C29-C30
28	A	414	LMG	C14-C15-C16-C17
28	C	519	LMG	C37-C38-C39-C40
34	C	518	DGD	CAA-CBA-CCA-CDA
34	c	518	DGD	CAA-CBA-CCA-CDA
25	A	408	CLA	O1D-CGD-O2D-CED
25	a	408	CLA	O1D-CGD-O2D-CED
33	D	408	LHG	O6-C4-C5-C6
33	d	408	LHG	O6-C4-C5-C6
33	B	628	LHG	C28-C29-C30-C31
33	b	628	LHG	C28-C29-C30-C31
25	A	408	CLA	C11-C10-C8-C7
25	B	602	CLA	C11-C10-C8-C7
25	B	603	CLA	C6-C7-C8-C10
25	B	604	CLA	C6-C7-C8-C10
25	B	605	CLA	C11-C10-C8-C7
25	C	512	CLA	C6-C7-C8-C10
25	C	512	CLA	C12-C13-C15-C16
25	C	514	CLA	C6-C7-C8-C10
25	C	514	CLA	C12-C13-C15-C16
25	D	404	CLA	C11-C12-C13-C15
25	a	408	CLA	C11-C10-C8-C7
25	b	602	CLA	C11-C10-C8-C7
25	b	603	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	b	604	CLA	C6-C7-C8-C10
25	b	605	CLA	C11-C10-C8-C7
25	c	512	CLA	C6-C7-C8-C10
25	c	512	CLA	C12-C13-C15-C16
25	c	514	CLA	C6-C7-C8-C10
25	c	514	CLA	C12-C13-C15-C16
25	d	404	CLA	C11-C12-C13-C15
31	I	101	LMT	C1-C2-C3-C4
31	i	101	LMT	C1-C2-C3-C4
31	E	101	LMT	C3-C4-C5-C6
27	C	515	BCR	C9-C10-C11-C12
27	c	515	BCR	C9-C10-C11-C12
25	B	615	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C20
31	e	101	LMT	C3-C4-C5-C6
33	D	406	LHG	C30-C31-C32-C33
33	d	406	LHG	C30-C31-C32-C33
31	A	415	LMT	C11-C10-C9-C8
31	T	101	LMT	C4-C5-C6-C7
31	a	415	LMT	C11-C10-C9-C8
31	t	101	LMT	C4-C5-C6-C7
25	B	613	CLA	CBA-CGA-O2A-C1
25	b	613	CLA	CBA-CGA-O2A-C1
33	D	408	LHG	C24-C23-O8-C6
33	d	408	LHG	C24-C23-O8-C6
33	B	627	LHG	C12-C13-C14-C15
33	b	627	LHG	C12-C13-C14-C15
35	E	104	HEM	C2A-CAA-CBA-CGA
35	e	104	HEM	C2A-CAA-CBA-CGA
25	A	408	CLA	CBD-CGD-O2D-CED
25	a	408	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	CAD-CBD-CGD-O2D
25	B	616	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	b	616	CLA	CAD-CBD-CGD-O2D
30	B	620	SQD	C46-C45-O47-C7
30	F	102	SQD	C44-C45-O47-C7
30	b	620	SQD	C46-C45-O47-C7
30	f	102	SQD	C44-C45-O47-C7
31	B	625	LMT	C6-C7-C8-C9
31	b	625	LMT	C6-C7-C8-C9
31	E	101	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	X	101	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
31	x	101	LMT	O5'-C1'-O1'-C1
28	H	105	LMG	O1-C7-C8-C9
28	h	105	LMG	O1-C7-C8-C9
30	K	101	SQD	C44-C45-C46-O48
30	k	101	SQD	C44-C45-C46-O48
33	d	406	LHG	O10-C23-O8-C6
33	B	628	LHG	O6-C4-C5-O7
33	Z	102	LHG	O6-C4-C5-O7
33	b	628	LHG	O6-C4-C5-O7
33	z	102	LHG	O6-C4-C5-O7
33	D	406	LHG	O10-C23-O8-C6
25	D	403	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C19
28	c	519	LMG	C29-C30-C31-C32
33	E	102	LHG	C1-C2-C3-O3
33	e	102	LHG	C1-C2-C3-O3
25	B	603	CLA	CHA-CBD-CGD-O1D
25	B	603	CLA	CHA-CBD-CGD-O2D
25	B	605	CLA	CHA-CBD-CGD-O1D
25	B	607	CLA	CHA-CBD-CGD-O1D
25	B	607	CLA	CHA-CBD-CGD-O2D
25	B	609	CLA	CHA-CBD-CGD-O1D
25	C	505	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	b	603	CLA	CHA-CBD-CGD-O1D
25	b	603	CLA	CHA-CBD-CGD-O2D
25	b	605	CLA	CHA-CBD-CGD-O1D
25	b	607	CLA	CHA-CBD-CGD-O1D
25	b	607	CLA	CHA-CBD-CGD-O2D
25	b	609	CLA	CHA-CBD-CGD-O1D
25	c	505	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
28	C	519	LMG	C29-C30-C31-C32
34	C	516	DGD	C2E-C1E-O5D-C6D
34	c	516	DGD	C2E-C1E-O5D-C6D
25	B	615	CLA	C5-C6-C7-C8
25	b	615	CLA	C5-C6-C7-C8
31	D	411	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	d	411	LMT	C7-C8-C9-C10
26	D	402	PHO	O1D-CGD-O2D-CED
26	d	402	PHO	O1D-CGD-O2D-CED
31	I	101	LMT	C6-C7-C8-C9
31	i	101	LMT	C6-C7-C8-C9
33	D	406	LHG	C15-C16-C17-C18
33	D	408	LHG	C11-C10-C9-C8
33	d	406	LHG	C15-C16-C17-C18
33	d	408	LHG	C11-C10-C9-C8
25	B	613	CLA	O1A-CGA-O2A-C1
25	b	613	CLA	O1A-CGA-O2A-C1
25	C	512	CLA	C6-C7-C8-C9
25	C	512	CLA	C14-C13-C15-C16
25	D	403	CLA	C11-C12-C13-C14
25	c	512	CLA	C6-C7-C8-C9
25	c	512	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C14
31	M	101	LMT	C7-C8-C9-C10
31	m	101	LMT	C7-C8-C9-C10
31	T	101	LMT	C2-C3-C4-C5
31	t	101	LMT	C2-C3-C4-C5
31	c	522	LMT	C2-C3-C4-C5
31	C	522	LMT	C2-C3-C4-C5
33	D	407	LHG	C28-C29-C30-C31
33	d	407	LHG	C28-C29-C30-C31
30	A	412	SQD	C9-C10-C11-C12
30	a	412	SQD	C9-C10-C11-C12
25	B	603	CLA	C16-C17-C18-C19
25	C	512	CLA	C16-C17-C18-C20
25	b	603	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C20
25	B	612	CLA	C13-C15-C16-C17
25	b	612	CLA	C13-C15-C16-C17
25	B	616	CLA	C2-C1-O2A-CGA
25	b	616	CLA	C2-C1-O2A-CGA
31	e	103	LMT	C5-C6-C7-C8
27	K	103	BCR	C9-C10-C11-C12
27	k	103	BCR	C9-C10-C11-C12
33	E	102	LHG	C3-O3-P-O6
33	e	102	LHG	C3-O3-P-O6
31	E	103	LMT	C5-C6-C7-C8
31	I	101	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	i	101	LMT	C9-C10-C11-C12
33	D	408	LHG	C2-C3-O3-P
33	E	102	LHG	C2-C3-O3-P
33	d	408	LHG	C2-C3-O3-P
33	e	102	LHG	C2-C3-O3-P
34	h	104	DGD	CCA-CDA-CEA-CFA
33	B	627	LHG	C3-O3-P-O5
33	B	627	LHG	C4-O6-P-O5
33	B	628	LHG	C4-O6-P-O5
33	D	407	LHG	C4-O6-P-O5
33	E	102	LHG	C4-O6-P-O4
33	E	102	LHG	C4-O6-P-O5
33	b	627	LHG	C3-O3-P-O5
33	b	627	LHG	C4-O6-P-O5
33	b	628	LHG	C4-O6-P-O5
33	d	407	LHG	C4-O6-P-O5
33	e	102	LHG	C4-O6-P-O4
33	e	102	LHG	C4-O6-P-O5
25	B	613	CLA	C16-C17-C18-C20
25	b	613	CLA	C16-C17-C18-C20
34	H	104	DGD	CCA-CDA-CEA-CFA
31	T	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
25	B	614	CLA	C13-C15-C16-C17
25	b	614	CLA	C13-C15-C16-C17
33	E	102	LHG	O6-C4-C5-C6
33	Z	102	LHG	O6-C4-C5-C6
33	e	102	LHG	O6-C4-C5-C6
33	z	102	LHG	O6-C4-C5-C6
30	c	501	SQD	C10-C11-C12-C13
31	D	412	LMT	O1'-C1-C2-C3
31	d	412	LMT	O1'-C1-C2-C3
30	C	501	SQD	C10-C11-C12-C13
25	B	603	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	607	CLA	CAD-CBD-CGD-O1D
25	B	609	CLA	CAD-CBD-CGD-O1D
25	C	505	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CAD-CBD-CGD-O1D
25	b	603	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	607	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	b	609	CLA	CAD-CBD-CGD-O1D
25	c	505	CLA	CAD-CBD-CGD-O1D
25	c	507	CLA	CAD-CBD-CGD-O1D
30	A	412	SQD	C5-C6-S-O7
30	A	412	SQD	C5-C6-S-O9
30	H	103	SQD	O5-C5-C6-S
30	a	412	SQD	C5-C6-S-O7
30	a	412	SQD	C5-C6-S-O9
30	h	103	SQD	O5-C5-C6-S
28	C	523	LMG	O7-C10-C11-C12
28	c	523	LMG	O7-C10-C11-C12
31	D	410	LMT	C2-C3-C4-C5
31	d	410	LMT	C2-C3-C4-C5
33	D	408	LHG	C25-C26-C27-C28
33	d	408	LHG	C25-C26-C27-C28
30	B	620	SQD	C15-C16-C17-C18
30	b	620	SQD	C15-C16-C17-C18
25	A	406	CLA	C11-C10-C8-C7
25	B	603	CLA	C11-C10-C8-C7
25	B	607	CLA	C12-C13-C15-C16
25	B	612	CLA	C11-C10-C8-C7
25	B	615	CLA	C12-C13-C15-C16
25	D	403	CLA	C11-C12-C13-C15
25	a	406	CLA	C11-C10-C8-C7
25	b	603	CLA	C11-C10-C8-C7
25	b	607	CLA	C12-C13-C15-C16
25	b	612	CLA	C11-C10-C8-C7
25	b	615	CLA	C12-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C15
33	E	102	LHG	O6-C4-C5-O7
33	e	102	LHG	O6-C4-C5-O7
31	X	101	LMT	C7-C8-C9-C10
31	x	101	LMT	C7-C8-C9-C10
33	d	408	LHG	O10-C23-O8-C6
28	d	409	LMG	C4-C5-C6-O5
30	B	620	SQD	C7-C8-C9-C10
30	b	620	SQD	C7-C8-C9-C10
33	D	407	LHG	C23-C24-C25-C26
33	d	407	LHG	C23-C24-C25-C26
28	D	409	LMG	C4-C5-C6-O5
30	F	102	SQD	C44-C45-C46-O48
30	f	102	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
33	Z	102	LHG	C4-C5-C6-O8
33	z	102	LHG	C4-C5-C6-O8
33	D	408	LHG	O10-C23-O8-C6
30	A	412	SQD	O6-C44-C45-O47
30	a	412	SQD	O6-C44-C45-O47
33	D	407	LHG	O7-C5-C6-O8
33	Z	102	LHG	O7-C5-C6-O8
33	d	407	LHG	O7-C5-C6-O8
33	z	102	LHG	O7-C5-C6-O8
31	B	629	LMT	C7-C8-C9-C10
31	b	629	LMT	C7-C8-C9-C10
25	B	608	CLA	C13-C15-C16-C17
33	B	628	LHG	C34-C35-C36-C37
33	b	628	LHG	C34-C35-C36-C37
28	C	523	LMG	C33-C34-C35-C36
28	c	523	LMG	C33-C34-C35-C36
30	C	501	SQD	C11-C12-C13-C14
30	c	501	SQD	C11-C12-C13-C14
28	H	105	LMG	C8-C7-O1-C1
28	h	105	LMG	C8-C7-O1-C1
34	C	517	DGD	C2G-C3G-O3G-C1D
34	c	517	DGD	C2G-C3G-O3G-C1D
25	b	608	CLA	C13-C15-C16-C17
25	B	602	CLA	C11-C10-C8-C9
25	B	604	CLA	C6-C7-C8-C9
25	B	605	CLA	C11-C10-C8-C9
25	B	612	CLA	C11-C10-C8-C9
25	D	404	CLA	C11-C12-C13-C14
25	b	602	CLA	C11-C10-C8-C9
25	b	604	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C10-C8-C9
25	b	612	CLA	C11-C10-C8-C9
25	d	404	CLA	C11-C12-C13-C14
25	B	611	CLA	C3-C5-C6-C7
25	b	611	CLA	C3-C5-C6-C7
25	C	507	CLA	C16-C17-C18-C19
25	c	507	CLA	C16-C17-C18-C19
28	D	409	LMG	C33-C34-C35-C36
28	d	409	LMG	C33-C34-C35-C36
34	c	516	DGD	C2B-C3B-C4B-C5B
34	C	516	DGD	C2B-C3B-C4B-C5B
34	C	516	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
34	c	516	DGD	O2G-C1B-C2B-C3B
27	K	102	BCR	C18-C19-C20-C21
27	k	102	BCR	C18-C19-C20-C21
31	A	415	LMT	C6-C7-C8-C9
31	D	410	LMT	C4-C5-C6-C7
31	d	410	LMT	C4-C5-C6-C7
31	a	415	LMT	C6-C7-C8-C9
31	I	101	LMT	C5-C6-C7-C8
31	i	101	LMT	C5-C6-C7-C8
30	A	413	SQD	O47-C7-C8-C9
30	a	413	SQD	O47-C7-C8-C9
28	b	621	LMG	C15-C16-C17-C18
25	C	512	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C19
28	B	621	LMG	C15-C16-C17-C18
28	C	523	LMG	C36-C37-C38-C39
28	c	523	LMG	C36-C37-C38-C39
28	D	409	LMG	C13-C14-C15-C16
28	d	409	LMG	C13-C14-C15-C16
33	Z	102	LHG	C25-C26-C27-C28
33	z	102	LHG	C25-C26-C27-C28
31	F	103	LMT	C4'-C5'-C6'-O6'
31	f	103	LMT	C4'-C5'-C6'-O6'
25	B	603	CLA	C2A-CAA-CBA-CGA
25	C	506	CLA	C2A-CAA-CBA-CGA
25	b	603	CLA	C2A-CAA-CBA-CGA
25	c	506	CLA	C2A-CAA-CBA-CGA
25	B	604	CLA	C2-C1-O2A-CGA
25	C	504	CLA	C2-C1-O2A-CGA
25	C	512	CLA	C2-C1-O2A-CGA
25	b	604	CLA	C2-C1-O2A-CGA
25	c	504	CLA	C2-C1-O2A-CGA
25	c	512	CLA	C2-C1-O2A-CGA
33	E	102	LHG	C19-C20-C21-C22
33	e	102	LHG	C19-C20-C21-C22
33	E	102	LHG	C26-C27-C28-C29
33	e	102	LHG	C26-C27-C28-C29
27	F	101	BCR	C19-C20-C21-C22
27	f	101	BCR	C19-C20-C21-C22
25	C	512	CLA	C3-C5-C6-C7
25	c	512	CLA	C3-C5-C6-C7
27	B	618	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	K	103	BCR	C23-C24-C25-C30
27	b	618	BCR	C5-C6-C7-C8
27	k	103	BCR	C23-C24-C25-C30
31	b	623	LMT	C9-C10-C11-C12
28	H	105	LMG	O6-C1-O1-C7
28	h	105	LMG	O6-C1-O1-C7
31	B	623	LMT	C9-C10-C11-C12
33	D	408	LHG	C19-C20-C21-C22
33	d	408	LHG	C19-C20-C21-C22
28	H	105	LMG	C2-C1-O1-C7
28	h	105	LMG	C2-C1-O1-C7
30	C	501	SQD	C2-C1-O6-C44
30	c	501	SQD	C2-C1-O6-C44
33	D	407	LHG	C3-O3-P-O6
33	D	408	LHG	C4-O6-P-O3
33	d	407	LHG	C3-O3-P-O6
33	d	408	LHG	C4-O6-P-O3
28	C	519	LMG	C15-C16-C17-C18
28	c	519	LMG	C15-C16-C17-C18
31	X	102	LMT	C1-C2-C3-C4
31	x	102	LMT	C1-C2-C3-C4
33	D	406	LHG	C4-C5-C6-O8
33	d	406	LHG	C4-C5-C6-O8
28	A	410	LMG	C31-C32-C33-C34
28	C	519	LMG	C19-C20-C21-C22
28	c	519	LMG	C19-C20-C21-C22
25	A	406	CLA	C6-C7-C8-C10
25	C	514	CLA	C2-C3-C5-C6
25	a	406	CLA	C6-C7-C8-C10
25	c	514	CLA	C2-C3-C5-C6
28	a	410	LMG	C31-C32-C33-C34
25	B	603	CLA	C11-C10-C8-C9
25	B	615	CLA	C14-C13-C15-C16
25	b	603	CLA	C11-C10-C8-C9
25	b	615	CLA	C14-C13-C15-C16
25	b	614	CLA	C5-C6-C7-C8
27	B	618	BCR	C9-C10-C11-C12
27	C	515	BCR	C19-C20-C21-C22
27	K	102	BCR	C19-C20-C21-C22
27	k	102	BCR	C19-C20-C21-C22
25	C	507	CLA	C16-C17-C18-C20
25	c	507	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	m	102	LMT	C9-C10-C11-C12
25	B	614	CLA	C5-C6-C7-C8
31	M	102	LMT	C9-C10-C11-C12
34	H	104	DGD	O1B-C1B-C2B-C3B
34	h	104	DGD	O1B-C1B-C2B-C3B
31	T	101	LMT	C1-C2-C3-C4
31	t	101	LMT	C1-C2-C3-C4
27	Z	101	BCR	C11-C12-C13-C35
27	z	101	BCR	C11-C12-C13-C35
25	B	613	CLA	C16-C17-C18-C19
25	b	613	CLA	C16-C17-C18-C19
25	B	603	CLA	CBA-CGA-O2A-C1
30	K	101	SQD	C29-C30-C31-C32
31	B	625	LMT	C4'-C5'-C6'-O6'
30	k	101	SQD	C29-C30-C31-C32
31	b	625	LMT	C4'-C5'-C6'-O6'
25	b	603	CLA	CBA-CGA-O2A-C1
33	Z	102	LHG	C24-C23-O8-C6
33	z	102	LHG	C24-C23-O8-C6
34	C	517	DGD	C2A-C1A-O1G-C1G
34	c	517	DGD	C2A-C1A-O1G-C1G
30	C	501	SQD	C28-C29-C30-C31
34	C	517	DGD	O1A-C1A-O1G-C1G
34	c	517	DGD	O1A-C1A-O1G-C1G
30	c	501	SQD	C28-C29-C30-C31
31	T	101	LMT	C5-C6-C7-C8
31	t	101	LMT	C5-C6-C7-C8
30	A	412	SQD	C28-C29-C30-C31
30	a	412	SQD	C28-C29-C30-C31
34	c	517	DGD	C9A-CAA-CBA-CCA
25	A	405	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	CBA-CGA-O2A-C1
34	C	517	DGD	C9A-CAA-CBA-CCA
27	b	618	BCR	C9-C10-C11-C12
27	c	515	BCR	C19-C20-C21-C22
29	A	411	PL9	C19-C21-C22-C23
29	a	411	PL9	C19-C21-C22-C23
30	k	101	SQD	C28-C29-C30-C31
25	D	401	CLA	C2C-C3C-CAC-CBC
25	d	401	CLA	C2C-C3C-CAC-CBC
30	K	101	SQD	C28-C29-C30-C31
35	E	104	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
35	e	104	HEM	CAA-CBA-CGA-O1A
30	B	620	SQD	C29-C30-C31-C32
30	b	620	SQD	C29-C30-C31-C32
29	A	411	PL9	C45-C44-C46-C47
29	a	411	PL9	C45-C44-C46-C47
33	B	627	LHG	C28-C29-C30-C31
33	D	408	LHG	C31-C32-C33-C34
33	b	627	LHG	C28-C29-C30-C31
33	d	408	LHG	C31-C32-C33-C34
35	V	201	HEM	CAD-CBD-CGD-O1D
35	v	201	HEM	CAD-CBD-CGD-O1D
25	B	602	CLA	C2-C1-O2A-CGA
25	b	602	CLA	C2-C1-O2A-CGA
26	A	407	PHO	C15-C16-C17-C18
26	a	407	PHO	C15-C16-C17-C18
30	C	501	SQD	C16-C17-C18-C19
30	c	501	SQD	C16-C17-C18-C19
25	C	503	CLA	C2A-CAA-CBA-CGA
25	c	503	CLA	C2A-CAA-CBA-CGA
28	A	410	LMG	O7-C8-C9-O8
28	a	410	LMG	O7-C8-C9-O8
28	H	105	LMG	C32-C33-C34-C35
28	h	105	LMG	C32-C33-C34-C35
33	D	406	LHG	C31-C32-C33-C34
31	J	101	LMT	C3-C4-C5-C6
33	d	406	LHG	C31-C32-C33-C34
35	V	201	HEM	CAD-CBD-CGD-O2D
35	v	201	HEM	CAD-CBD-CGD-O2D
31	j	101	LMT	C3-C4-C5-C6
33	B	628	LHG	O9-C7-O7-C5
33	b	628	LHG	O9-C7-O7-C5
25	c	511	CLA	C5-C6-C7-C8
31	B	629	LMT	C5-C6-C7-C8
31	b	629	LMT	C5-C6-C7-C8
34	C	518	DGD	C2A-C3A-C4A-C5A
34	c	518	DGD	C2A-C3A-C4A-C5A
30	K	101	SQD	C25-C26-C27-C28
25	A	406	CLA	C11-C10-C8-C9
25	B	609	CLA	C6-C7-C8-C9
25	a	406	CLA	C11-C10-C8-C9
25	b	609	CLA	C6-C7-C8-C9
25	C	511	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	k	101	SQD	C25-C26-C27-C28
33	D	406	LHG	C11-C10-C9-C8
27	K	102	BCR	C20-C21-C22-C37
27	k	102	BCR	C20-C21-C22-C37
30	A	413	SQD	C44-C45-C46-O48
30	a	413	SQD	C44-C45-C46-O48
34	H	104	DGD	O1G-C1G-C2G-C3G
34	h	104	DGD	O1G-C1G-C2G-C3G
28	C	519	LMG	C21-C22-C23-C24
28	c	519	LMG	C21-C22-C23-C24
33	d	406	LHG	C11-C10-C9-C8
28	B	621	LMG	C32-C33-C34-C35
28	b	621	LMG	C32-C33-C34-C35
30	A	413	SQD	C30-C31-C32-C33
34	C	517	DGD	O6D-C1D-O3G-C3G
34	c	517	DGD	O6D-C1D-O3G-C3G
30	a	413	SQD	C30-C31-C32-C33
31	I	103	LMT	C7-C8-C9-C10
31	i	103	LMT	C7-C8-C9-C10
31	F	103	LMT	C4B-C5B-C6B-O6B
31	f	103	LMT	C4B-C5B-C6B-O6B
25	a	406	CLA	C3-C5-C6-C7
25	B	604	CLA	C10-C11-C12-C13
25	b	604	CLA	C10-C11-C12-C13
25	D	404	CLA	C4-C3-C5-C6
25	d	404	CLA	C4-C3-C5-C6
25	B	608	CLA	C1A-C2A-CAA-CBA
25	b	608	CLA	C1A-C2A-CAA-CBA
34	C	518	DGD	CAB-CBB-CCB-CDB
34	c	518	DGD	CAB-CBB-CCB-CDB
25	B	602	CLA	C11-C12-C13-C15
25	B	606	CLA	C11-C10-C8-C7
25	B	615	CLA	C6-C7-C8-C10
25	b	602	CLA	C11-C12-C13-C15
25	b	606	CLA	C11-C10-C8-C7
25	b	615	CLA	C6-C7-C8-C10
25	A	406	CLA	C3-C5-C6-C7
27	K	102	BCR	C13-C14-C15-C16
27	k	102	BCR	C13-C14-C15-C16
30	A	412	SQD	C18-C19-C20-C21
30	a	412	SQD	C18-C19-C20-C21
33	B	628	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
33	b	628	LHG	C3-O3-P-O6
34	C	517	DGD	C5B-C6B-C7B-C8B
34	c	517	DGD	C5B-C6B-C7B-C8B
25	A	405	CLA	O1A-CGA-O2A-C1
25	a	405	CLA	O1A-CGA-O2A-C1
25	C	506	CLA	C6-C7-C8-C10
25	c	506	CLA	C6-C7-C8-C10
31	B	625	LMT	O5'-C5'-C6'-O6'
31	i	101	LMT	C4'-C5'-C6'-O6'
28	a	410	LMG	C16-C17-C18-C19
31	b	625	LMT	O5'-C5'-C6'-O6'
28	A	410	LMG	C16-C17-C18-C19
30	c	501	SQD	C31-C32-C33-C34
31	F	103	LMT	C7-C8-C9-C10
30	C	501	SQD	C31-C32-C33-C34
31	f	103	LMT	C7-C8-C9-C10
25	B	607	CLA	C15-C16-C17-C18
31	I	101	LMT	C4'-C5'-C6'-O6'
31	J	101	LMT	C11-C10-C9-C8
31	j	101	LMT	C11-C10-C9-C8
33	B	628	LHG	C17-C18-C19-C20
31	I	102	LMT	C11-C10-C9-C8
33	b	628	LHG	C17-C18-C19-C20
31	I	103	LMT	C4B-C5B-C6B-O6B
31	i	103	LMT	C4B-C5B-C6B-O6B
25	b	607	CLA	C15-C16-C17-C18
31	i	102	LMT	C11-C10-C9-C8
34	C	517	DGD	CAB-CBB-CCB-CDB
34	c	517	DGD	CAB-CBB-CCB-CDB
25	C	508	CLA	O1A-CGA-O2A-C1
25	c	508	CLA	O1A-CGA-O2A-C1
28	C	519	LMG	O10-C28-O8-C9
28	c	519	LMG	O10-C28-O8-C9
25	B	603	CLA	CBD-CGD-O2D-CED
25	b	603	CLA	CBD-CGD-O2D-CED
27	K	102	BCR	C20-C21-C22-C23
27	k	102	BCR	C20-C21-C22-C23
27	F	101	BCR	C13-C14-C15-C16
27	f	101	BCR	C13-C14-C15-C16
33	D	406	LHG	C27-C28-C29-C30
25	C	512	CLA	C5-C6-C7-C8
25	c	512	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	d	406	LHG	C27-C28-C29-C30
25	B	603	CLA	O1A-CGA-O2A-C1
25	b	603	CLA	O1A-CGA-O2A-C1
35	E	104	HEM	CAA-CBA-CGA-O2A
35	e	104	HEM	CAA-CBA-CGA-O2A
25	C	502	CLA	C4-C3-C5-C6
25	c	502	CLA	C4-C3-C5-C6
31	b	624	LMT	C5-C6-C7-C8
31	i	102	LMT	C6-C7-C8-C9
25	c	502	CLA	O1D-CGD-O2D-CED
31	B	624	LMT	C5-C6-C7-C8
33	Z	102	LHG	O10-C23-O8-C6
33	z	102	LHG	O10-C23-O8-C6
31	E	103	LMT	O1'-C1-C2-C3
31	I	102	LMT	C6-C7-C8-C9
31	e	103	LMT	O1'-C1-C2-C3
30	A	412	SQD	C24-C25-C26-C27
30	a	412	SQD	C24-C25-C26-C27
25	A	408	CLA	C2A-CAA-CBA-CGA
25	a	408	CLA	C2A-CAA-CBA-CGA
31	C	524	LMT	C11-C10-C9-C8
31	c	524	LMT	C11-C10-C9-C8
27	B	618	BCR	C1-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C26
27	B	618	BCR	C23-C24-C25-C30
27	b	618	BCR	C1-C6-C7-C8
27	b	618	BCR	C23-C24-C25-C26
27	b	618	BCR	C23-C24-C25-C30
25	C	502	CLA	O1D-CGD-O2D-CED
34	C	516	DGD	C1G-C2G-C3G-O3G
34	c	516	DGD	C1G-C2G-C3G-O3G
30	H	103	SQD	C10-C11-C12-C13
30	h	103	SQD	C10-C11-C12-C13
27	B	619	BCR	C21-C22-C23-C24
27	b	619	BCR	C21-C22-C23-C24
25	B	614	CLA	C15-C16-C17-C18
25	b	614	CLA	C15-C16-C17-C18
30	A	413	SQD	C45-C44-O6-C1
30	a	413	SQD	C45-C44-O6-C1
34	C	516	DGD	C5D-C6D-O5D-C1E
34	c	516	DGD	C5D-C6D-O5D-C1E
33	B	628	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
34	H	104	DGD	C9A-CAA-CBA-CCA
34	h	104	DGD	C9A-CAA-CBA-CCA
33	B	627	LHG	C29-C30-C31-C32
33	b	627	LHG	C29-C30-C31-C32
34	c	517	DGD	C2A-C3A-C4A-C5A
31	E	101	LMT	C1-C2-C3-C4
31	e	101	LMT	C1-C2-C3-C4
34	C	517	DGD	C2A-C3A-C4A-C5A
28	A	410	LMG	C15-C16-C17-C18
28	a	410	LMG	C15-C16-C17-C18
30	c	501	SQD	C26-C27-C28-C29
30	C	501	SQD	C26-C27-C28-C29
33	b	628	LHG	C8-C7-O7-C5
25	C	512	CLA	C8-C10-C11-C12
25	c	512	CLA	C8-C10-C11-C12
34	C	517	DGD	C6B-C7B-C8B-C9B
34	c	517	DGD	C6B-C7B-C8B-C9B
31	b	629	LMT	C11-C10-C9-C8
30	K	101	SQD	O48-C23-C24-C25
30	k	101	SQD	O48-C23-C24-C25
31	B	629	LMT	C11-C10-C9-C8
25	B	609	CLA	C2A-CAA-CBA-CGA
25	b	609	CLA	C2A-CAA-CBA-CGA
28	C	519	LMG	C29-C28-O8-C9
28	c	519	LMG	C29-C28-O8-C9
30	b	620	SQD	C30-C31-C32-C33
31	x	102	LMT	C2-C3-C4-C5
36	H	101	RRX	C11-C10-C9-C34
36	h	101	RRX	C11-C10-C9-C34
28	A	410	LMG	O7-C10-C11-C12
30	B	620	SQD	C30-C31-C32-C33
25	C	509	CLA	C4-C3-C5-C6
25	C	511	CLA	C4-C3-C5-C6
25	c	509	CLA	C4-C3-C5-C6
25	c	511	CLA	C4-C3-C5-C6
29	A	411	PL9	C25-C24-C26-C27
29	a	411	PL9	C25-C24-C26-C27
31	X	102	LMT	C2-C3-C4-C5
25	B	608	CLA	C16-C17-C18-C19
25	b	608	CLA	C16-C17-C18-C19
28	a	410	LMG	O7-C10-C11-C12
25	B	607	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	514	CLA	C11-C10-C8-C9
25	b	607	CLA	C14-C13-C15-C16
25	c	514	CLA	C11-C10-C8-C9
25	D	401	CLA	C3A-C2A-CAA-CBA
25	d	401	CLA	C3A-C2A-CAA-CBA
28	C	523	LMG	O8-C28-C29-C30
28	c	523	LMG	O8-C28-C29-C30
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	510	CLA	CAD-CBD-CGD-O2D
25	C	511	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
25	c	511	CLA	CAD-CBD-CGD-O2D
28	A	410	LMG	C39-C40-C41-C42
33	E	102	LHG	O8-C23-C24-C25
33	e	102	LHG	O8-C23-C24-C25
28	a	410	LMG	C39-C40-C41-C42
31	b	624	LMT	C4-C5-C6-C7
28	h	105	LMG	C33-C34-C35-C36
28	H	105	LMG	C33-C34-C35-C36
31	B	624	LMT	C4-C5-C6-C7
29	A	411	PL9	C23-C24-C26-C27
29	a	411	PL9	C23-C24-C26-C27
25	B	614	CLA	CAA-CBA-CGA-O2A
25	C	506	CLA	CAA-CBA-CGA-O2A
25	b	614	CLA	CAA-CBA-CGA-O2A
25	c	506	CLA	CAA-CBA-CGA-O2A
33	b	628	LHG	C15-C16-C17-C18
31	K	105	LMT	C11-C10-C9-C8
31	k	105	LMT	C11-C10-C9-C8
33	B	628	LHG	C15-C16-C17-C18
33	E	102	LHG	C17-C18-C19-C20
30	F	102	SQD	O6-C44-C45-C46
30	f	102	SQD	O6-C44-C45-C46
33	e	102	LHG	C17-C18-C19-C20
30	C	501	SQD	O47-C7-C8-C9
30	c	501	SQD	O47-C7-C8-C9
25	B	602	CLA	O2A-C1-C2-C3
25	b	602	CLA	O2A-C1-C2-C3
26	A	407	PHO	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	a	407	PHO	O2A-C1-C2-C3
33	D	407	LHG	O8-C23-C24-C25
33	d	407	LHG	O8-C23-C24-C25
25	B	604	CLA	CHA-CBD-CGD-O1D
25	B	604	CLA	CHA-CBD-CGD-O2D
25	B	605	CLA	CHA-CBD-CGD-O2D
25	B	609	CLA	CHA-CBD-CGD-O2D
25	B	611	CLA	CHA-CBD-CGD-O2D
25	B	614	CLA	CHA-CBD-CGD-O1D
25	B	614	CLA	CHA-CBD-CGD-O2D
25	C	505	CLA	CHA-CBD-CGD-O2D
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	CHA-CBD-CGD-O1D
25	C	512	CLA	CHA-CBD-CGD-O2D
25	b	604	CLA	CHA-CBD-CGD-O1D
25	b	604	CLA	CHA-CBD-CGD-O2D
25	b	605	CLA	CHA-CBD-CGD-O2D
25	b	609	CLA	CHA-CBD-CGD-O2D
25	b	611	CLA	CHA-CBD-CGD-O2D
25	b	614	CLA	CHA-CBD-CGD-O1D
25	b	614	CLA	CHA-CBD-CGD-O2D
25	c	505	CLA	CHA-CBD-CGD-O2D
25	c	508	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O2D
25	c	512	CLA	CHA-CBD-CGD-O1D
25	c	512	CLA	CHA-CBD-CGD-O2D
25	B	612	CLA	CAA-CBA-CGA-O2A
25	b	612	CLA	CAA-CBA-CGA-O2A
25	C	511	CLA	CAA-CBA-CGA-O2A
25	c	511	CLA	CAA-CBA-CGA-O2A
30	c	501	SQD	O48-C23-C24-C25
31	H	102	LMT	C3-C4-C5-C6
31	h	102	LMT	C3-C4-C5-C6
26	A	407	PHO	CHA-CBD-CGD-O1D
26	D	402	PHO	CHA-CBD-CGD-O1D
26	a	407	PHO	CHA-CBD-CGD-O1D
26	d	402	PHO	CHA-CBD-CGD-O1D
25	c	505	CLA	C8-C10-C11-C12
30	C	501	SQD	O48-C23-C24-C25
33	D	406	LHG	C17-C18-C19-C20
33	d	406	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
34	H	104	DGD	CAB-CBB-CCB-CDB
25	B	614	CLA	C11-C10-C8-C7
25	D	401	CLA	C11-C10-C8-C7
25	D	401	CLA	C12-C13-C15-C16
25	D	404	CLA	C2-C3-C5-C6
25	b	614	CLA	C11-C10-C8-C7
25	d	401	CLA	C12-C13-C15-C16
25	d	404	CLA	C2-C3-C5-C6
25	B	602	CLA	C16-C17-C18-C19
25	B	614	CLA	C16-C17-C18-C20
25	C	509	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C20
25	c	509	CLA	C16-C17-C18-C20
29	A	411	PL9	C4-C3-C7-C8
29	D	405	PL9	C4-C3-C7-C8
29	a	411	PL9	C4-C3-C7-C8
29	d	405	PL9	C4-C3-C7-C8
34	h	104	DGD	CAB-CBB-CCB-CDB
31	D	411	LMT	O5'-C1'-O1'-C1
31	d	411	LMT	O5'-C1'-O1'-C1
25	C	505	CLA	C8-C10-C11-C12
25	C	507	CLA	C3-C5-C6-C7
25	c	507	CLA	C3-C5-C6-C7
31	h	102	LMT	C1-C2-C3-C4
25	A	408	CLA	C11-C10-C8-C9
25	B	602	CLA	C14-C13-C15-C16
25	B	606	CLA	C11-C10-C8-C9
25	D	401	CLA	C14-C13-C15-C16
25	a	408	CLA	C11-C10-C8-C9
25	b	602	CLA	C14-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C9
25	d	401	CLA	C11-C10-C8-C9
25	d	401	CLA	C14-C13-C15-C16
29	D	405	PL9	C44-C46-C47-C48
29	d	405	PL9	C44-C46-C47-C48
36	H	101	RRX	C9-C10-C11-C12
36	h	101	RRX	C9-C10-C11-C12
31	H	102	LMT	C1-C2-C3-C4
31	f	103	LMT	C5-C6-C7-C8
30	K	101	SQD	O10-C23-C24-C25
30	k	101	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
30	A	412	SQD	C4-C5-C6-S
30	B	620	SQD	C4-C5-C6-S
30	a	412	SQD	C4-C5-C6-S
30	b	620	SQD	C4-C5-C6-S
31	F	103	LMT	C5-C6-C7-C8
25	B	612	CLA	CAA-CBA-CGA-O1A
25	b	612	CLA	CAA-CBA-CGA-O1A
30	A	412	SQD	C26-C27-C28-C29
30	a	412	SQD	C26-C27-C28-C29
28	c	523	LMG	C32-C33-C34-C35
28	h	105	LMG	C12-C13-C14-C15
33	D	406	LHG	C19-C20-C21-C22
33	d	406	LHG	C19-C20-C21-C22
28	C	523	LMG	C32-C33-C34-C35
28	H	105	LMG	C12-C13-C14-C15
25	A	406	CLA	C1A-C2A-CAA-CBA
25	B	607	CLA	C1A-C2A-CAA-CBA
25	a	406	CLA	C1A-C2A-CAA-CBA
25	b	607	CLA	C1A-C2A-CAA-CBA
25	B	608	CLA	C2-C1-O2A-CGA
25	b	608	CLA	C2-C1-O2A-CGA
31	X	105	LMT	C1-C2-C3-C4
31	x	105	LMT	C1-C2-C3-C4
33	D	407	LHG	C32-C33-C34-C35
33	b	628	LHG	C10-C11-C12-C13
33	d	407	LHG	C32-C33-C34-C35
28	A	410	LMG	C7-C8-C9-O8
28	a	410	LMG	C7-C8-C9-O8
25	C	513	CLA	CAA-CBA-CGA-O2A
25	c	513	CLA	CAA-CBA-CGA-O2A
25	A	405	CLA	C2A-CAA-CBA-CGA
25	a	405	CLA	C2A-CAA-CBA-CGA
25	c	502	CLA	CBD-CGD-O2D-CED
33	B	628	LHG	C10-C11-C12-C13
25	B	612	CLA	C16-C17-C18-C19
25	b	612	CLA	C16-C17-C18-C19
28	A	410	LMG	O9-C10-C11-C12
28	a	410	LMG	O9-C10-C11-C12
28	c	519	LMG	C32-C33-C34-C35
25	C	502	CLA	CBD-CGD-O2D-CED
28	C	519	LMG	C32-C33-C34-C35
30	C	501	SQD	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
28	D	409	LMG	O7-C10-C11-C12
28	d	409	LMG	O7-C10-C11-C12
30	c	501	SQD	C19-C20-C21-C22
28	C	523	LMG	O10-C28-C29-C30
33	E	102	LHG	O10-C23-C24-C25
33	e	102	LHG	O10-C23-C24-C25
31	I	101	LMT	C4-C5-C6-C7
31	i	101	LMT	C4-C5-C6-C7
33	B	628	LHG	C3-O3-P-O5
33	D	408	LHG	C4-O6-P-O5
33	b	628	LHG	C3-O3-P-O5
33	d	408	LHG	C4-O6-P-O5
28	A	410	LMG	C36-C37-C38-C39
25	B	614	CLA	CAA-CBA-CGA-O1A
25	b	614	CLA	CAA-CBA-CGA-O1A
25	c	506	CLA	CAA-CBA-CGA-O1A
28	c	523	LMG	O10-C28-C29-C30
33	D	407	LHG	O10-C23-C24-C25
33	d	407	LHG	O10-C23-C24-C25
30	C	501	SQD	O5-C1-O6-C44
30	c	501	SQD	O5-C1-O6-C44
29	D	405	PL9	C7-C8-C9-C10
29	d	405	PL9	C7-C8-C9-C10
27	Z	101	BCR	C1-C6-C7-C8
27	z	101	BCR	C1-C6-C7-C8
25	C	506	CLA	CAA-CBA-CGA-O1A
25	C	511	CLA	CAA-CBA-CGA-O1A
25	c	511	CLA	CAA-CBA-CGA-O1A
30	A	412	SQD	O49-C7-C8-C9
30	a	412	SQD	O49-C7-C8-C9
28	a	410	LMG	C36-C37-C38-C39
25	c	508	CLA	C8-C10-C11-C12
25	C	508	CLA	C8-C10-C11-C12
25	d	403	CLA	C10-C11-C12-C13
31	B	624	LMT	C3-C4-C5-C6
31	b	624	LMT	C3-C4-C5-C6
30	C	501	SQD	C34-C35-C36-C37
30	c	501	SQD	C34-C35-C36-C37
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	604	CLA	CAD-CBD-CGD-O1D
25	B	612	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	C	511	CLA	CAD-CBD-CGD-O1D
25	b	601	CLA	CAD-CBD-CGD-O1D
25	b	604	CLA	CAD-CBD-CGD-O1D
25	b	612	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	511	CLA	CAD-CBD-CGD-O1D
30	A	412	SQD	O5-C5-C6-S
30	a	412	SQD	O5-C5-C6-S
25	C	513	CLA	CAA-CBA-CGA-O1A
25	c	513	CLA	CAA-CBA-CGA-O1A
25	b	608	CLA	CAA-CBA-CGA-O2A
30	B	620	SQD	O48-C23-C24-C25
30	b	620	SQD	O48-C23-C24-C25
25	D	403	CLA	C10-C11-C12-C13
25	B	607	CLA	C6-C7-C8-C9
25	B	615	CLA	C6-C7-C8-C9
25	C	508	CLA	C11-C10-C8-C9
25	C	511	CLA	C14-C13-C15-C16
25	D	401	CLA	C11-C10-C8-C9
25	b	607	CLA	C6-C7-C8-C9
25	b	615	CLA	C6-C7-C8-C9
25	c	508	CLA	C11-C10-C8-C9
25	c	511	CLA	C14-C13-C15-C16
33	E	102	LHG	O1-C1-C2-O2
33	e	102	LHG	O1-C1-C2-O2
30	C	501	SQD	O10-C23-C24-C25
30	c	501	SQD	O10-C23-C24-C25
25	B	608	CLA	CAA-CBA-CGA-O2A
31	B	625	LMT	C4-C5-C6-C7
31	b	625	LMT	C4-C5-C6-C7
34	C	516	DGD	C6A-C7A-C8A-C9A
34	c	516	DGD	C6A-C7A-C8A-C9A
30	K	101	SQD	C11-C12-C13-C14
30	k	101	SQD	C11-C12-C13-C14
28	A	410	LMG	C29-C30-C31-C32
28	a	410	LMG	C29-C30-C31-C32
25	B	606	CLA	C4-C3-C5-C6
25	b	606	CLA	C4-C3-C5-C6
25	C	502	CLA	C2-C3-C5-C6
25	C	508	CLA	C11-C10-C8-C7
25	C	510	CLA	C11-C12-C13-C15
25	c	502	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	c	508	CLA	C11-C10-C8-C7
25	c	510	CLA	C11-C12-C13-C15
25	d	401	CLA	C11-C10-C8-C7
26	A	407	PHO	C3A-C2A-CAA-CBA
26	a	407	PHO	C3A-C2A-CAA-CBA
30	c	501	SQD	C24-C25-C26-C27
28	C	519	LMG	O7-C10-C11-C12
28	c	519	LMG	O7-C10-C11-C12
33	D	406	LHG	O8-C23-C24-C25
33	d	406	LHG	O8-C23-C24-C25
30	C	501	SQD	C24-C25-C26-C27
31	X	103	LMT	C1-C2-C3-C4
31	x	103	LMT	C1-C2-C3-C4
27	B	617	BCR	C17-C18-C19-C20
27	b	617	BCR	C17-C18-C19-C20
36	H	101	RRX	C7-C8-C9-C10
36	h	101	RRX	C7-C8-C9-C10
25	B	608	CLA	CAA-CBA-CGA-O1A
25	b	608	CLA	CAA-CBA-CGA-O1A
36	H	101	RRX	C15-C16-C17-C18
36	h	101	RRX	C15-C16-C17-C18
25	B	602	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C20
31	B	629	LMT	C2B-C1B-O1B-C4'
31	b	629	LMT	C2B-C1B-O1B-C4'
31	I	103	LMT	C2-C1-O1'-C1'
31	i	103	LMT	C2-C1-O1'-C1'
25	D	403	CLA	CAA-CBA-CGA-O2A
25	d	403	CLA	CAA-CBA-CGA-O2A
28	D	409	LMG	O9-C10-C11-C12
28	d	409	LMG	O9-C10-C11-C12
33	z	102	LHG	C24-C25-C26-C27
33	Z	102	LHG	C24-C25-C26-C27
30	B	620	SQD	O10-C23-C24-C25
30	b	620	SQD	O10-C23-C24-C25
31	A	415	LMT	C1-C2-C3-C4

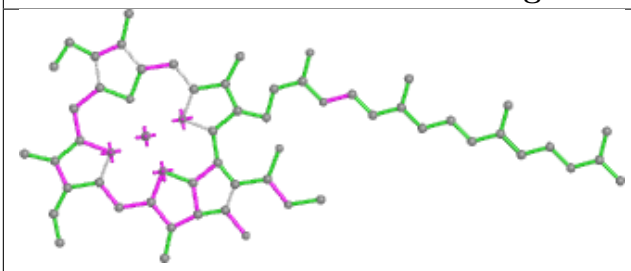
There are no ring outliers.

No monomer is involved in short contacts.

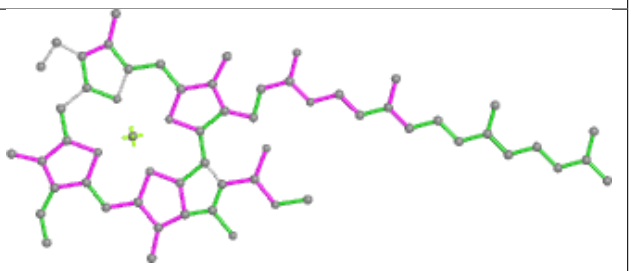
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

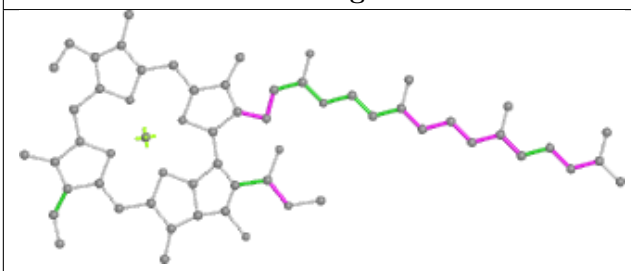
Ligand CLA A 408



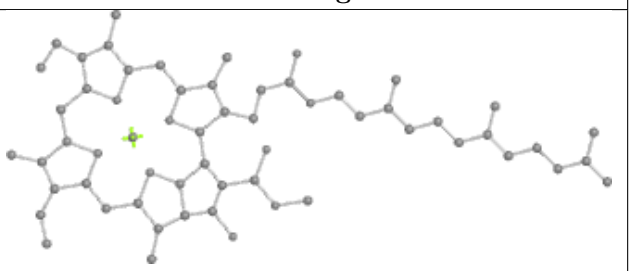
Bond lengths



Bond angles

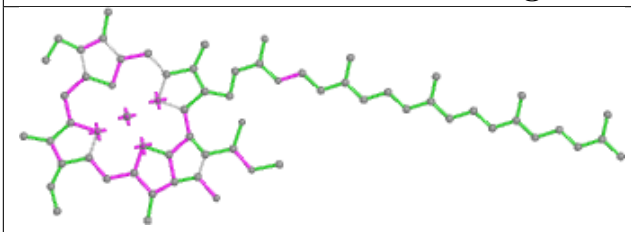


Torsions

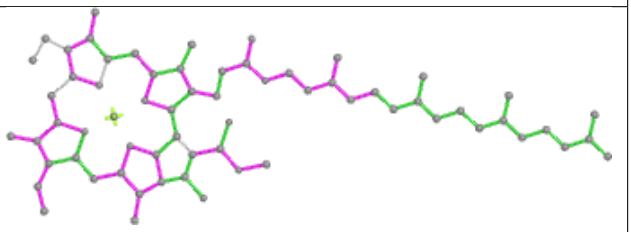


Rings

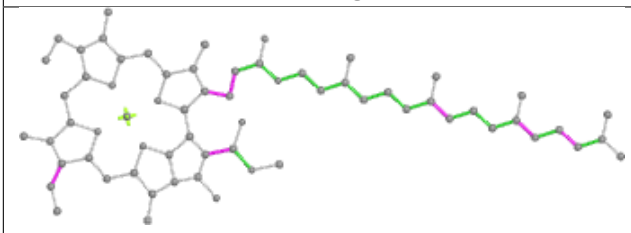
Ligand CLA D 401



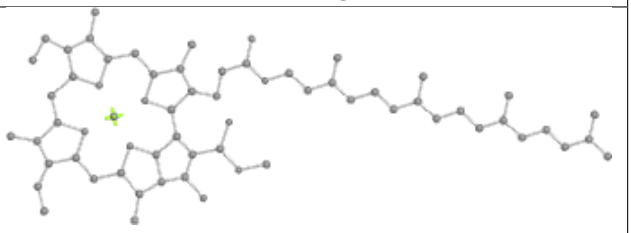
Bond lengths



Bond angles

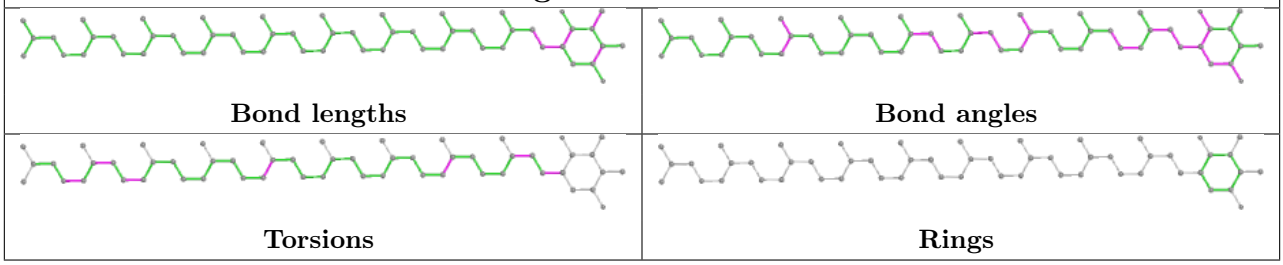


Torsions

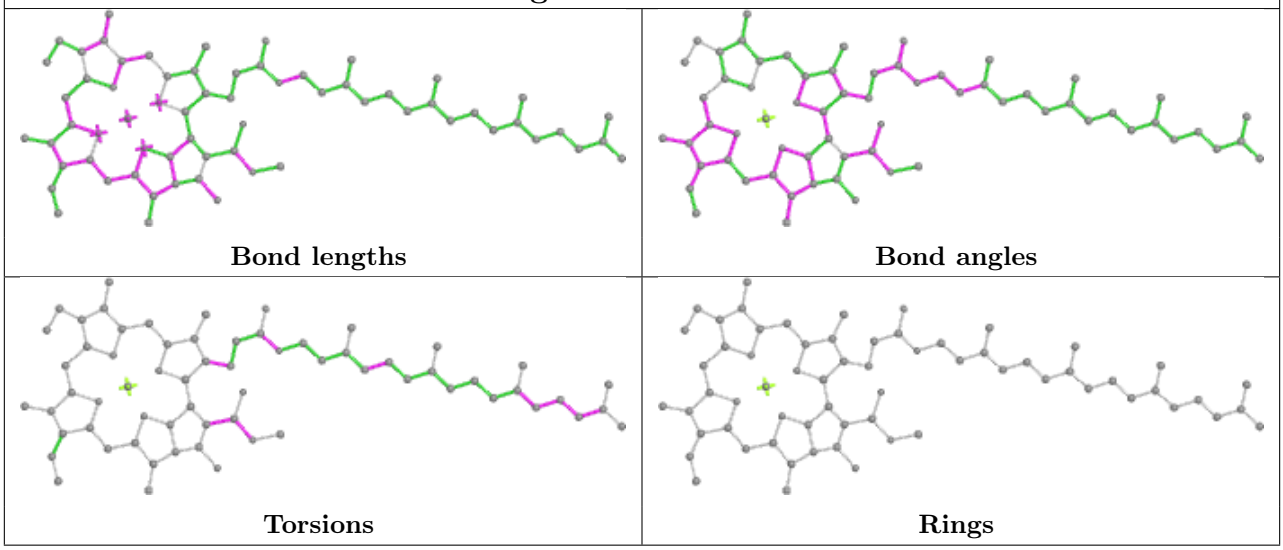


Rings

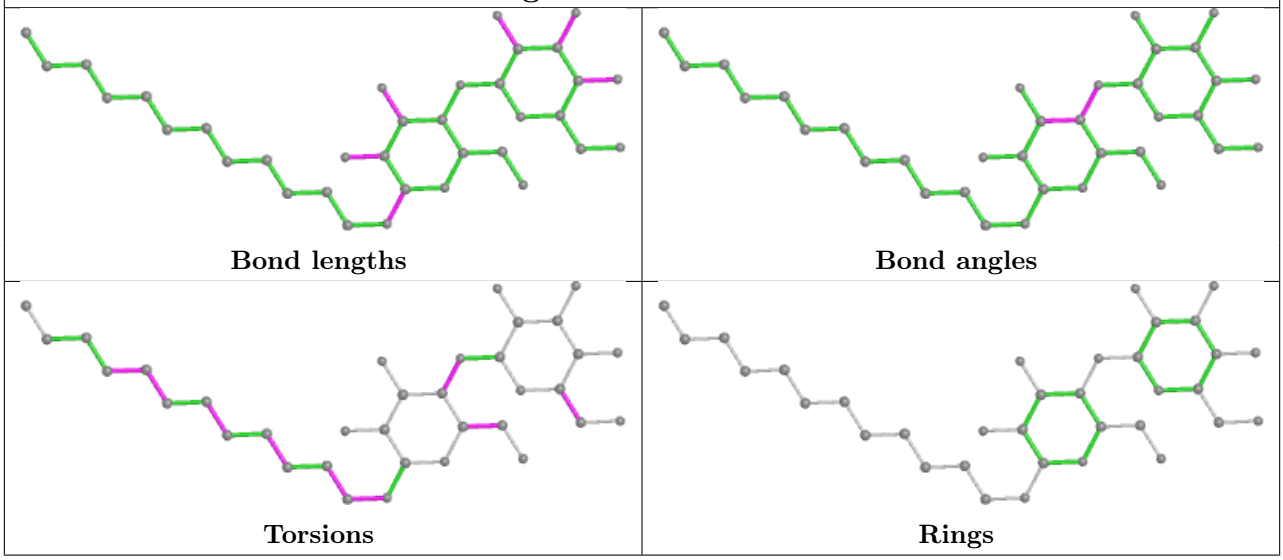
Ligand PL9 d 405



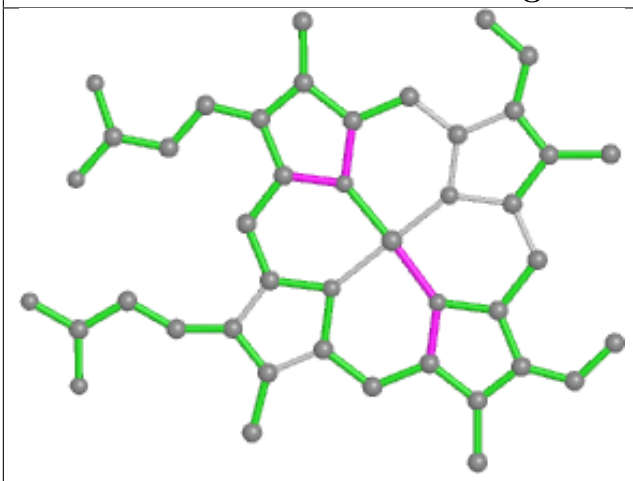
Ligand CLA c 507



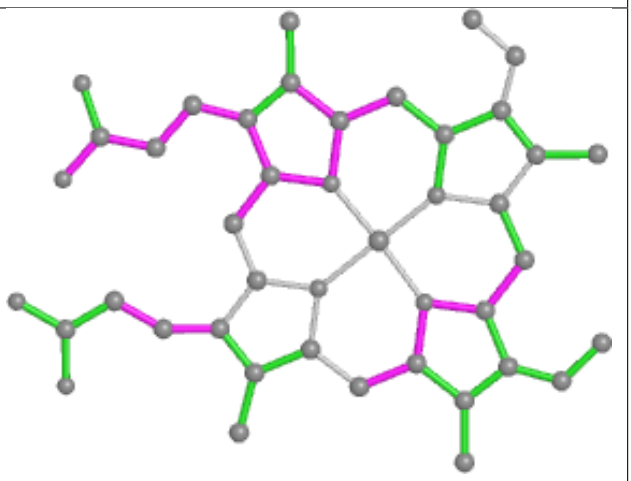
Ligand LMT B 625



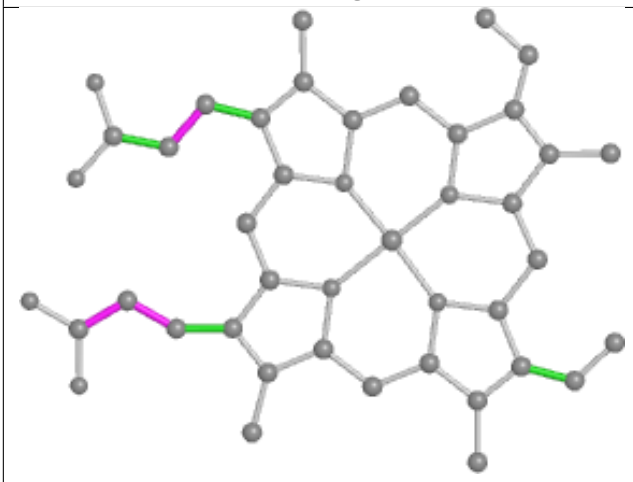
Ligand HEM e 104



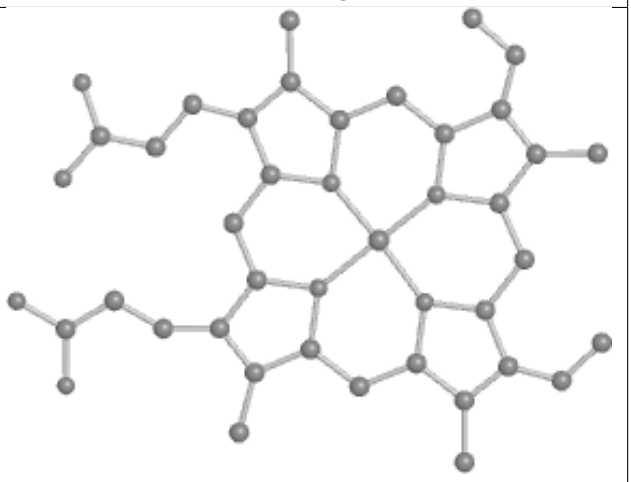
Bond lengths



Bond angles

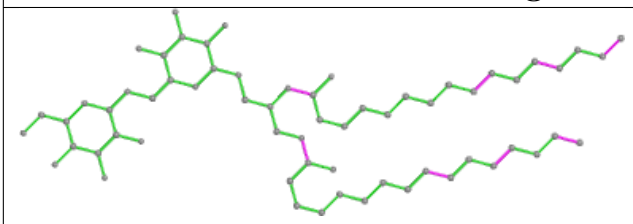


Torsions

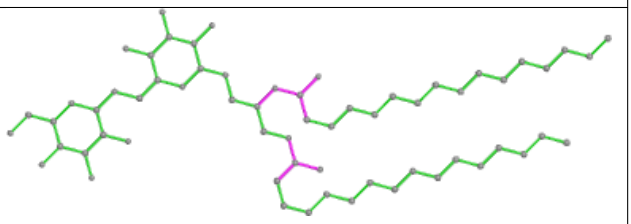


Rings

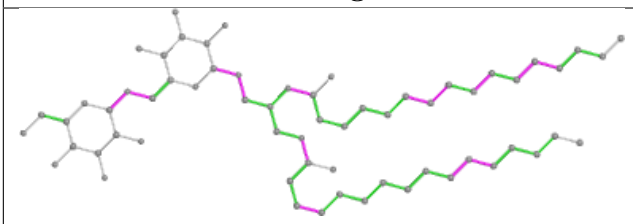
Ligand DGD c 517



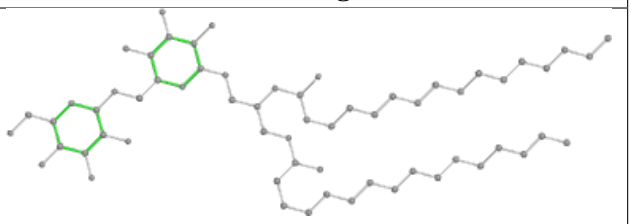
Bond lengths



Bond angles

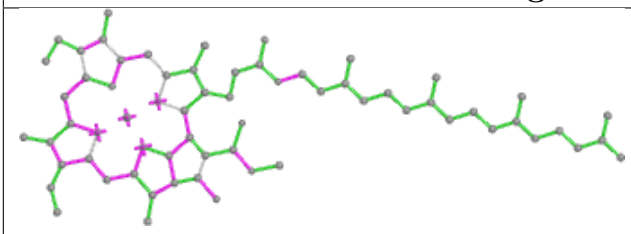


Torsions

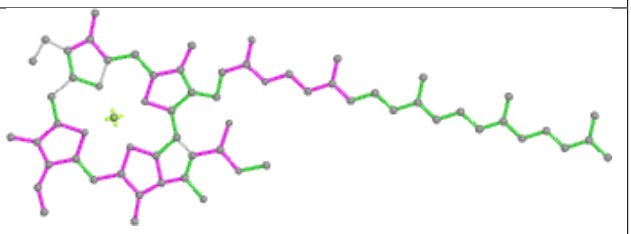


Rings

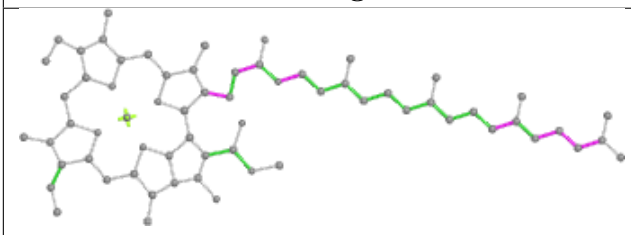
Ligand CLA b 608



Bond lengths



Bond angles



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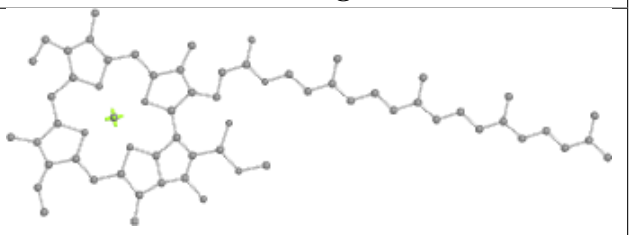
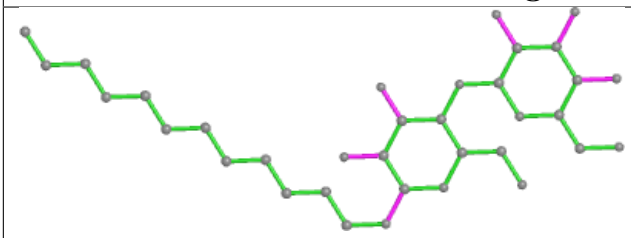
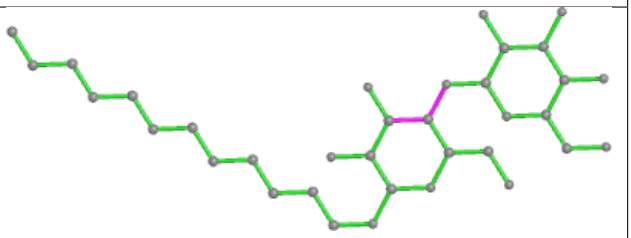


Rings

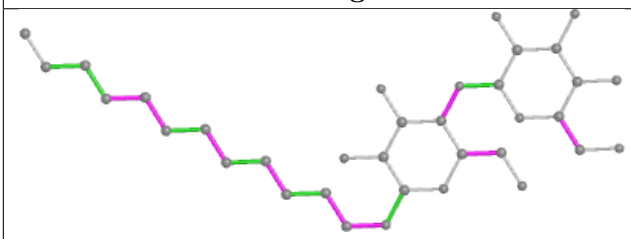
Ligand LMT b 625



Bond lengths



Bond angles



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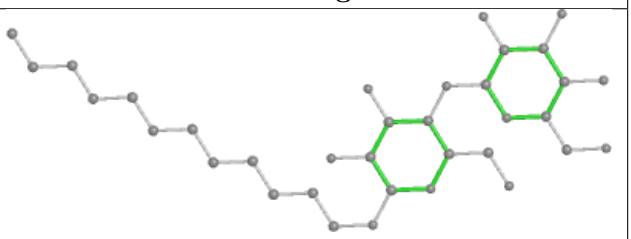
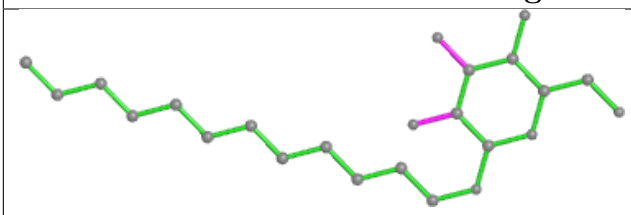
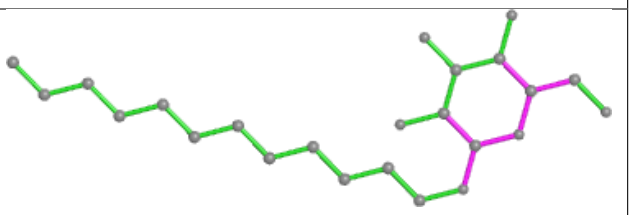


Rings

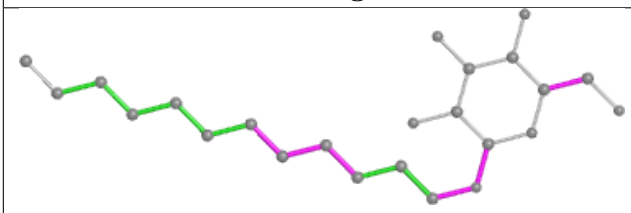
Ligand LMT d 410



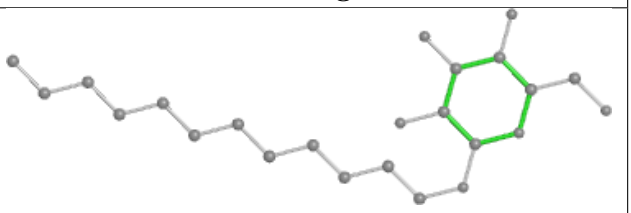
Bond lengths



Bond angles

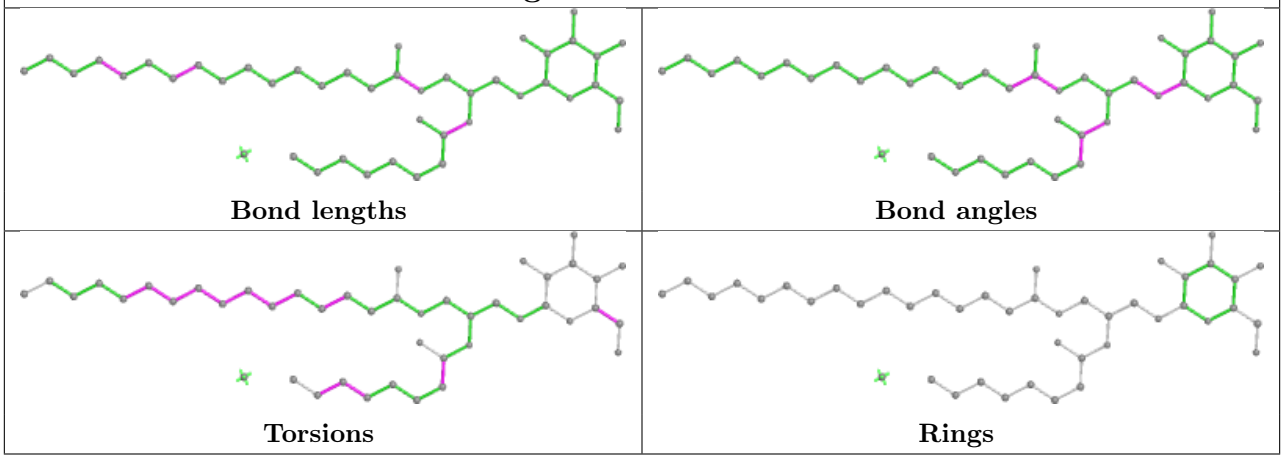


Torsions

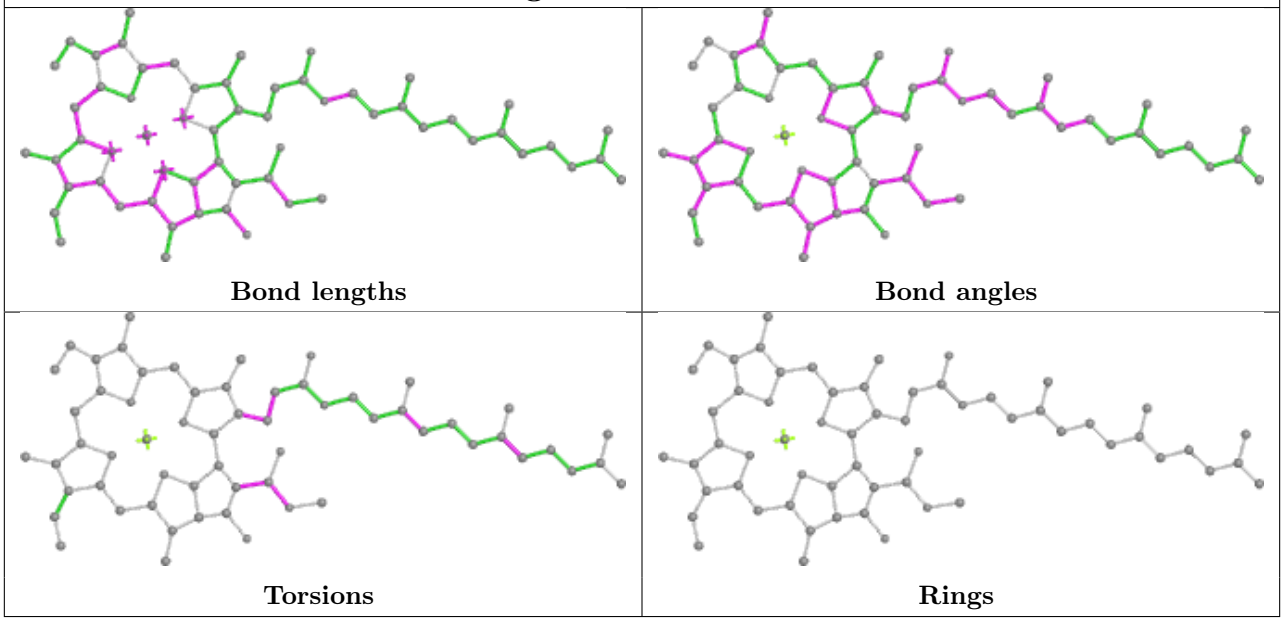


Rings

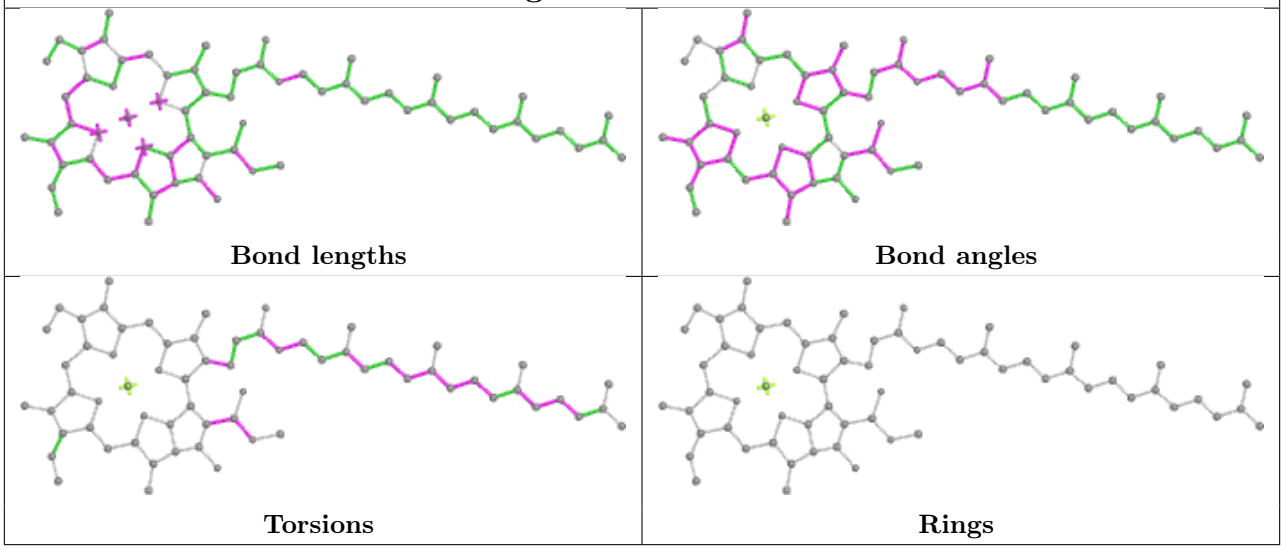
Ligand LMG d 409



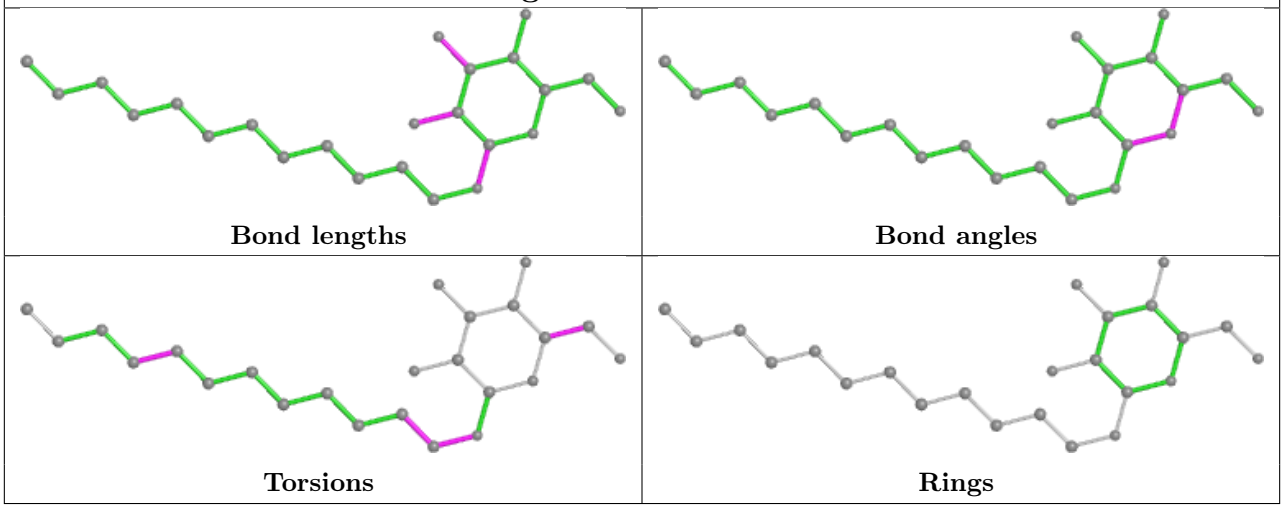
Ligand CLA B 606



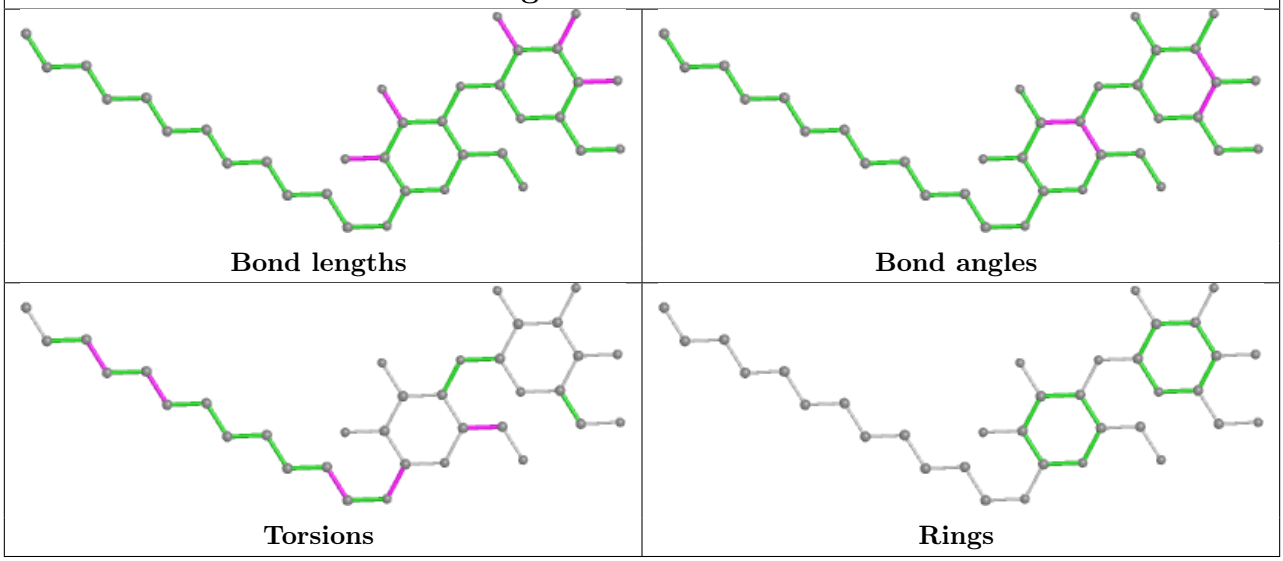
Ligand CLA C 514



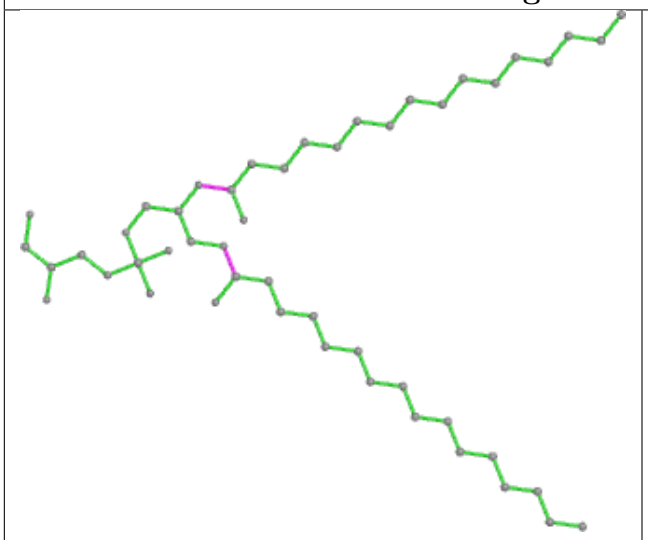
Ligand LMT A 416



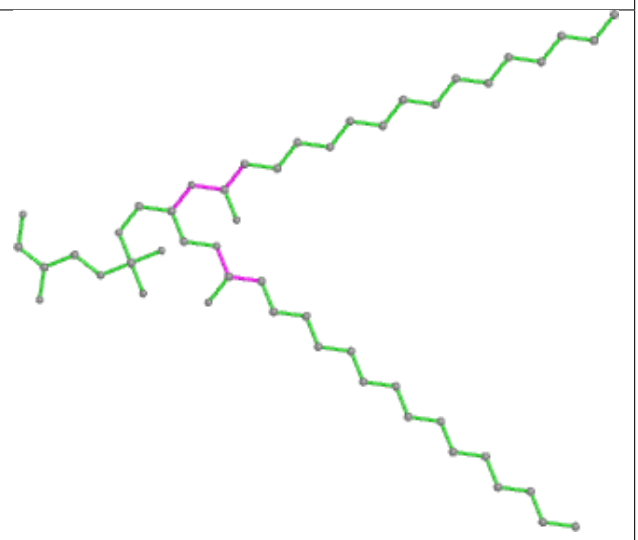
Ligand LMT D 412



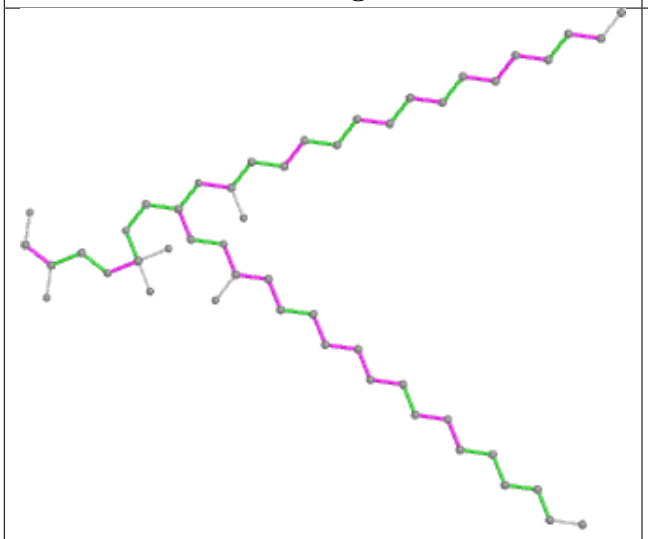
Ligand LHG D 406



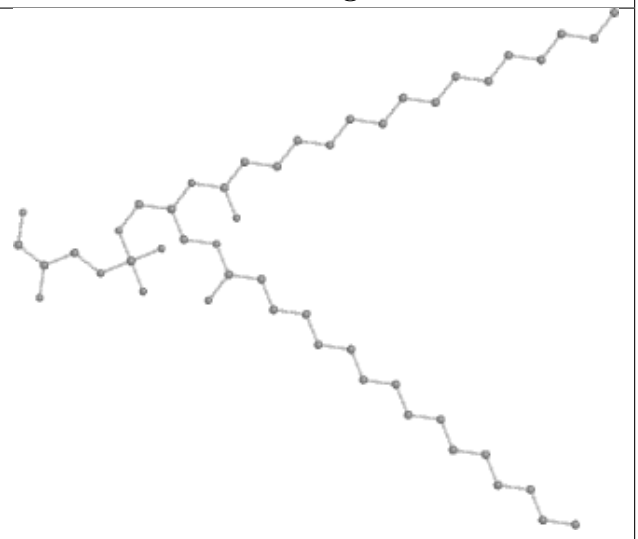
Bond lengths



Bond angles

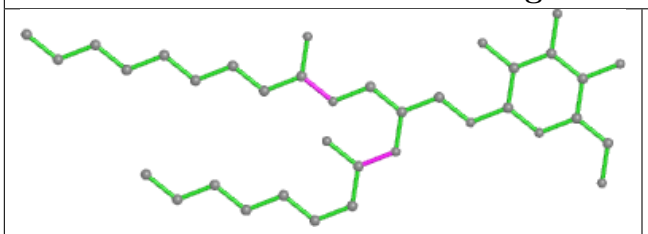


Torsions



Rings

Ligand LMG a 414



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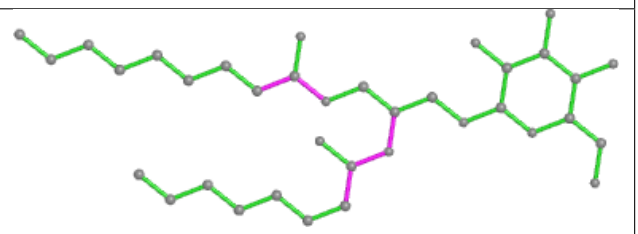
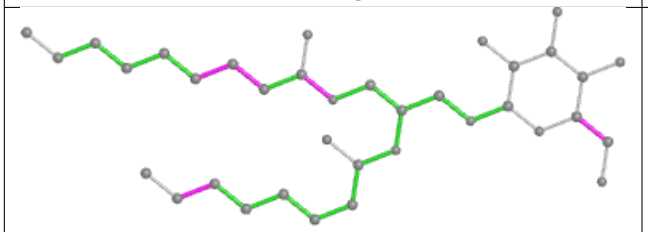
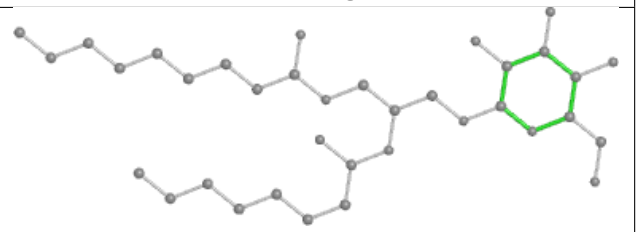


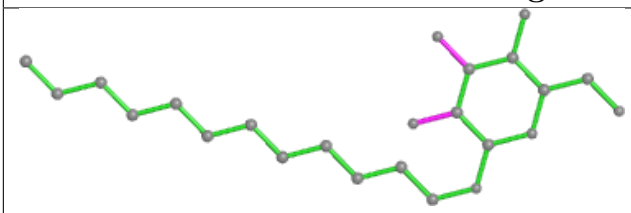
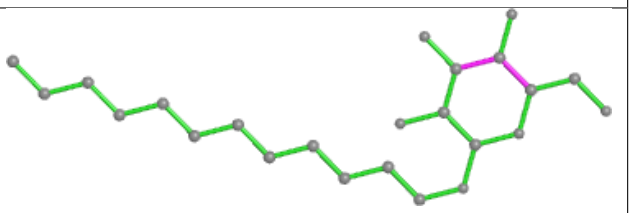
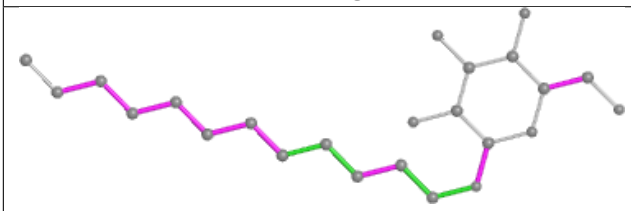
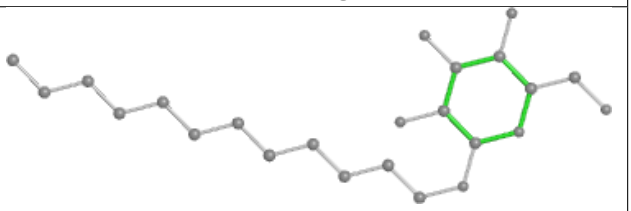
Bond angles

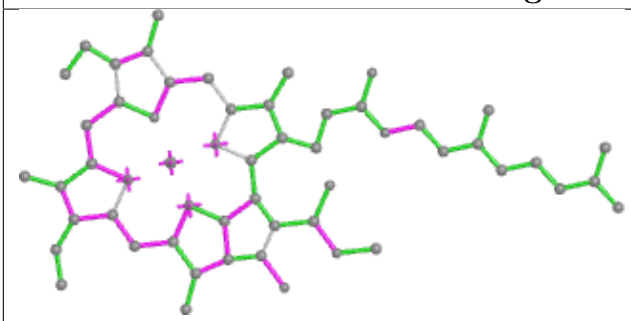
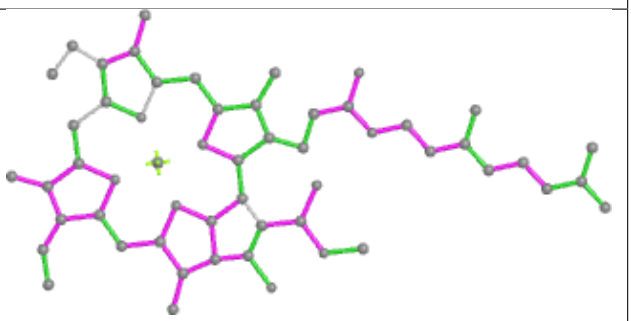
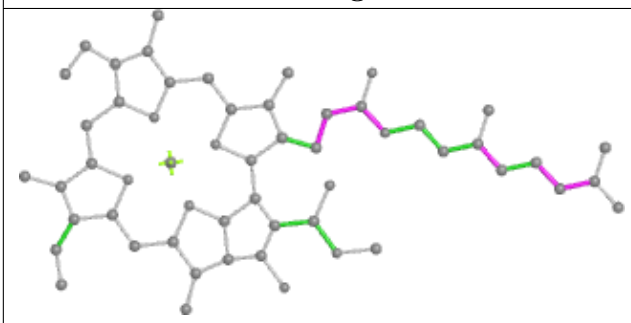
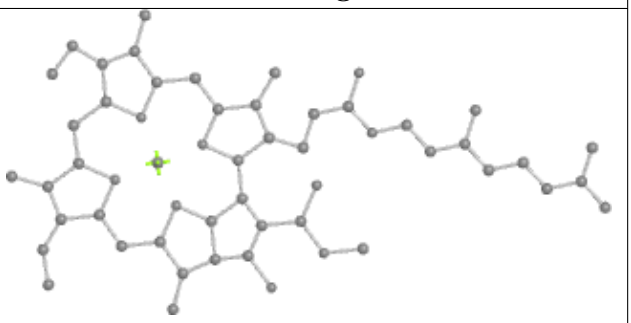


Torsions

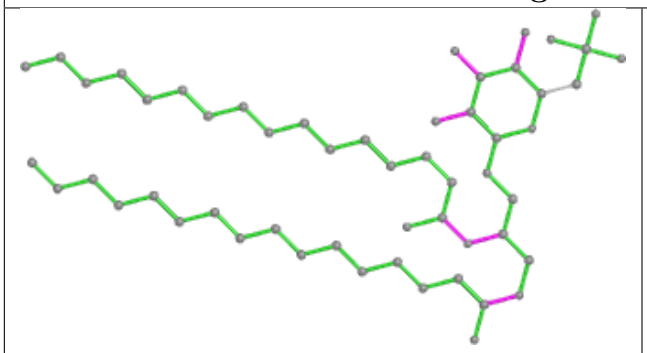


Rings

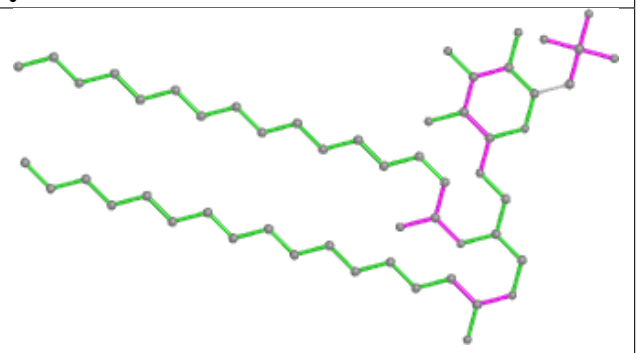
Ligand LMT I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

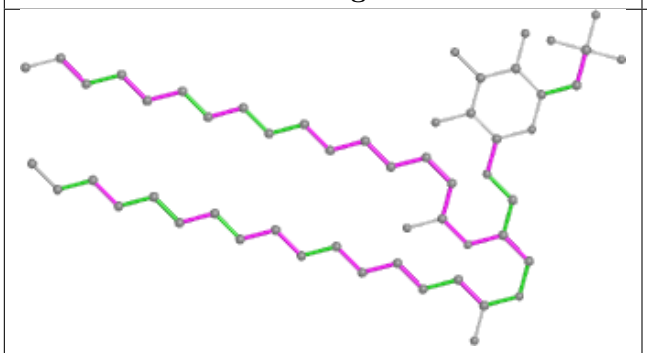
Ligand SQD c 501



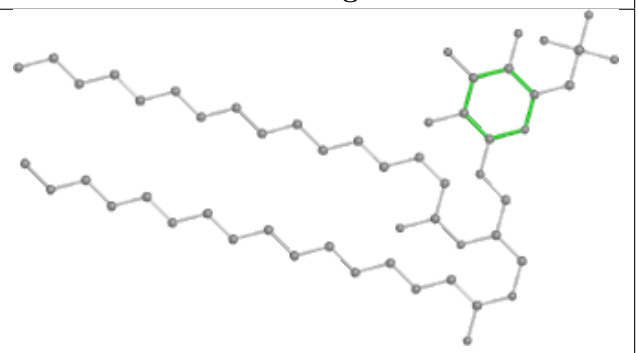
Bond lengths



Bond angles

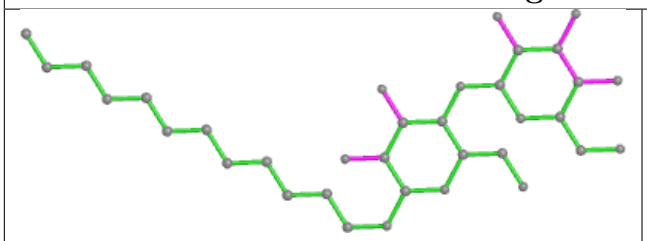


Torsions

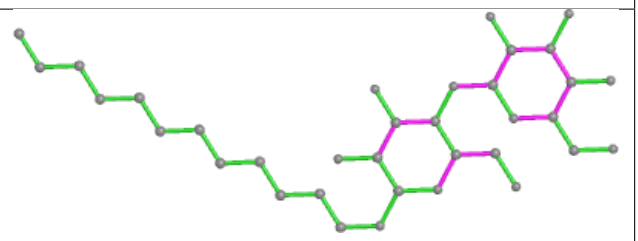


Rings

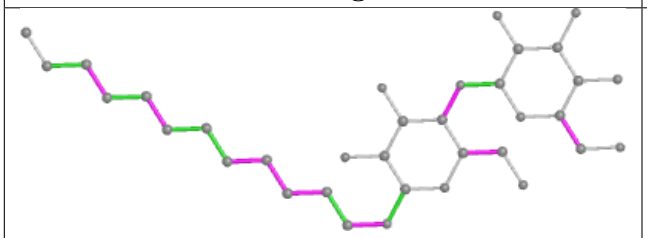
Ligand LMT k 105



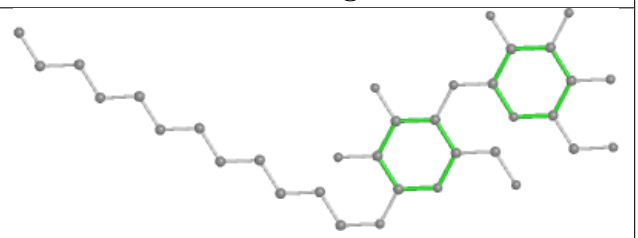
Bond lengths



Bond angles

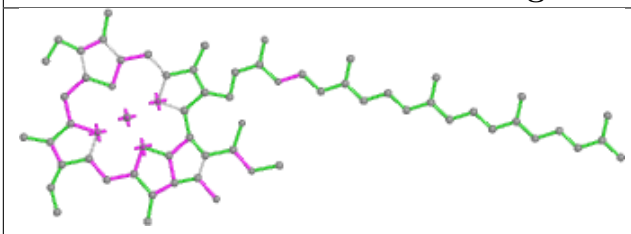


Torsions

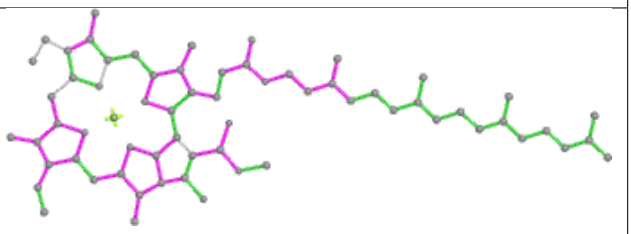


Rings

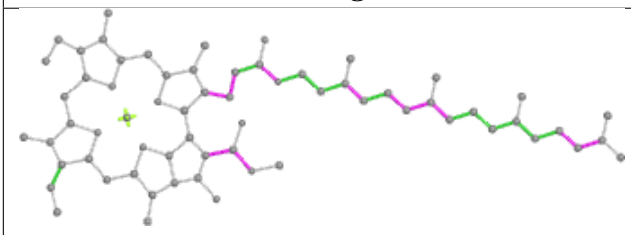
Ligand CLA b 603



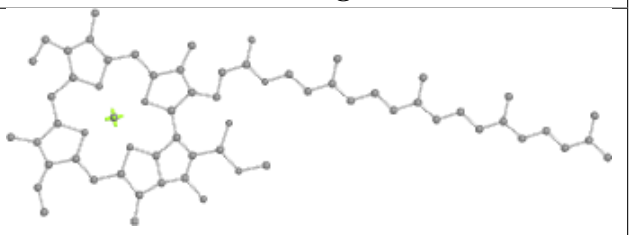
Bond lengths



Bond angles

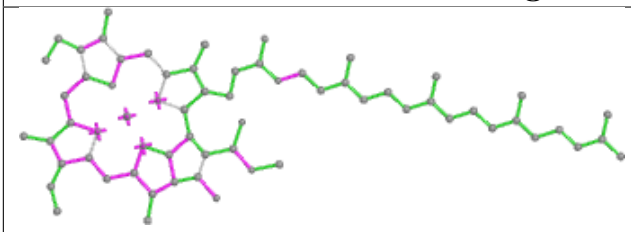


Torsions

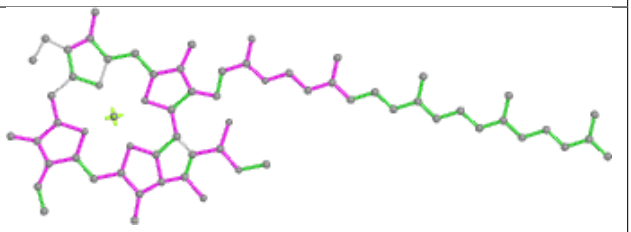


Rings

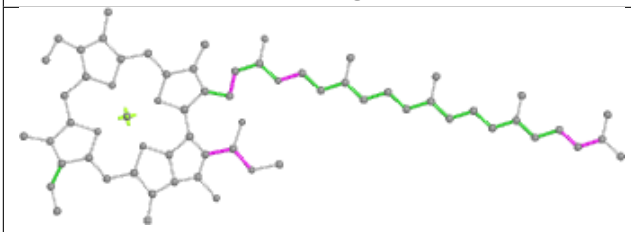
Ligand CLA B 610



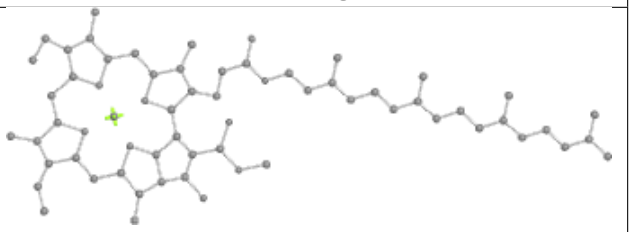
Bond lengths



Bond angles

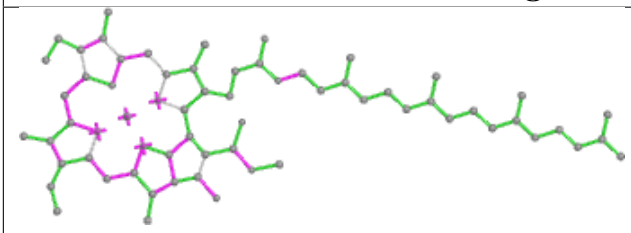


Torsions

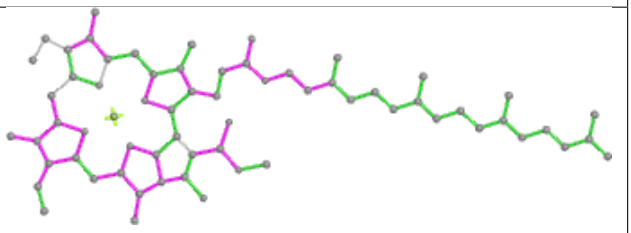


Rings

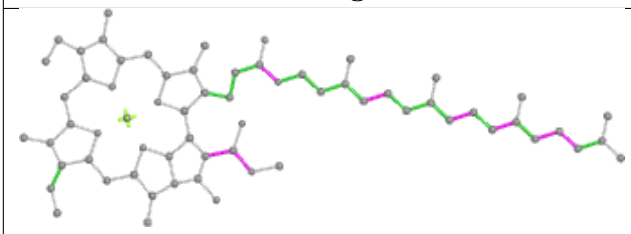
Ligand CLA B 611



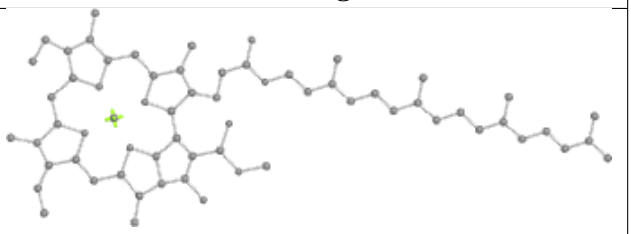
Bond lengths



Bond angles

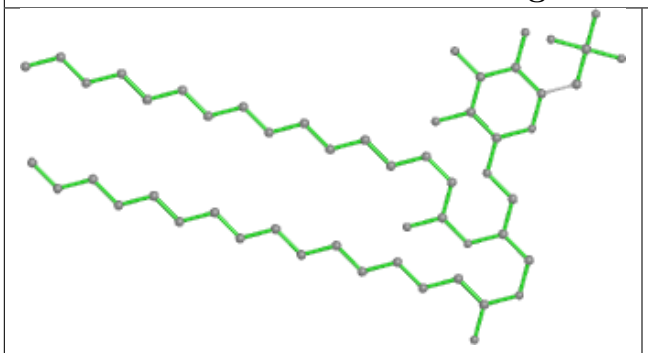


Torsions

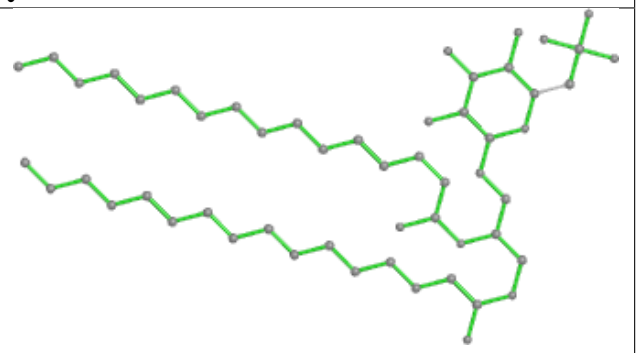


Rings

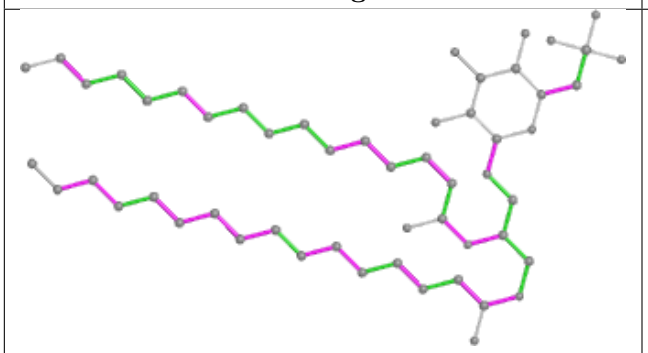
Ligand SQD b 620



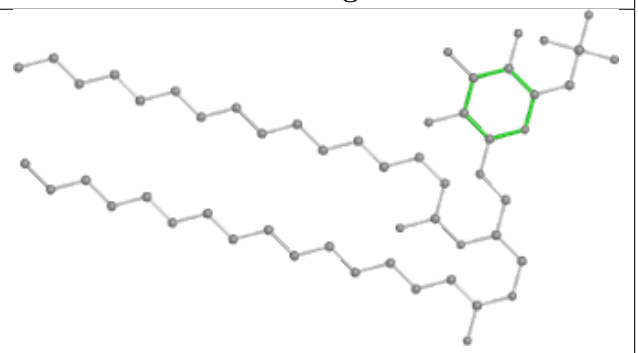
Bond lengths



Bond angles

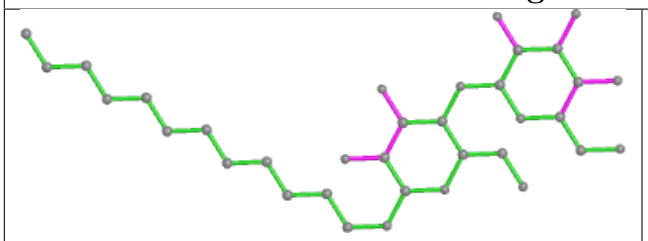


Torsions

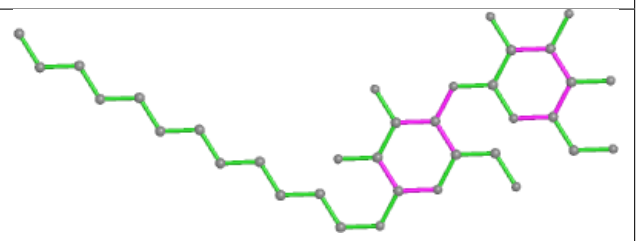


Rings

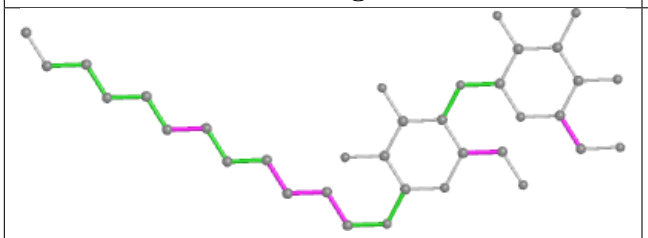
Ligand LMT e 103



Bond lengths



Bond angles



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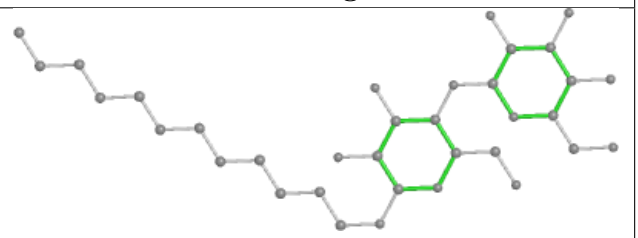
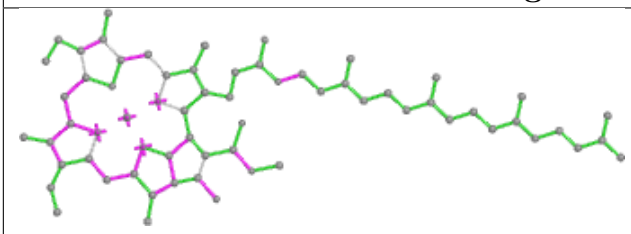
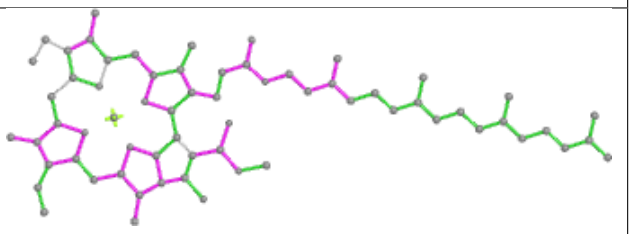


Rings

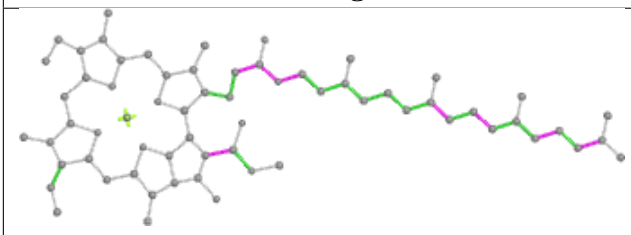
Ligand CLA B 612



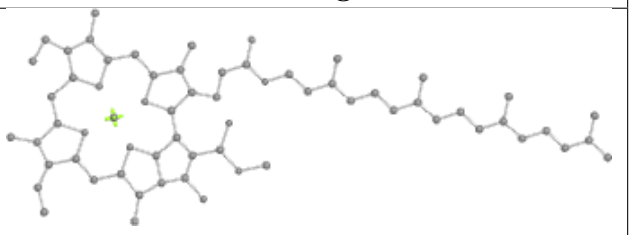
Bond lengths



Bond angles

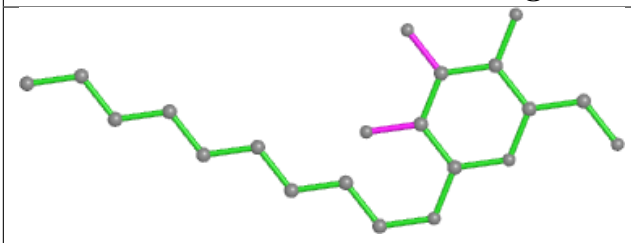


Torsions

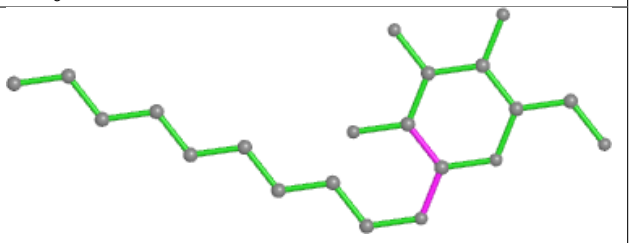


Rings

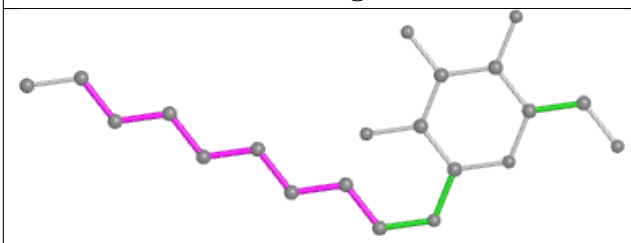
Ligand LMT y 101



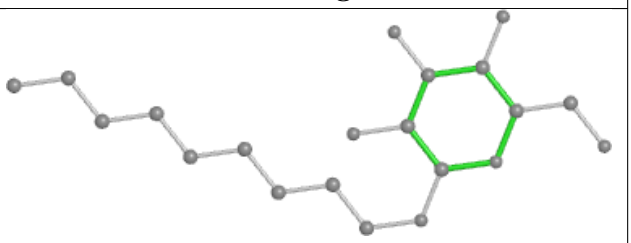
Bond lengths



Bond angles

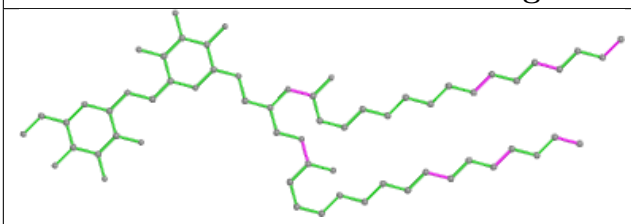


Torsions

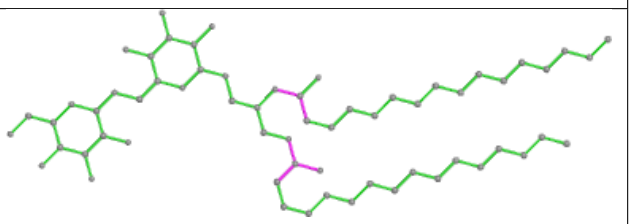


Rings

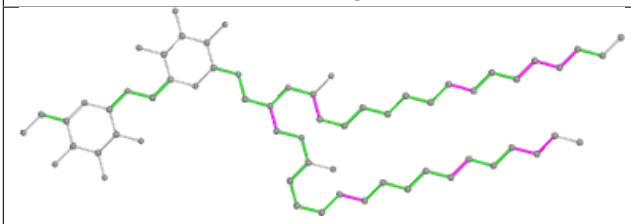
Ligand DGD h 104



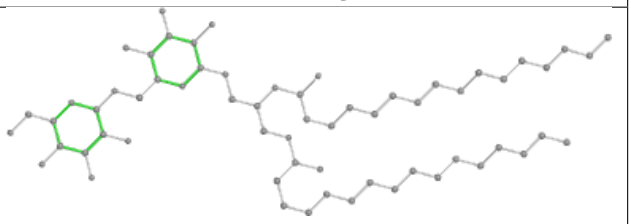
Bond lengths



Bond angles

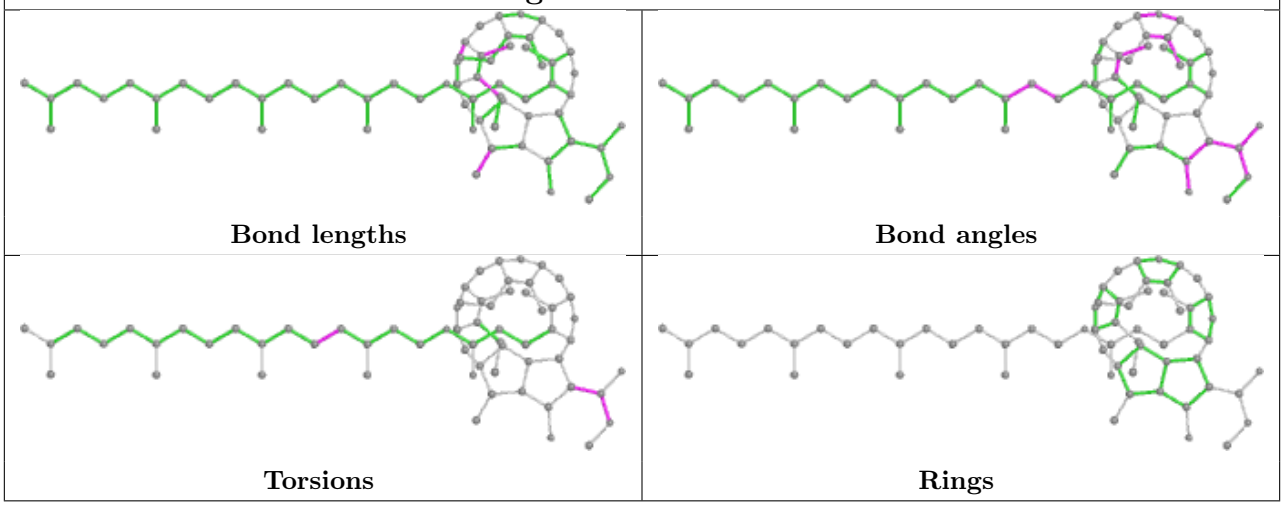


Torsions

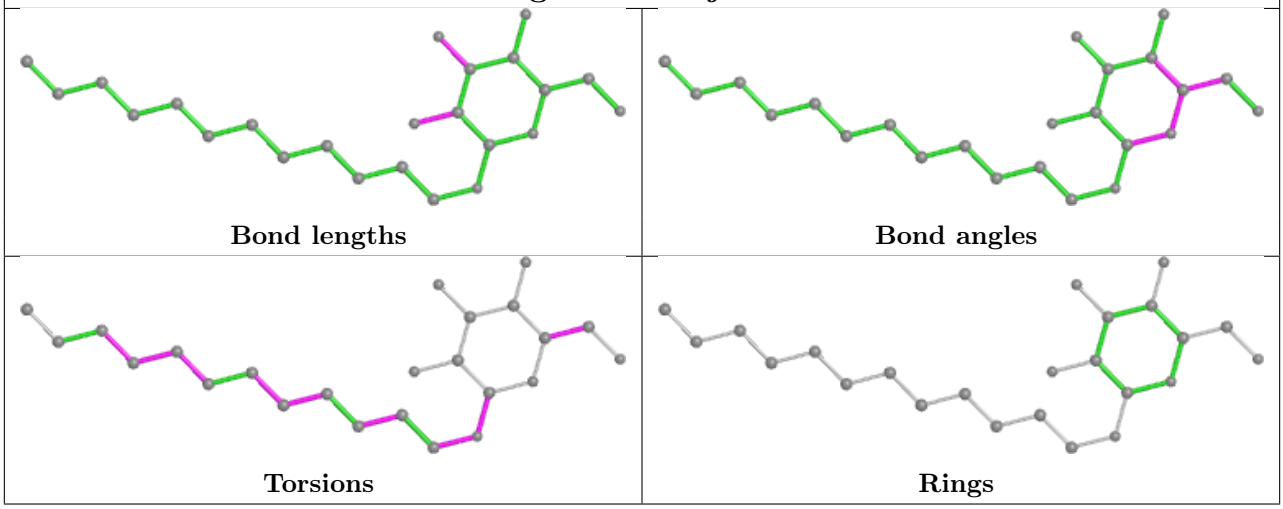


Rings

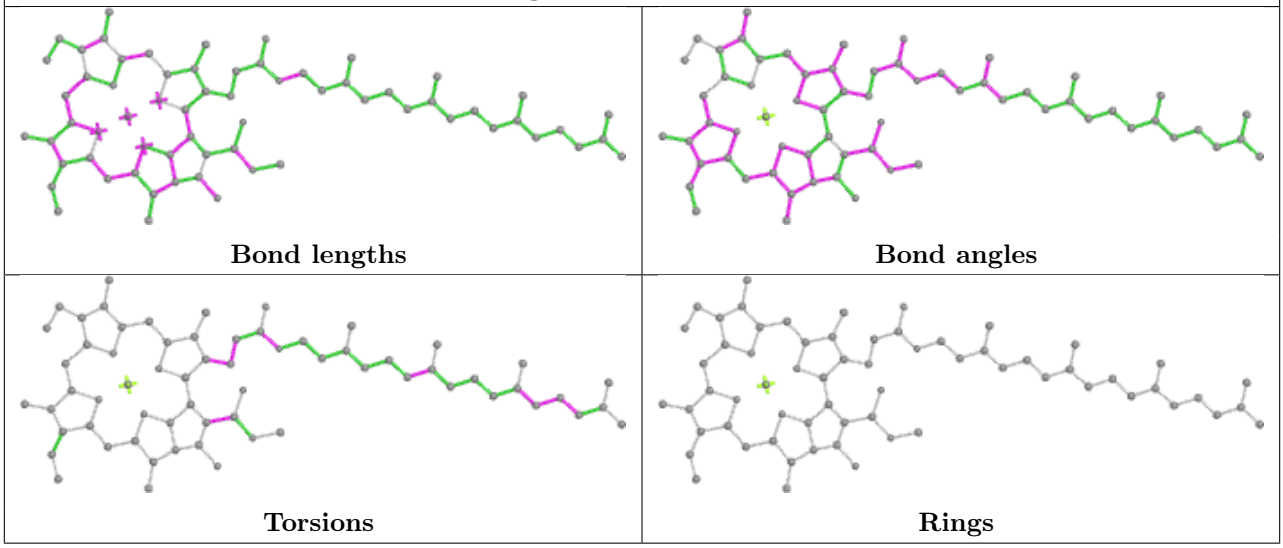
Ligand PHO d 402



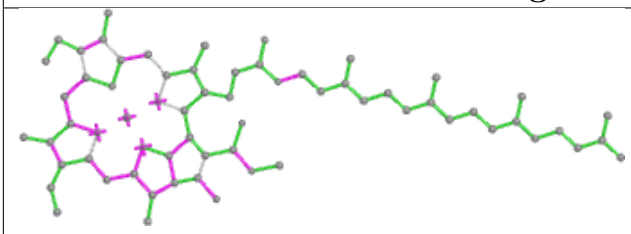
Ligand LMT j 101



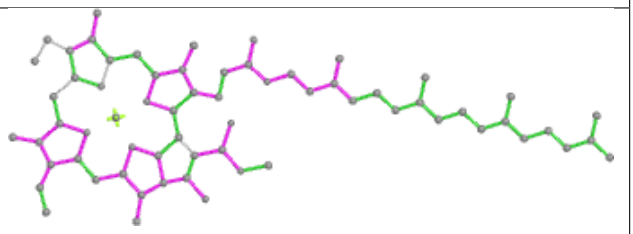
Ligand CLA B 607



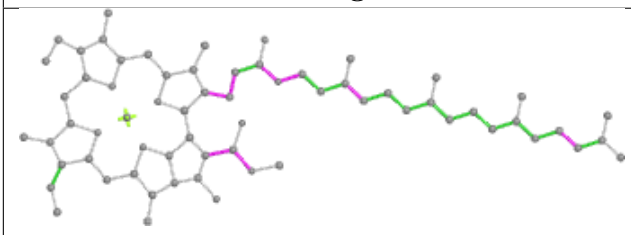
Ligand CLA c 502



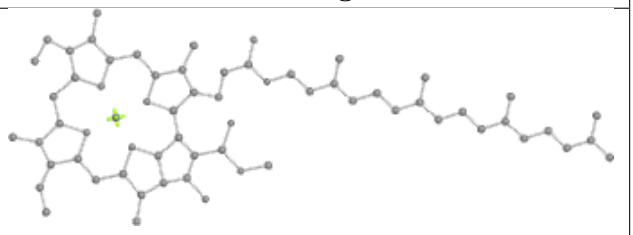
Bond lengths



Bond angles

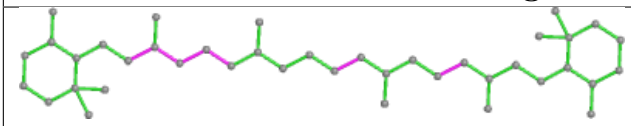


Torsions

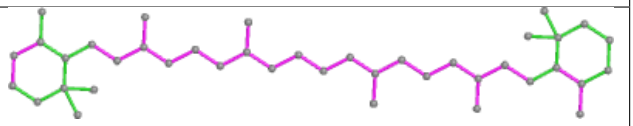


Rings

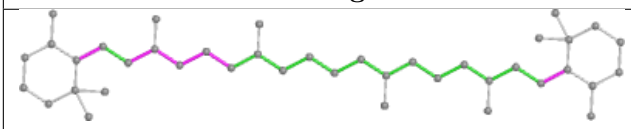
Ligand BCR B 618



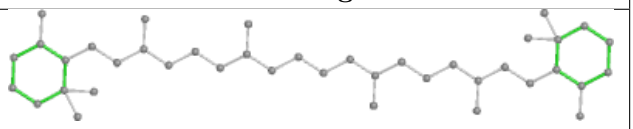
Bond lengths



Bond angles

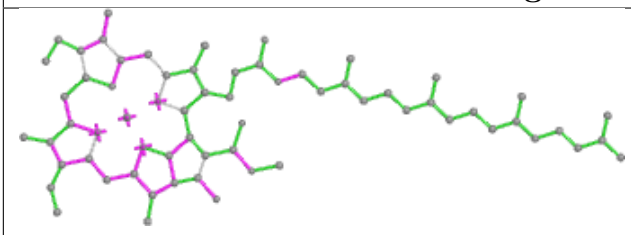


Torsions

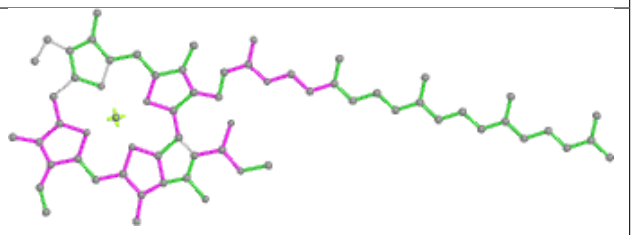


Rings

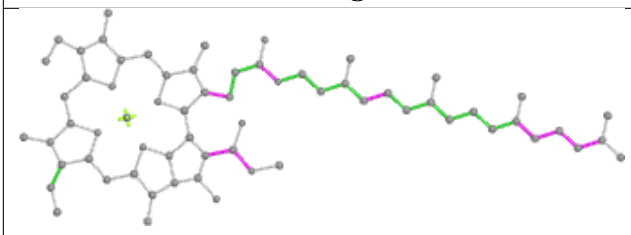
Ligand CLA C 507



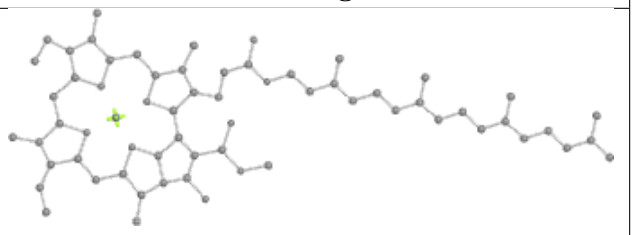
Bond lengths



Bond angles

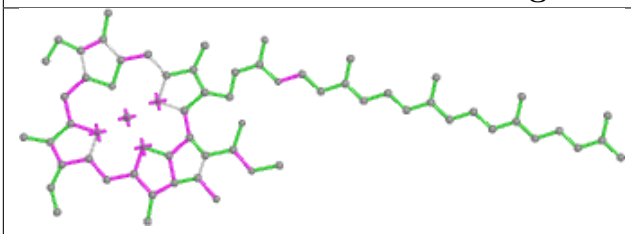


Torsions

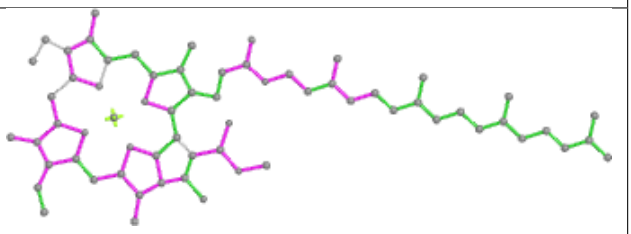


Rings

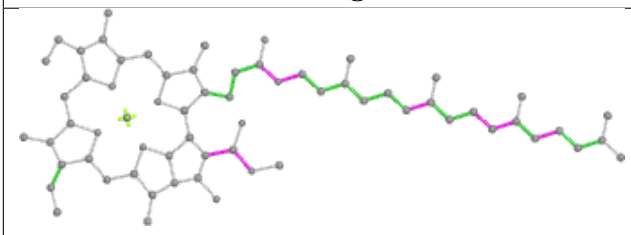
Ligand CLA c 510



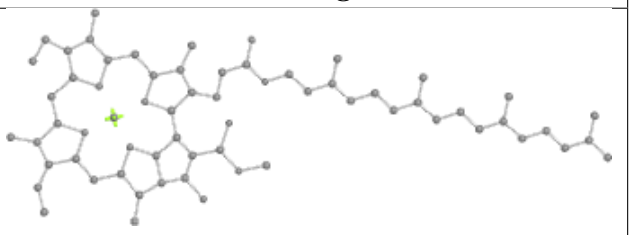
Bond lengths



Bond angles

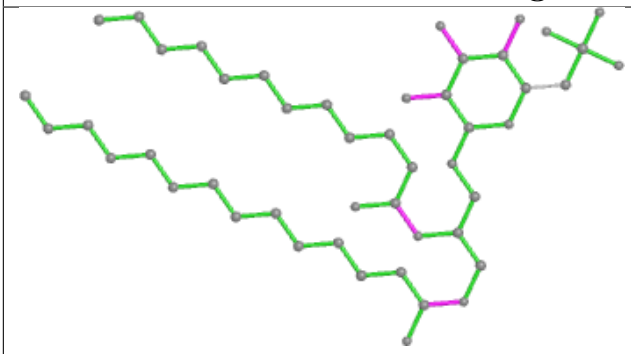


Torsions

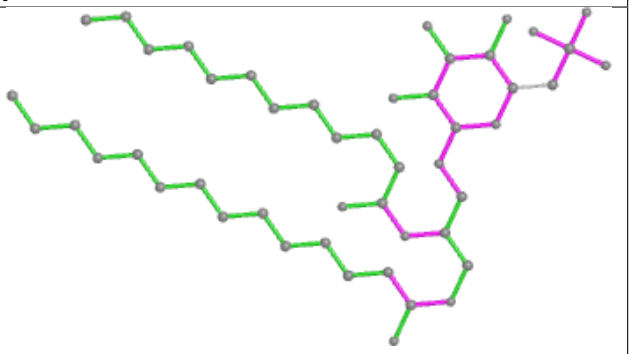


Rings

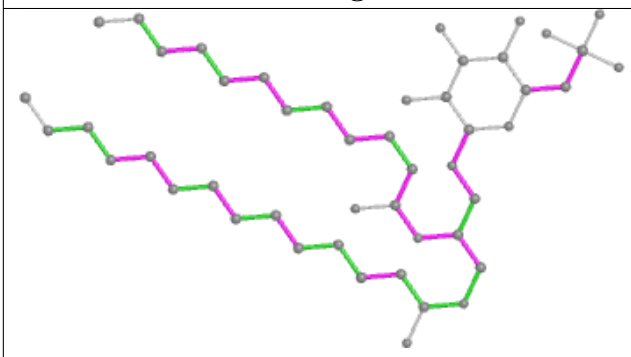
Ligand SQD a 413



Bond lengths



Bond angles



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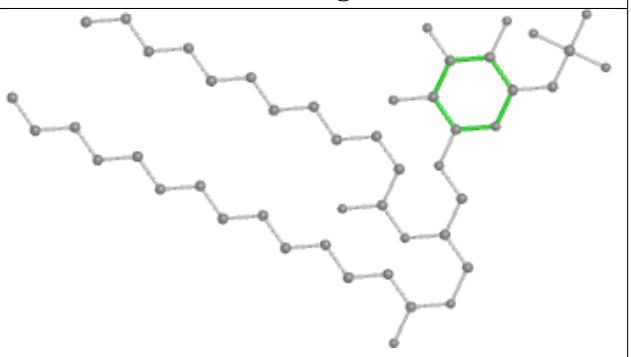
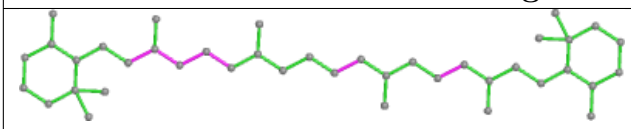
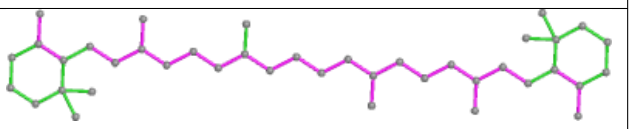


Rings

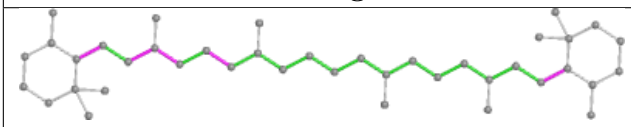
Ligand BCR A 409



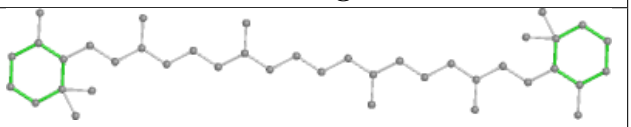
Bond lengths



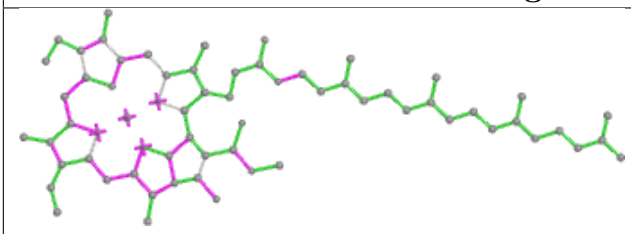
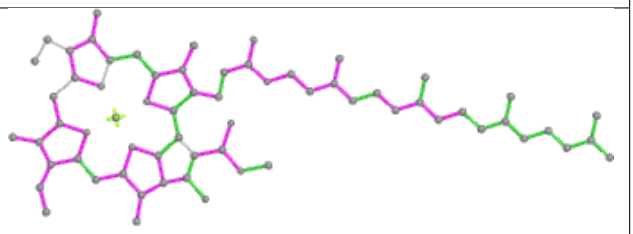
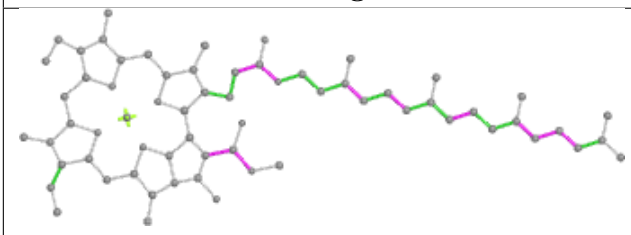
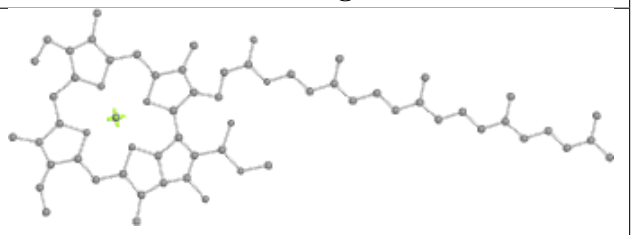
Bond angles

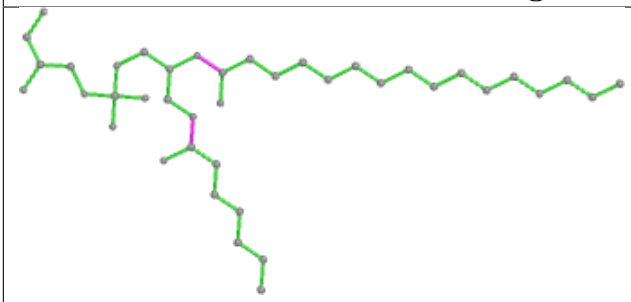
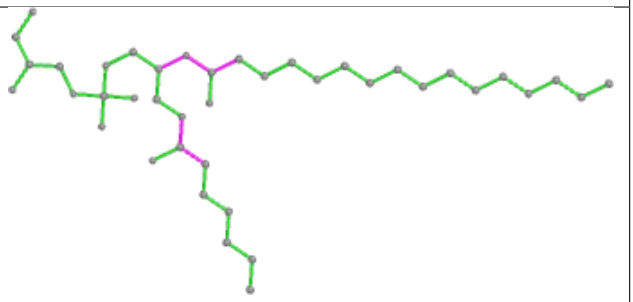
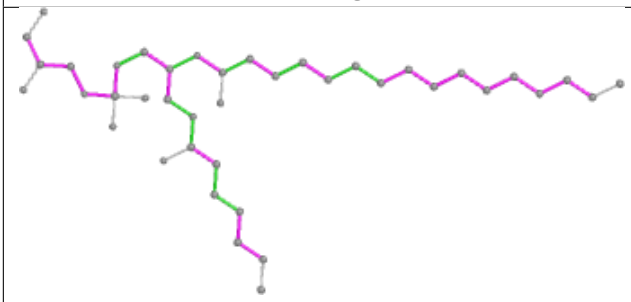
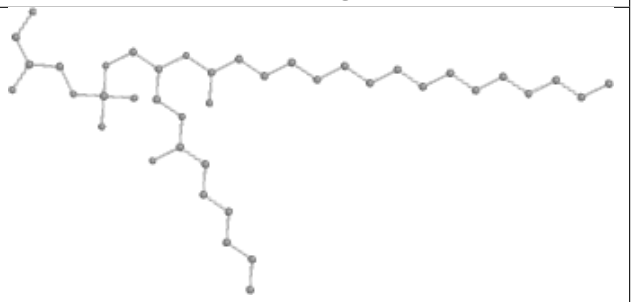


Torsions

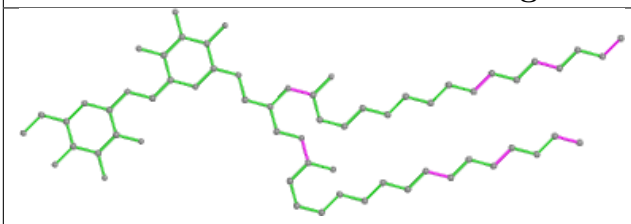


Rings

Ligand CLA C 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG e 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD C 517



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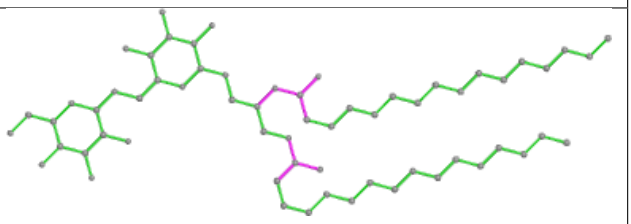

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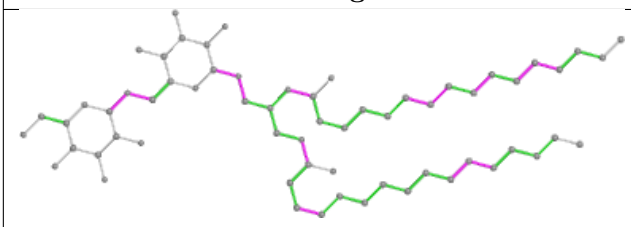

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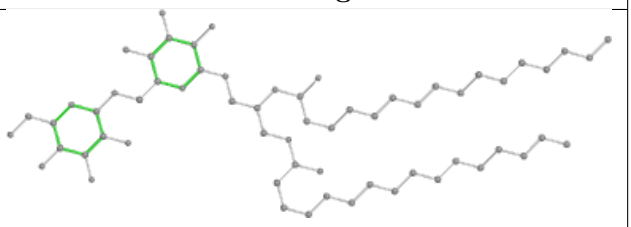
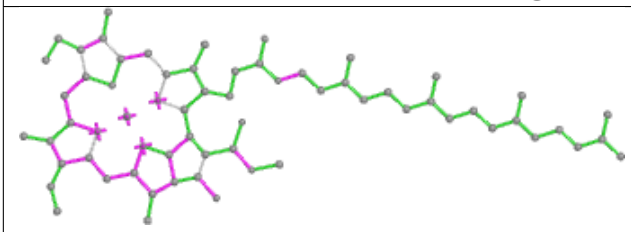


Rings

Ligand CLA a 406



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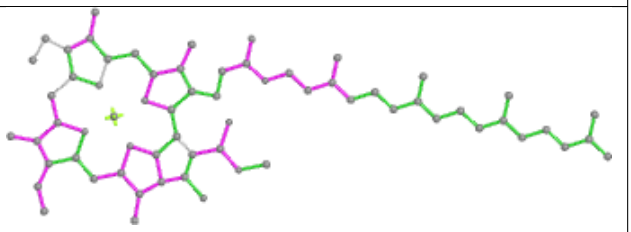

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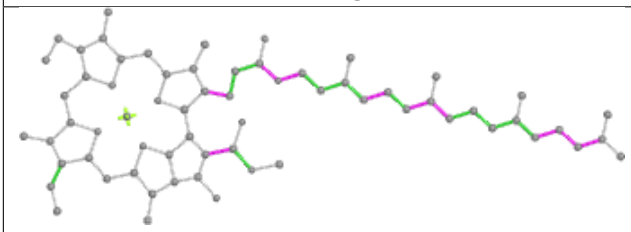

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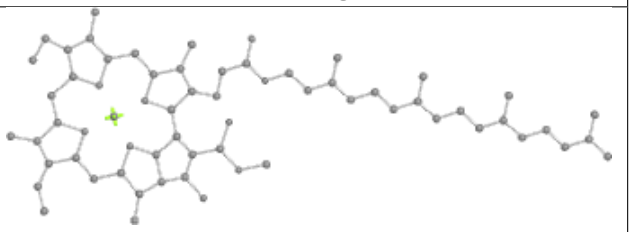
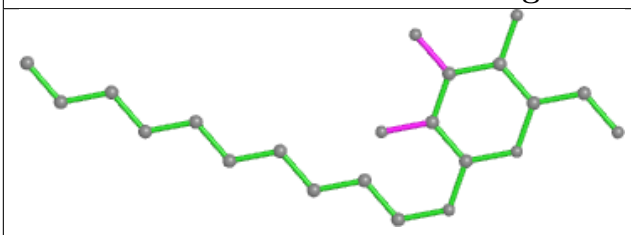


Rings

Ligand LMT E 101



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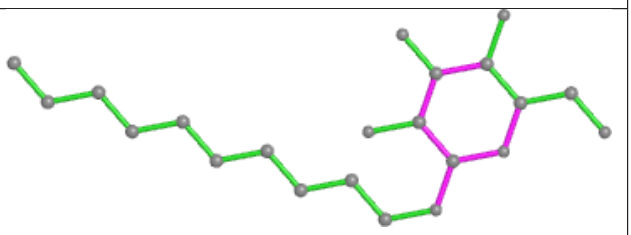
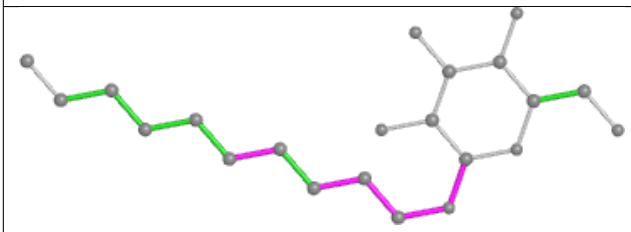


Bond angles



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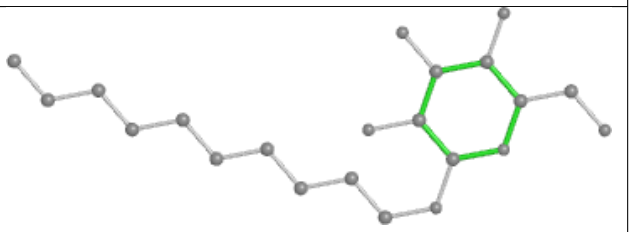
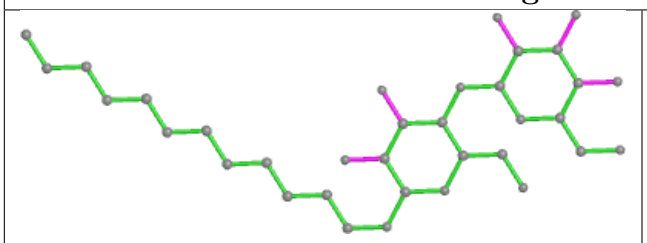


Rings

Ligand LMT A 415



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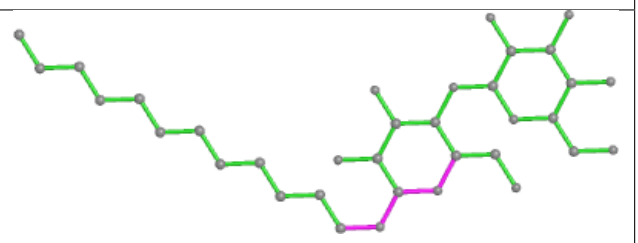

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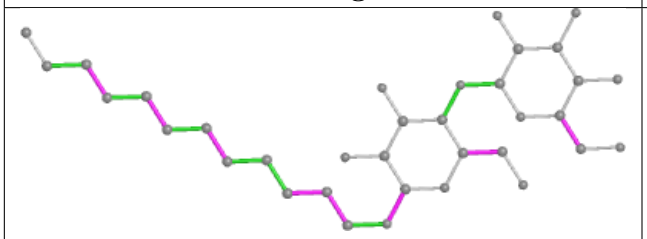

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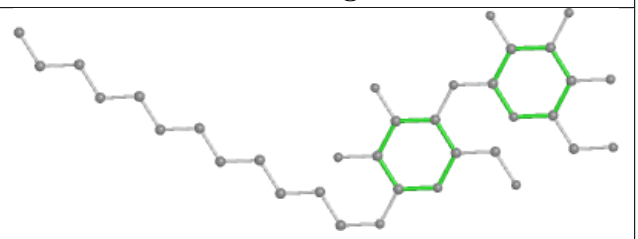
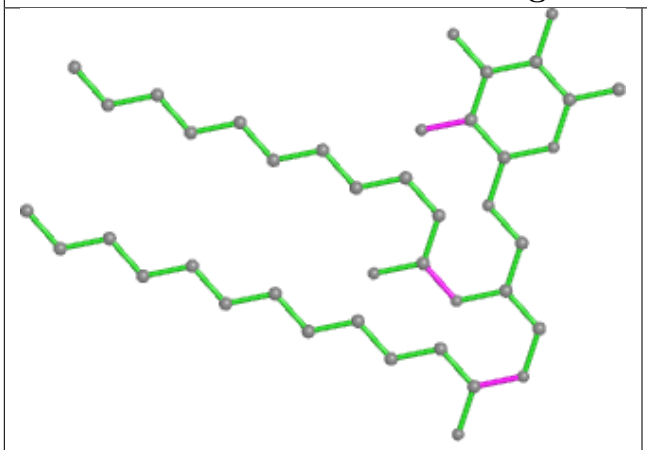


Rings

Ligand SQD k 101



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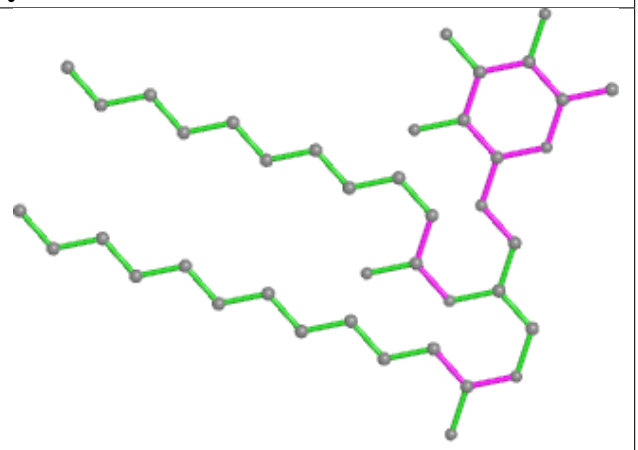
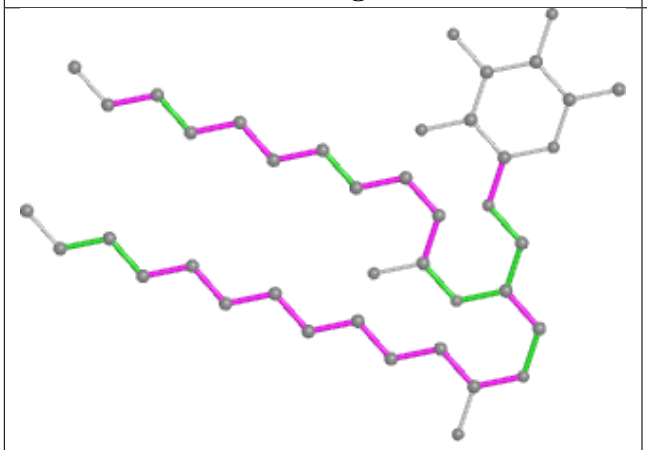


Bond angles



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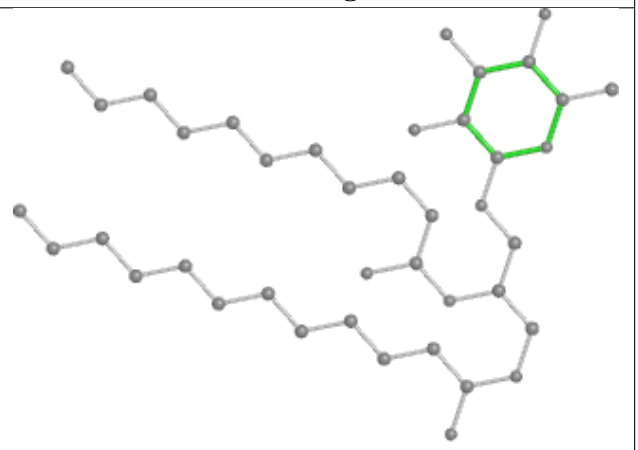
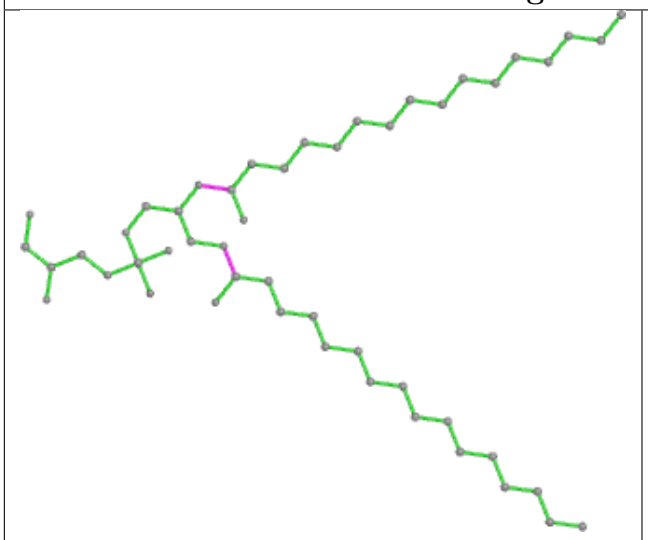


Rings

Ligand LHG b 628



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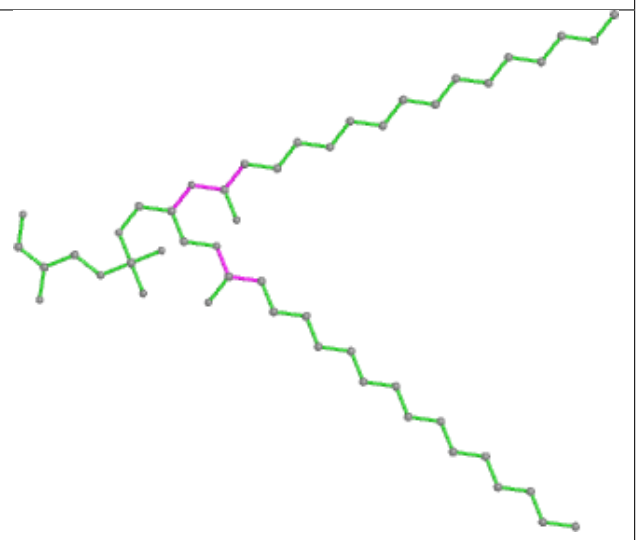
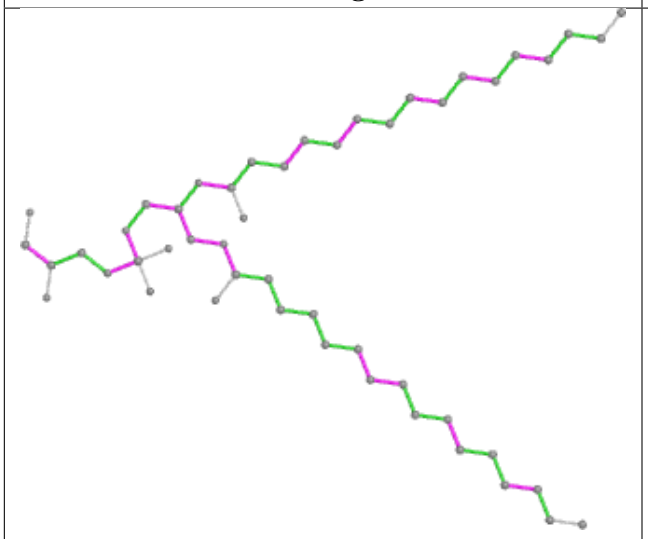


Bond angles



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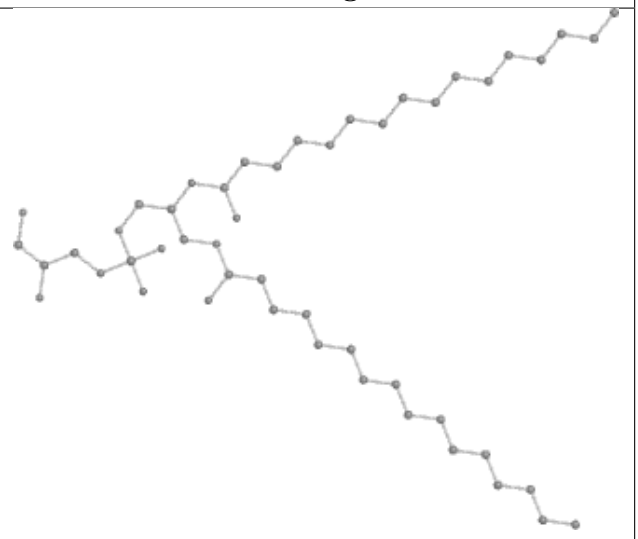
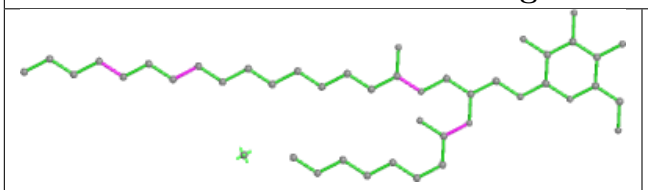
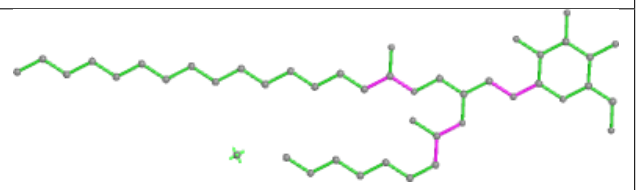


Rings

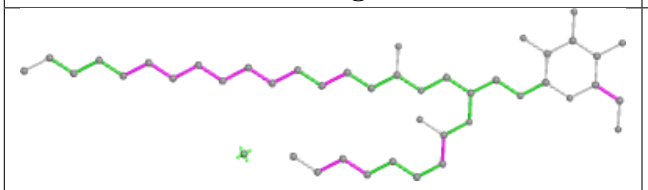
Ligand LMG D 409



Bond lengths



Bond angles



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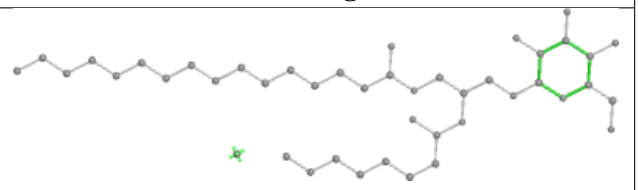
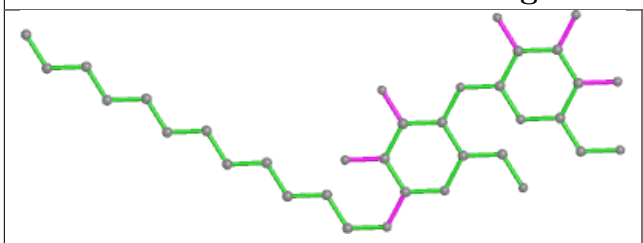
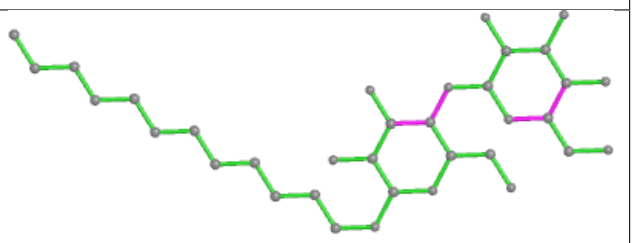
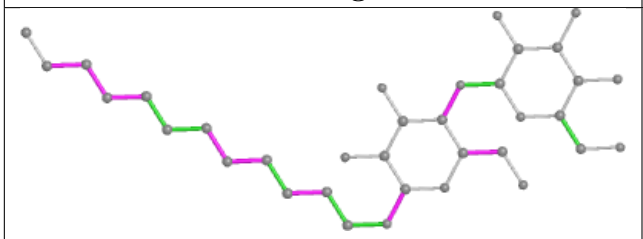
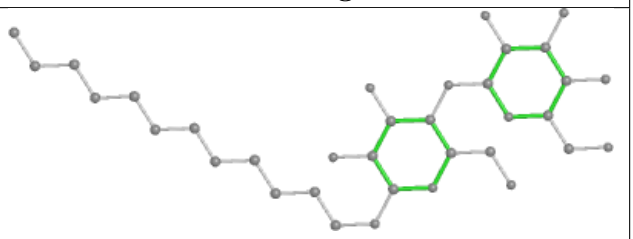
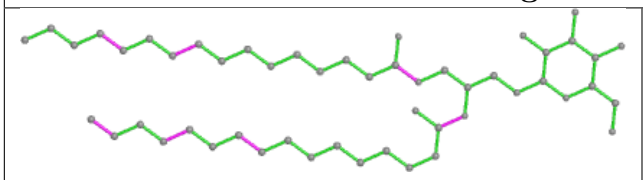
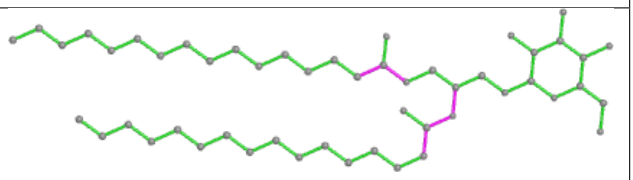
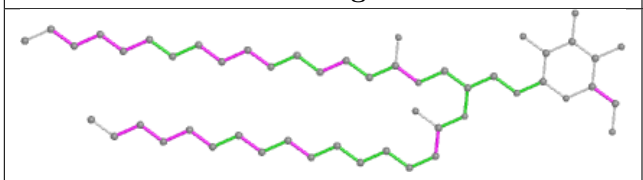
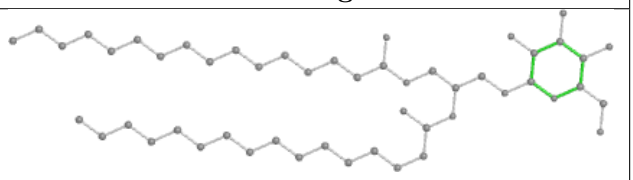
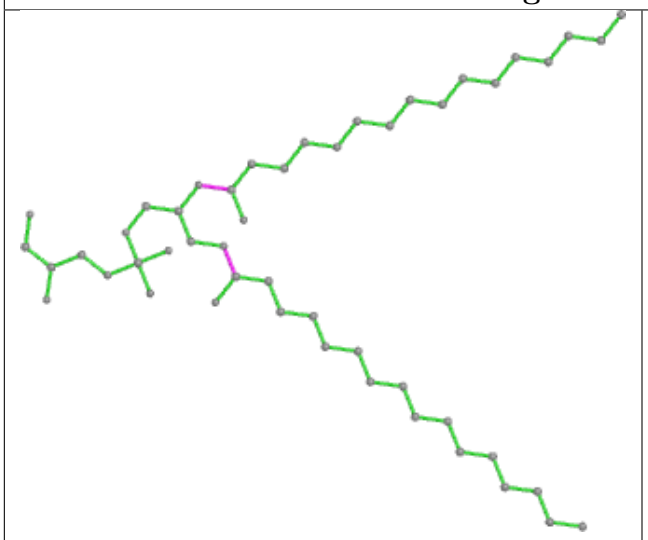


Rings

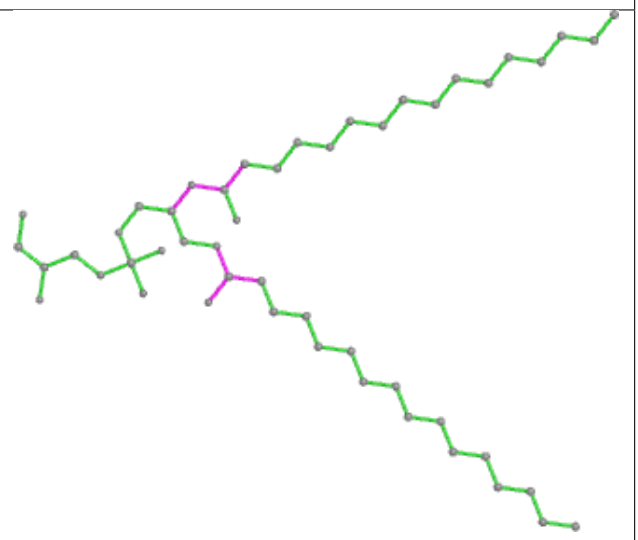
Ligand LMT m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG C 519	
 Bond lengths	 Bond angles
 Torsions	 Rings

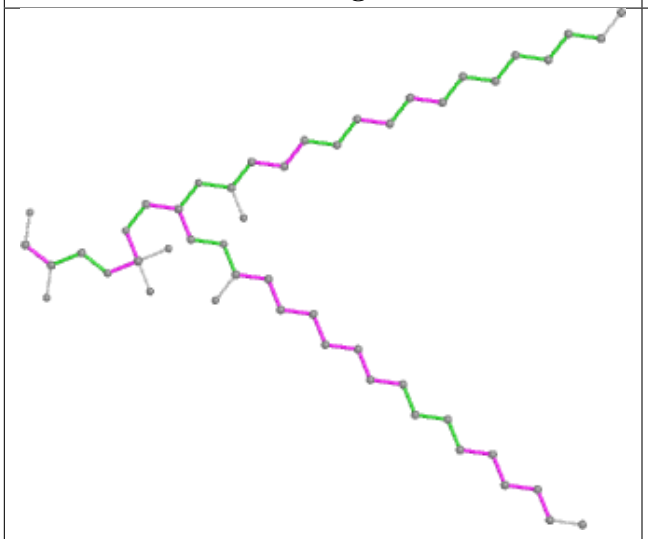
Ligand LHG D 407



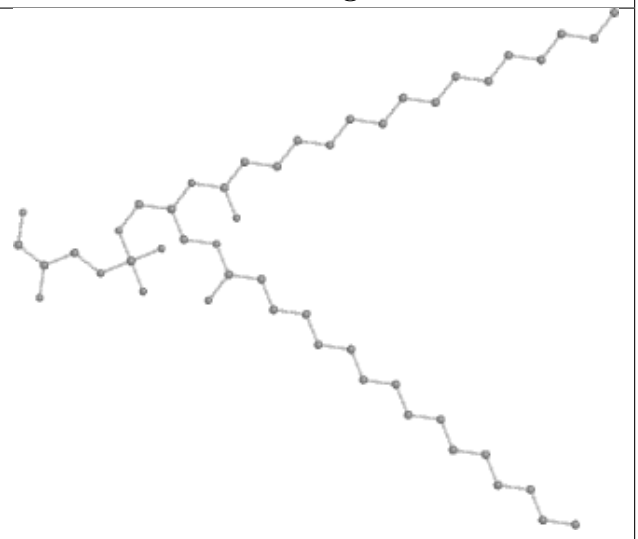
Bond lengths



Bond angles

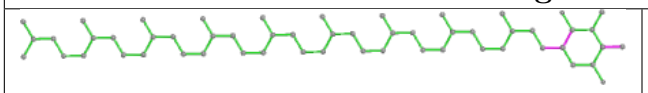


Torsions

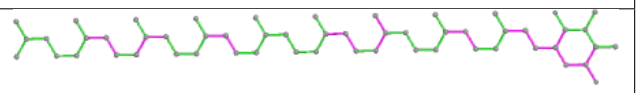


Rings

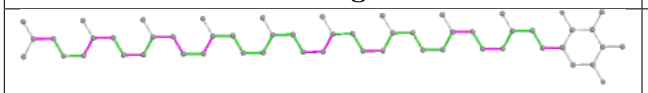
Ligand PL9 a 411



Bond lengths



Bond angles



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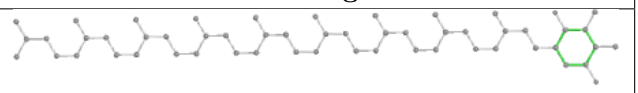
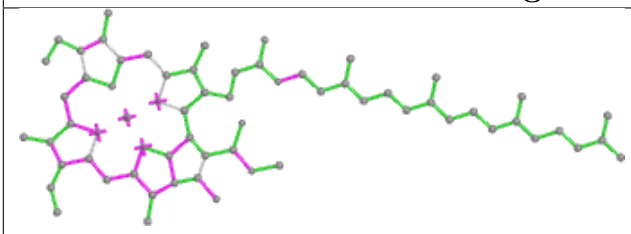
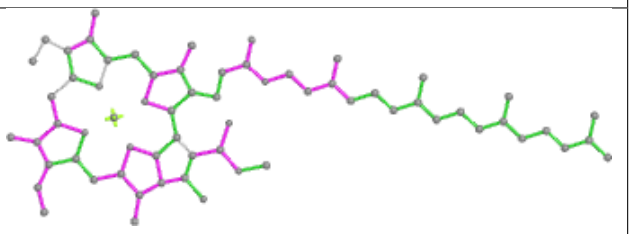


Rings

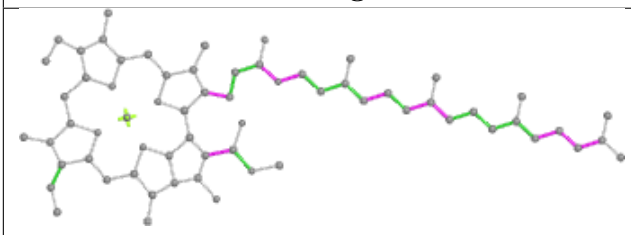
Ligand CLA A 406



Bond lengths



Bond angles



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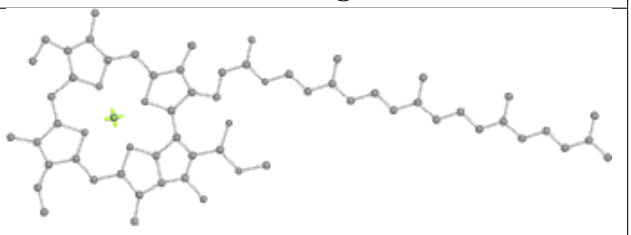
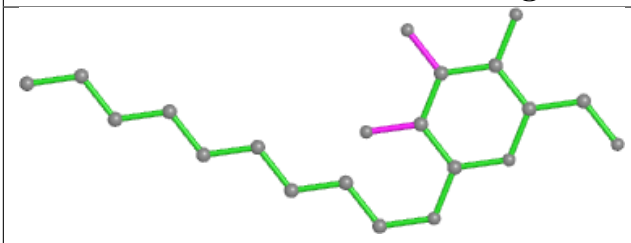
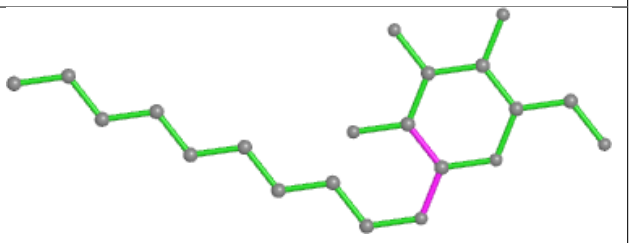


Rings

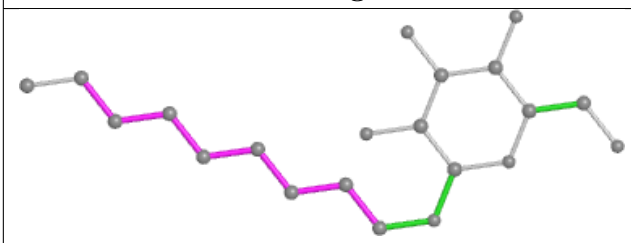
Ligand LMT Y 101



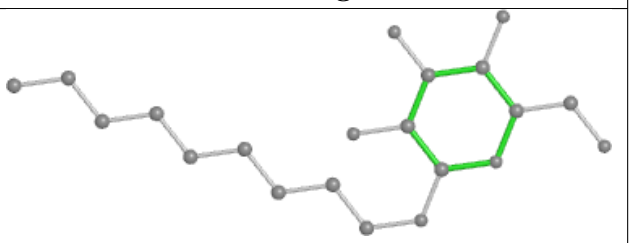
Bond lengths



Bond angles

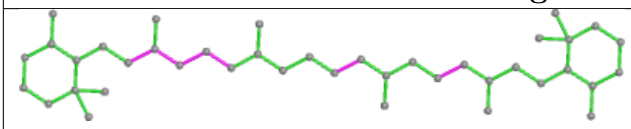


Torsions

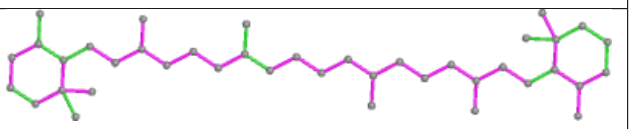


Rings

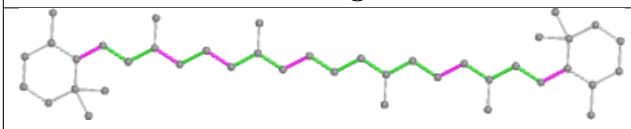
Ligand BCR f 101



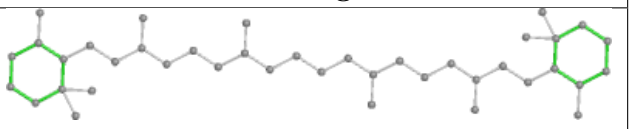
Bond lengths



Bond angles

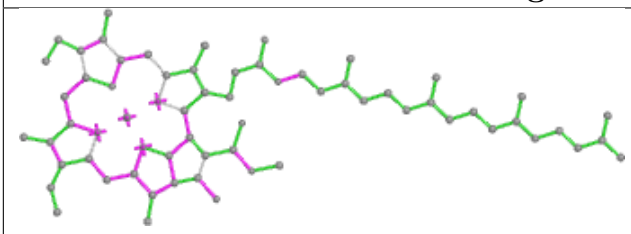


Torsions

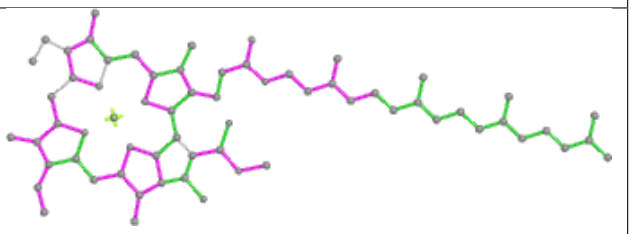


Rings

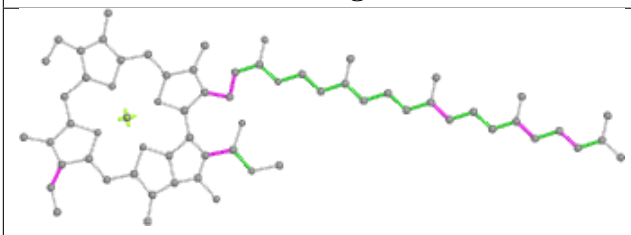
Ligand CLA d 401



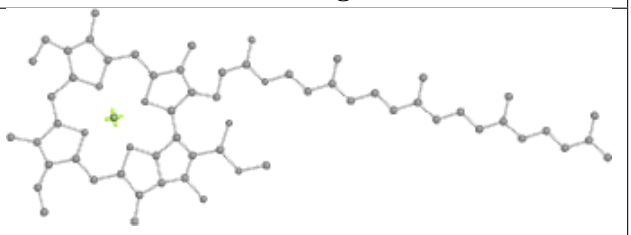
Bond lengths



Bond angles

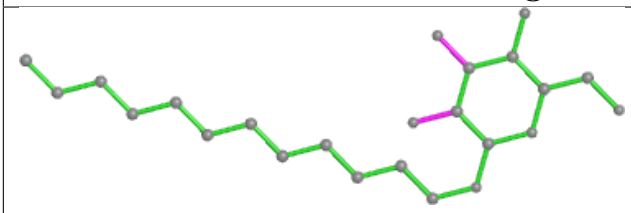


Torsions

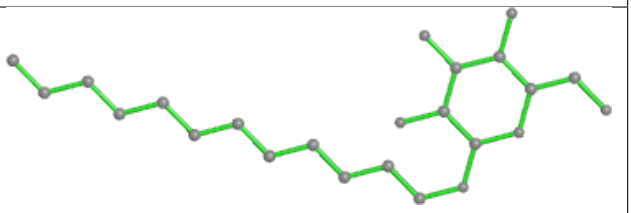


Rings

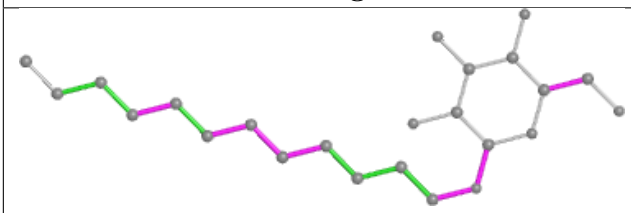
Ligand LMT b 624



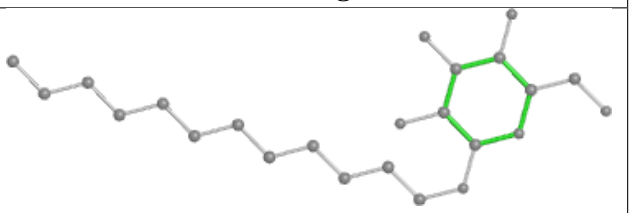
Bond lengths



Bond angles

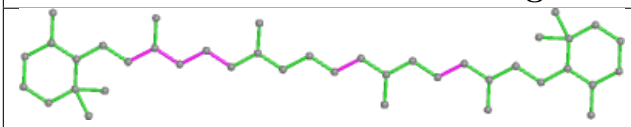


Torsions

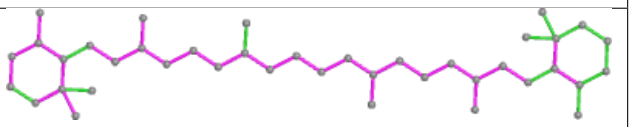


Rings

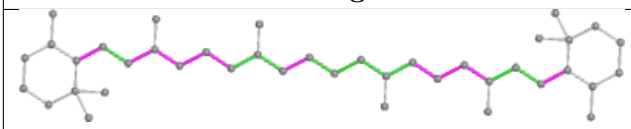
Ligand BCR k 102



Bond lengths



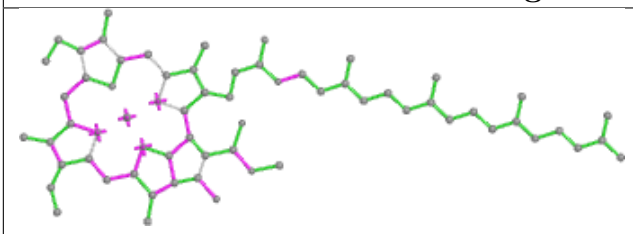
Bond angles



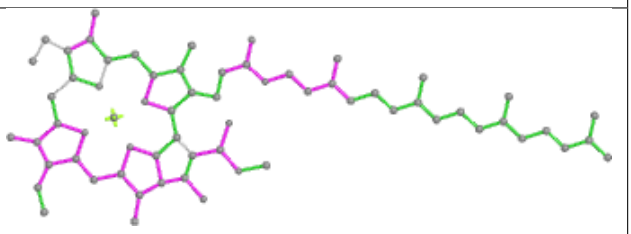
Torsions

Rings

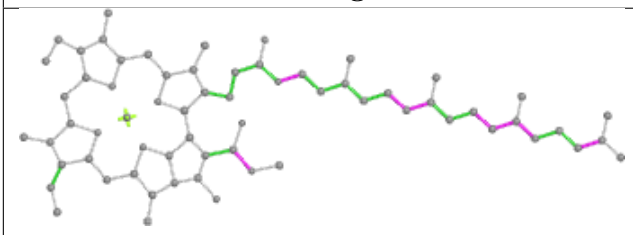
Ligand CLA B 615



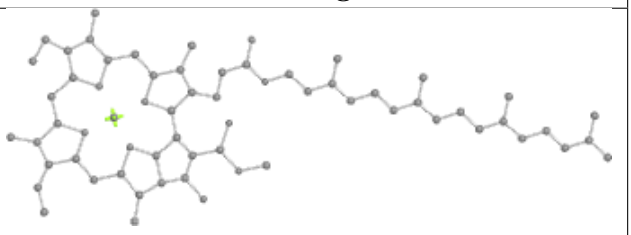
Bond lengths



Bond angles

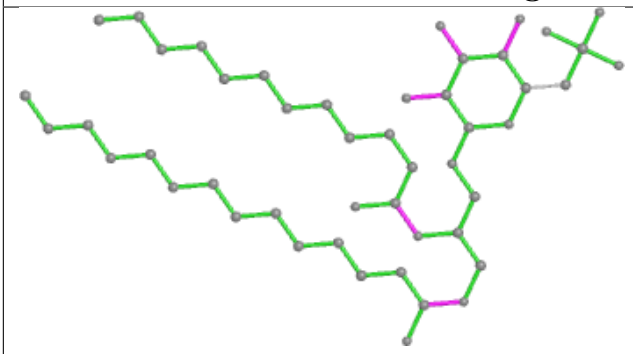


Torsions

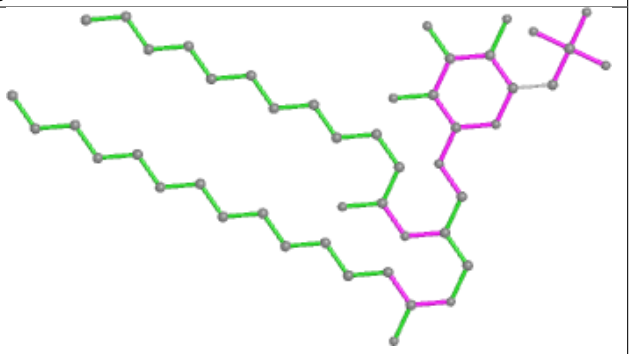


Rings

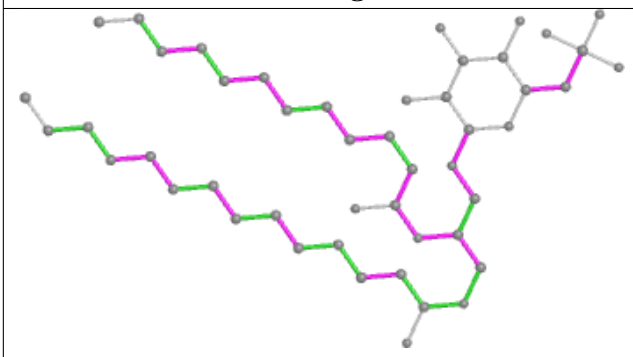
Ligand SQD A 413



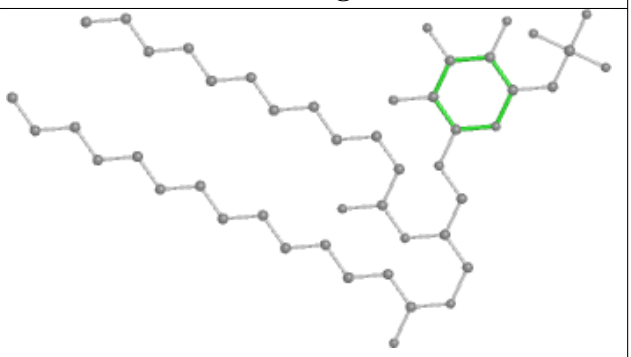
Bond lengths



Bond angles

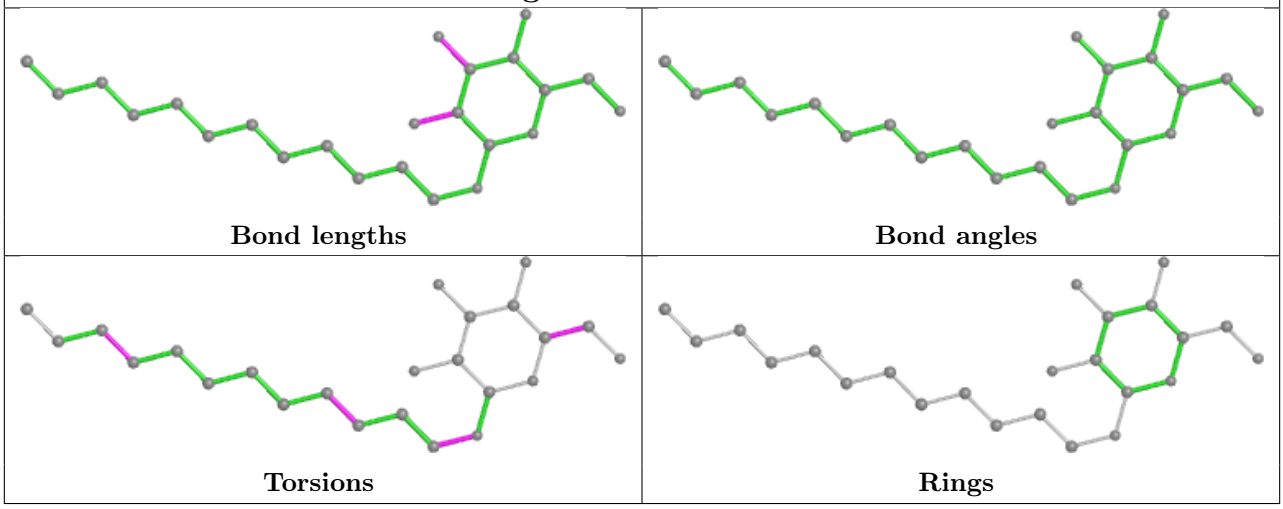


Torsions

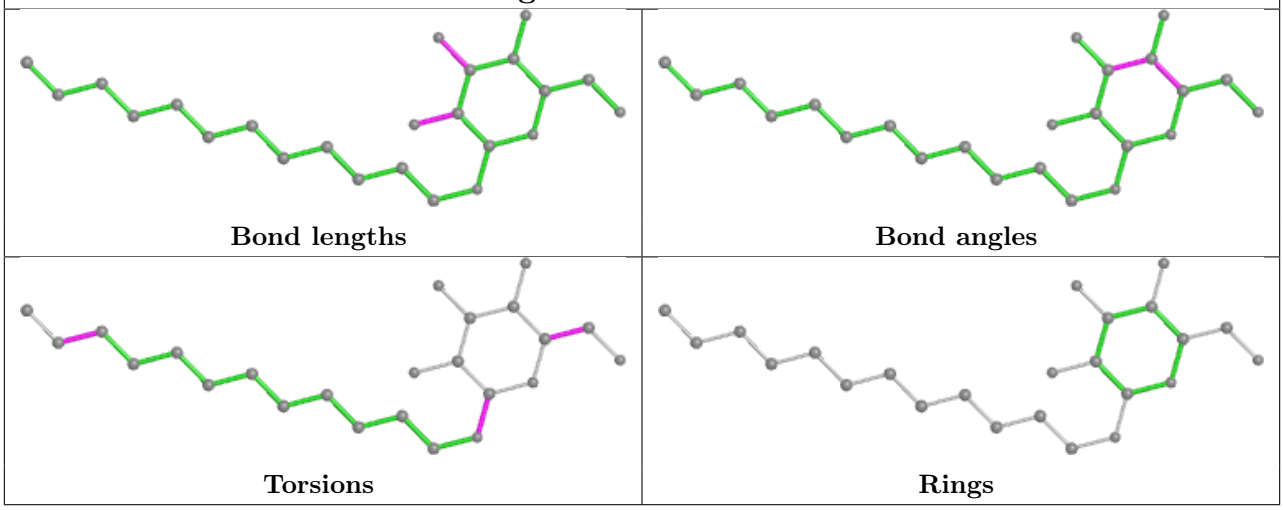


Rings

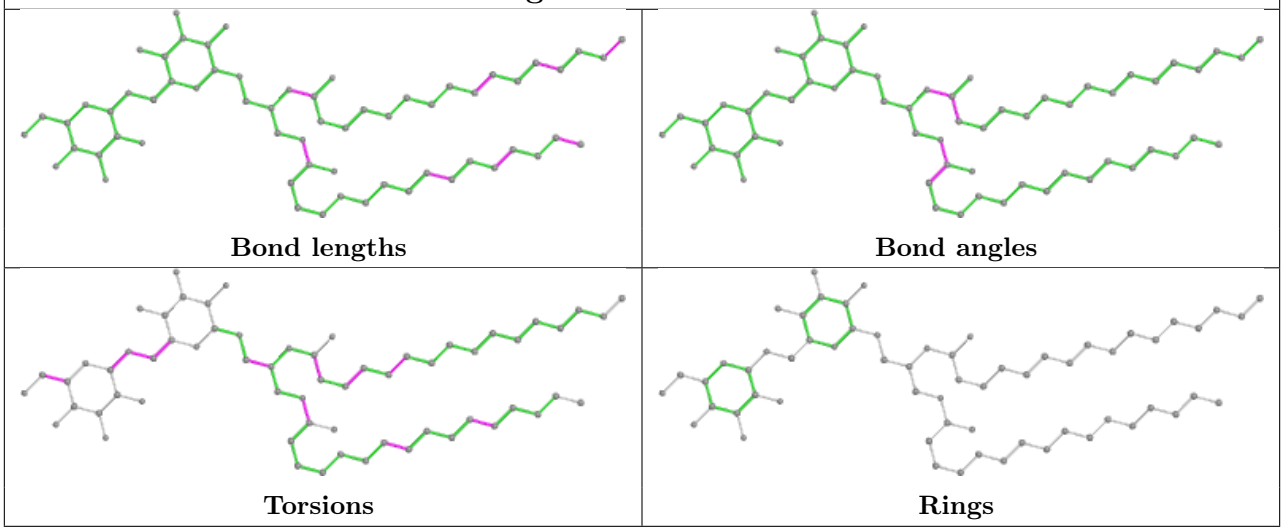
Ligand LMT B 626



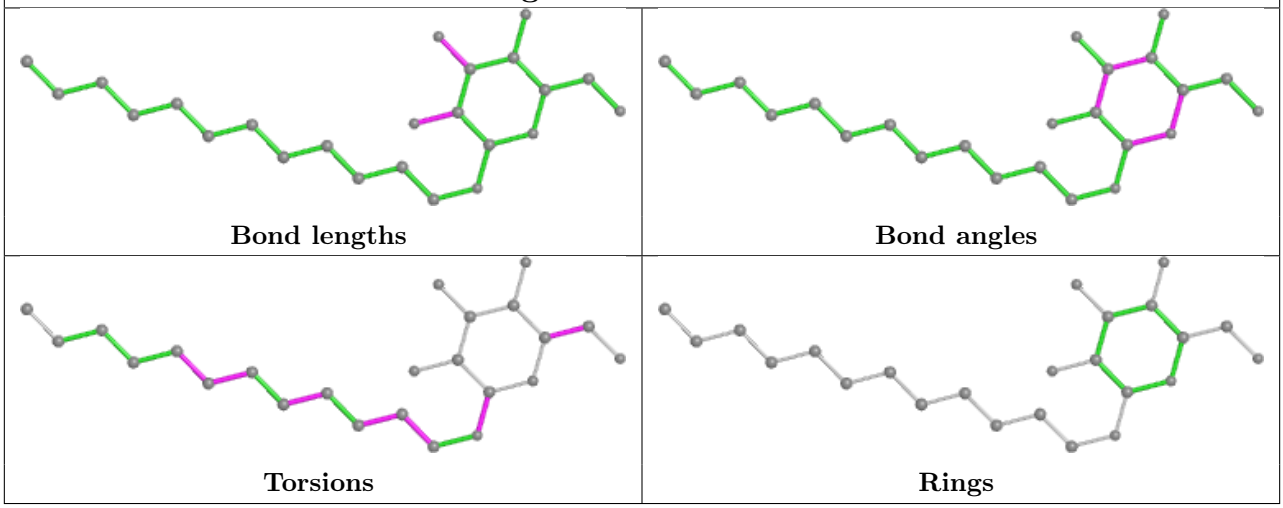
Ligand LMT M 102



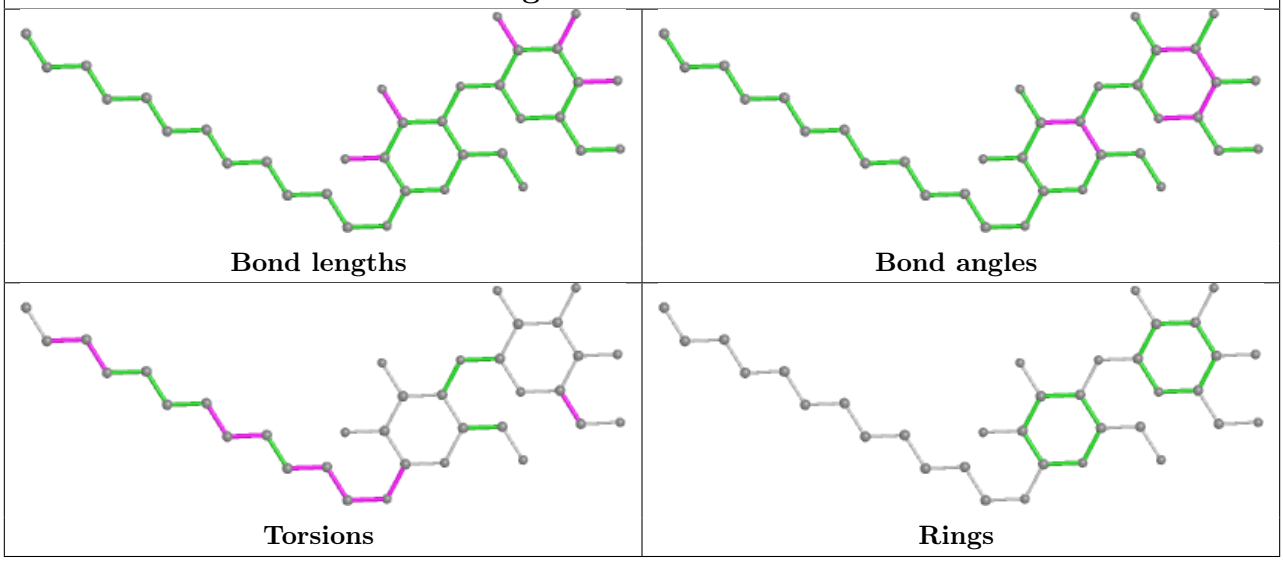
Ligand DGD c 516



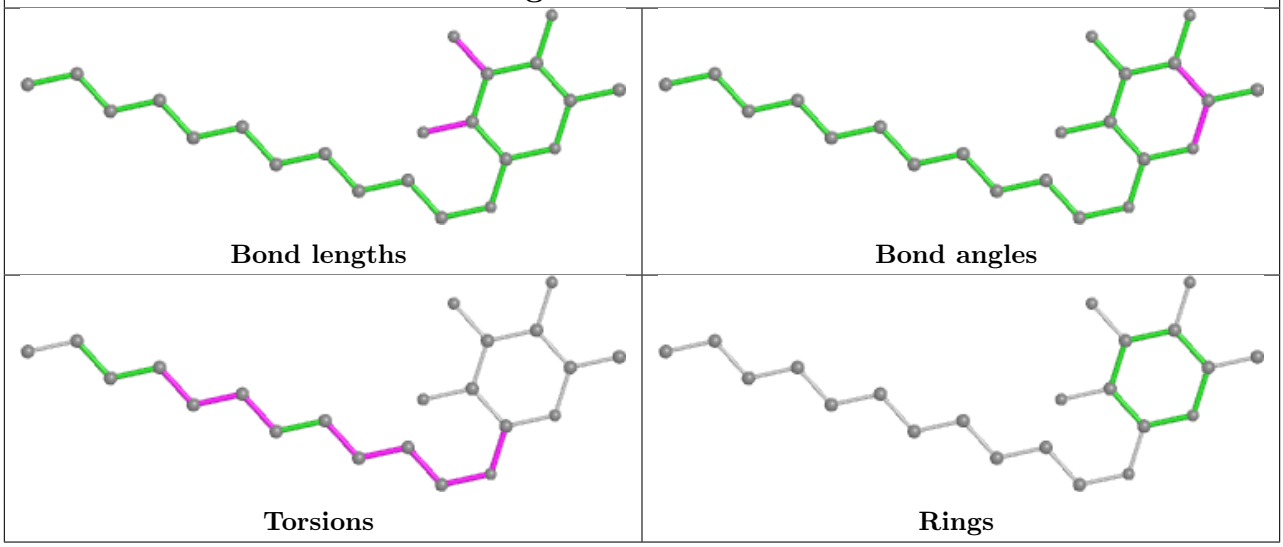
Ligand LMT H 102



Ligand LMT C 524



Ligand LMT x 102



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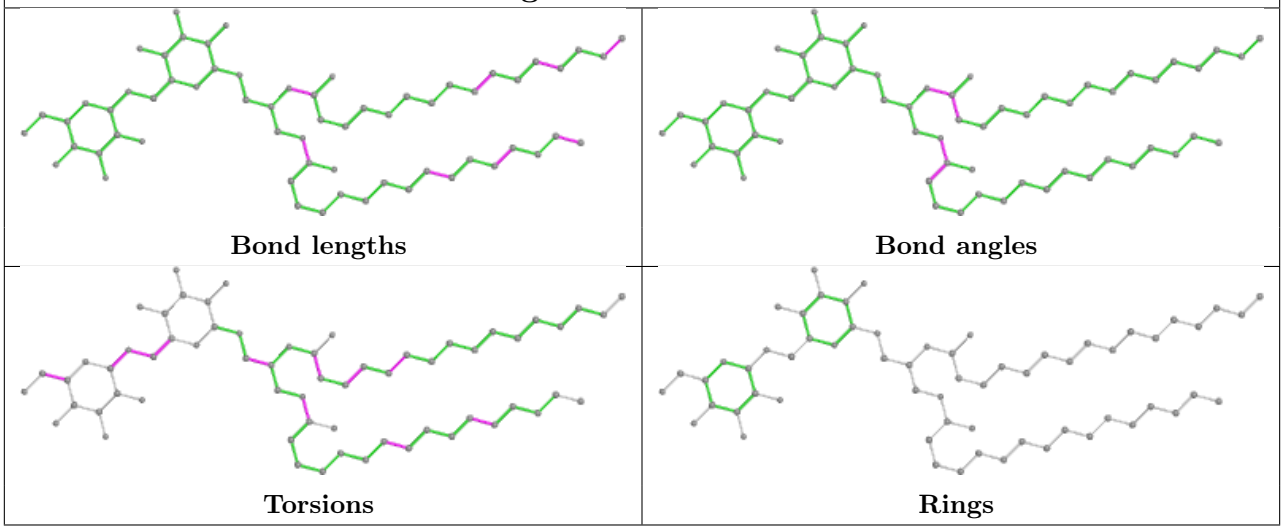
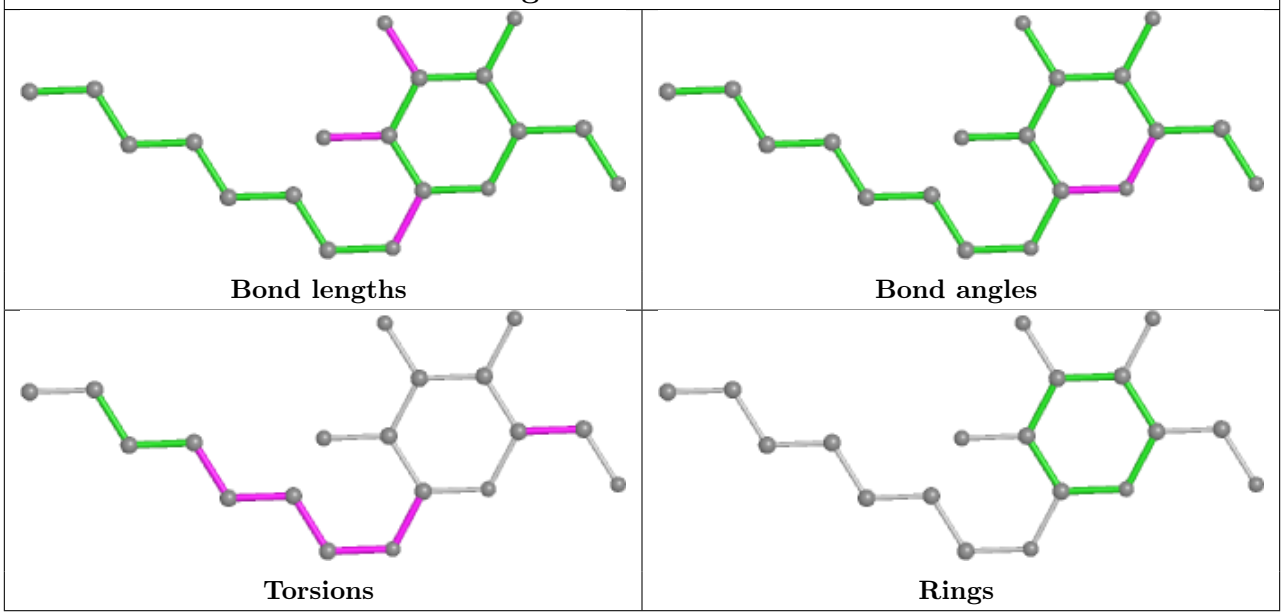
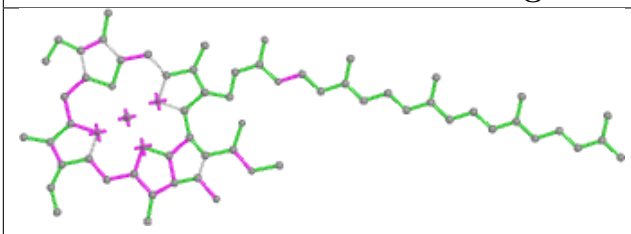


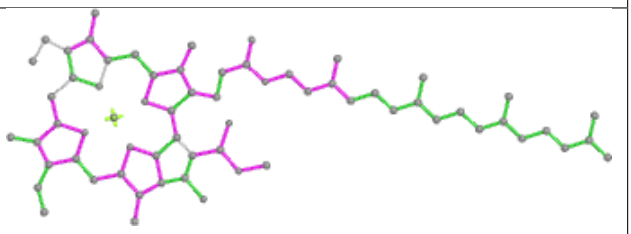
Ligand LMT X 104



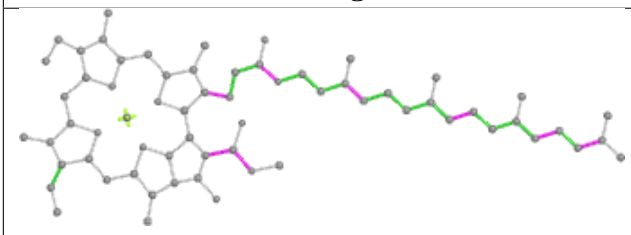
Ligand CLA C 509



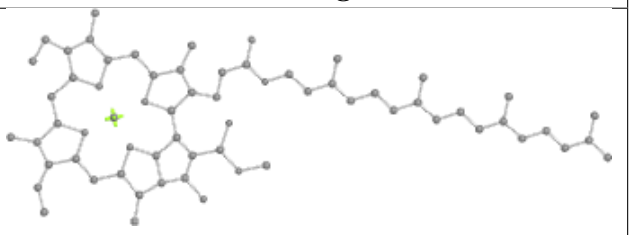
Bond lengths



Bond angles

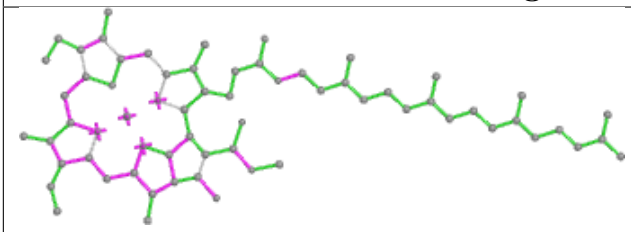


Torsions

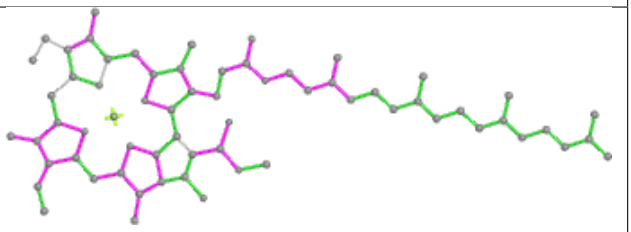


Rings

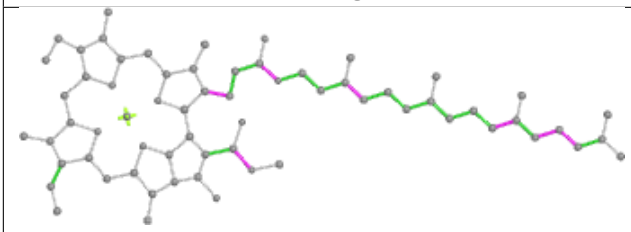
Ligand CLA D 404



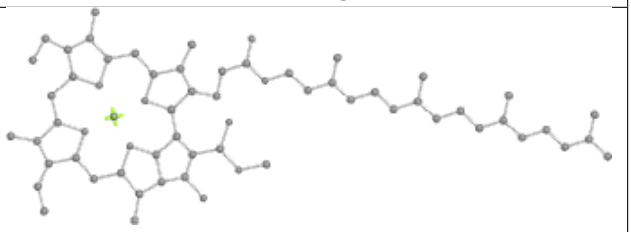
Bond lengths



Bond angles

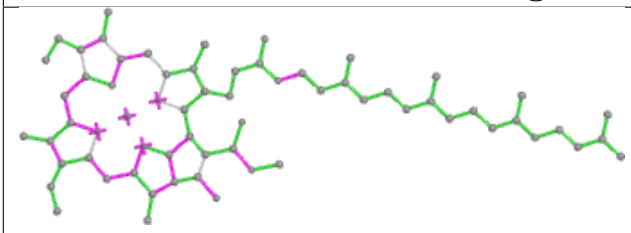


Torsions

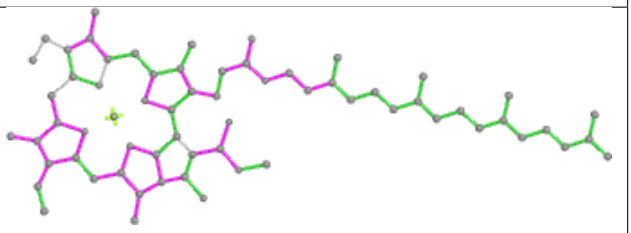


Rings

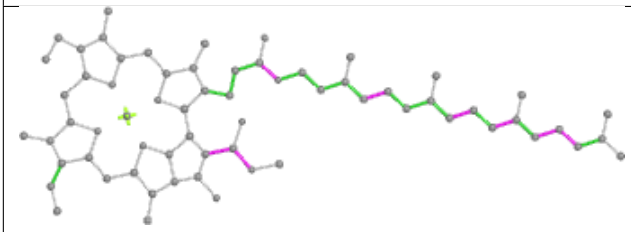
Ligand CLA b 611



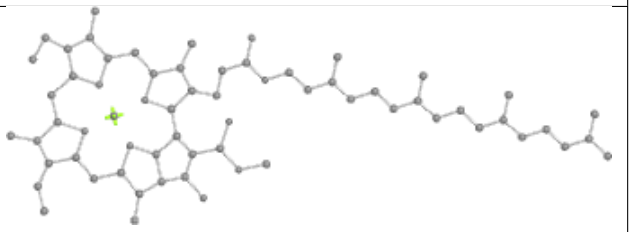
Bond lengths



Bond angles

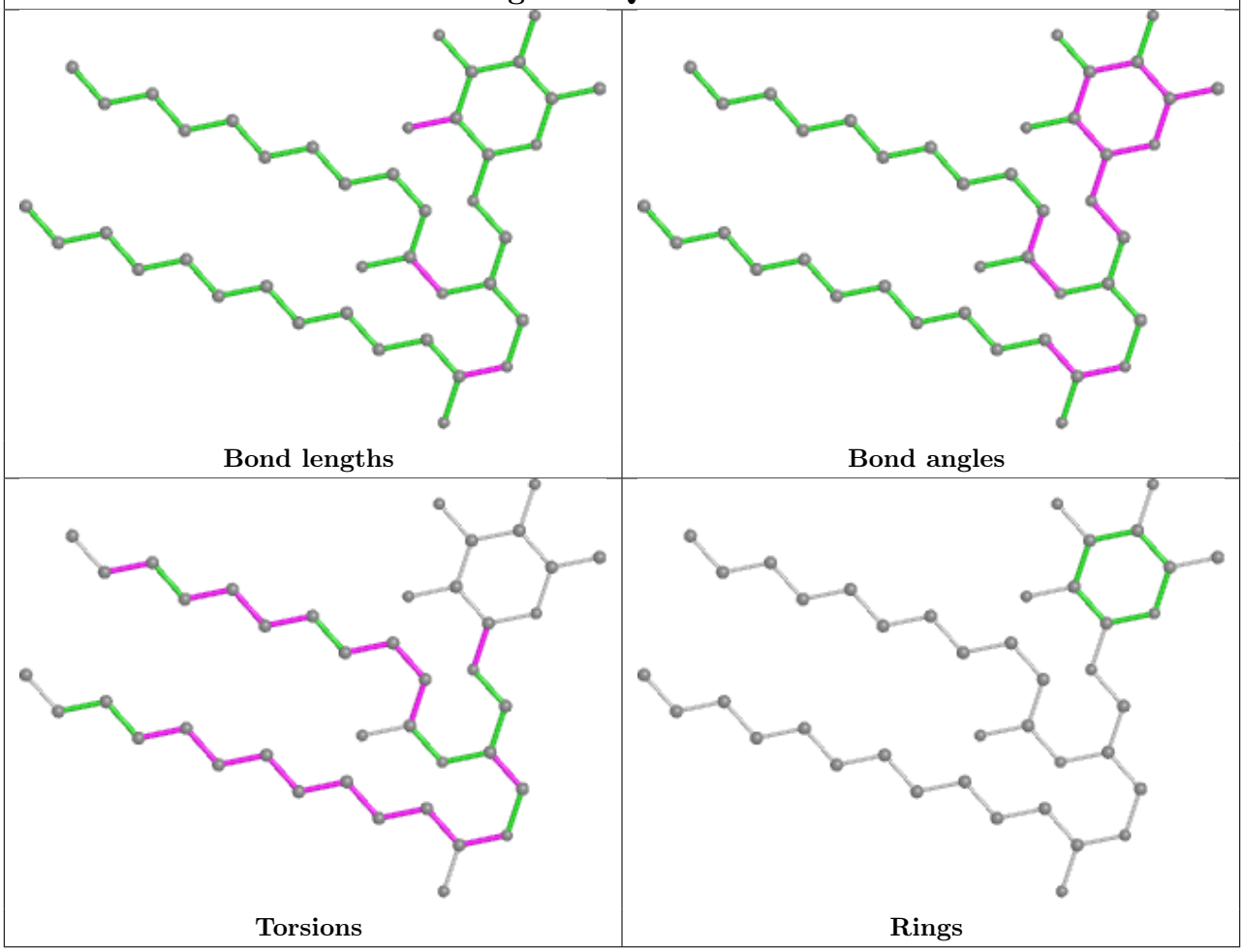


Torsions

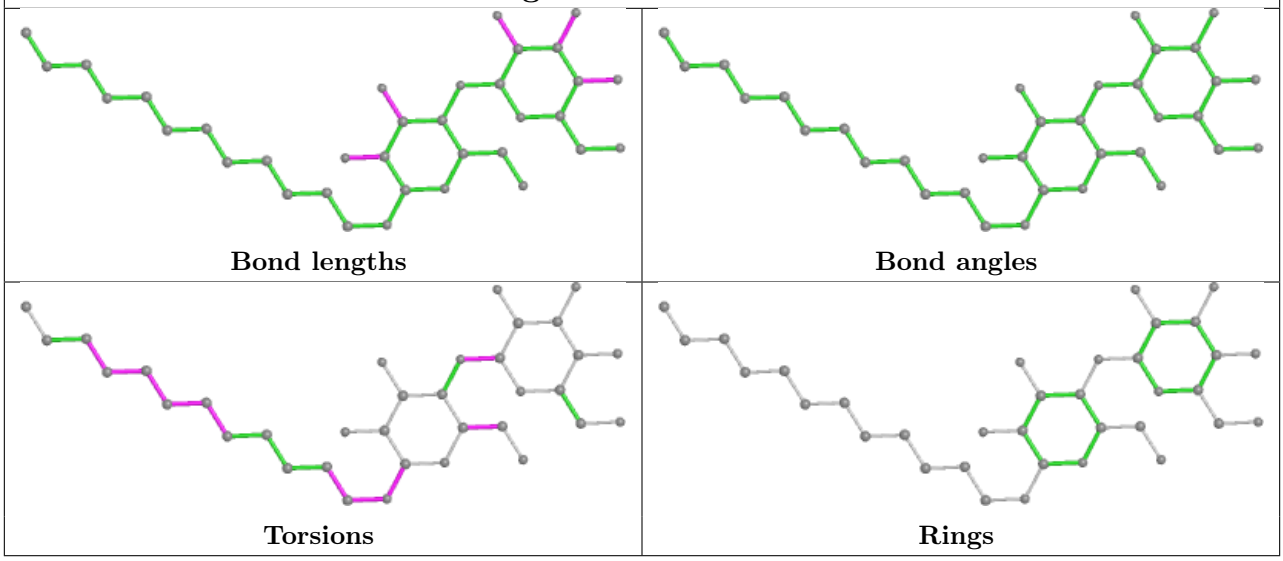


Rings

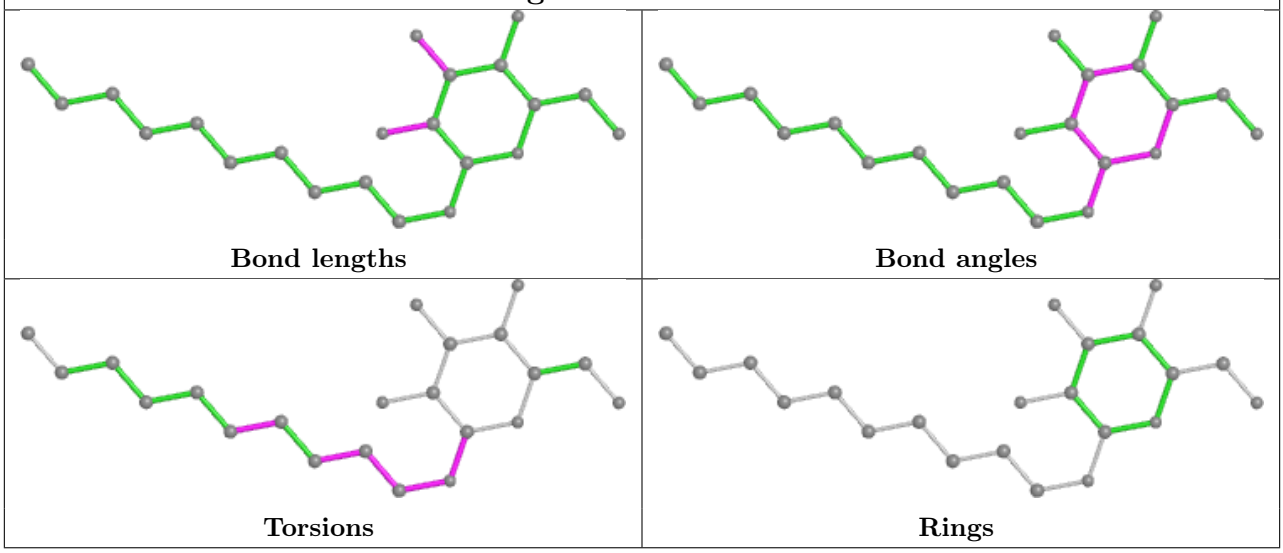
Ligand SQD K 101



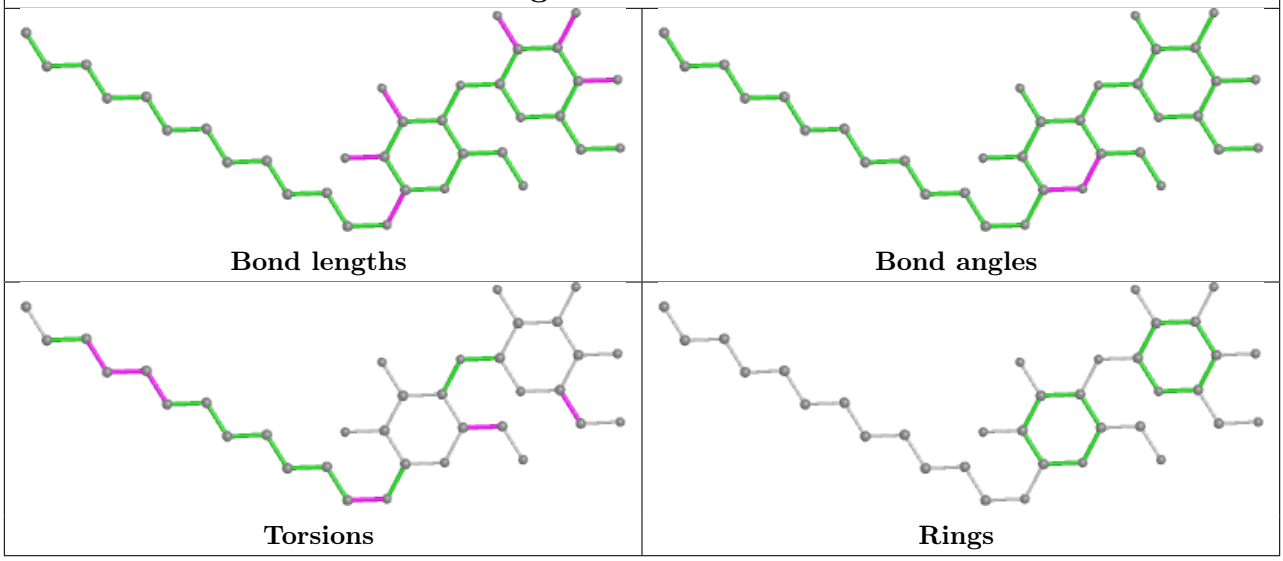
Ligand LMT B 629



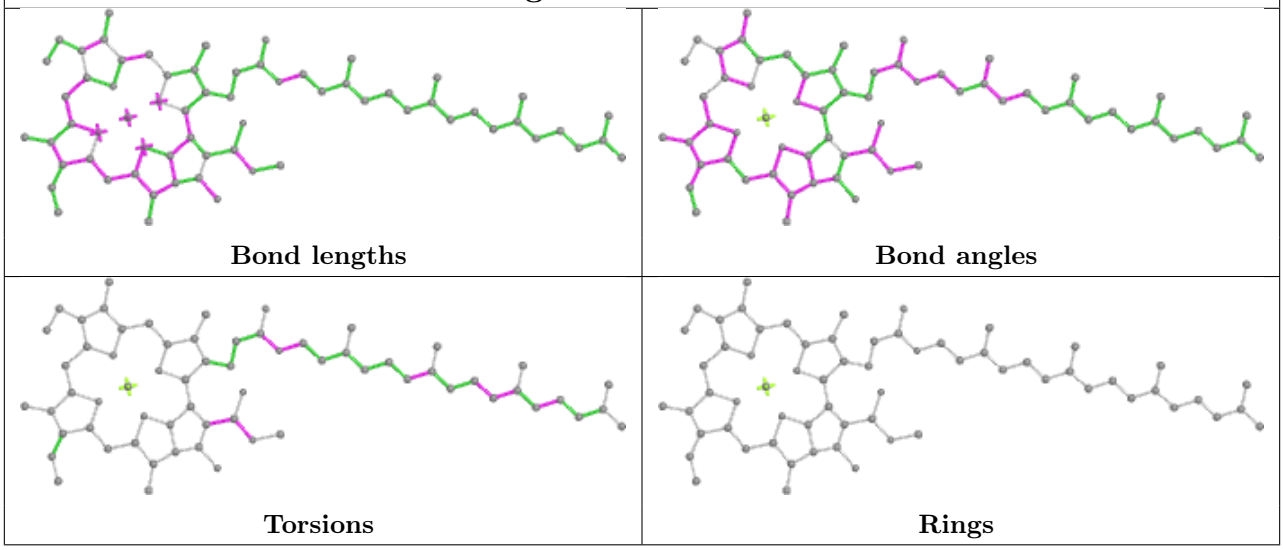
Ligand LMT e 101



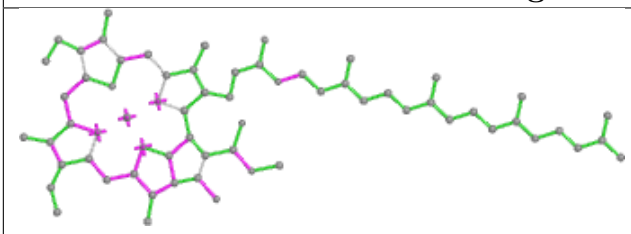
Ligand LMT i 103



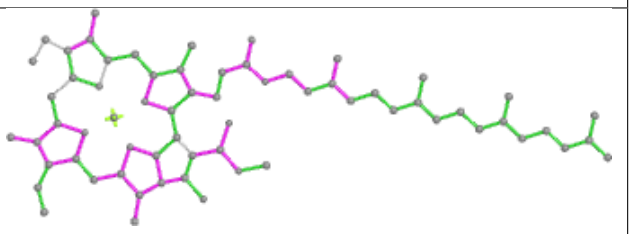
Ligand CLA C 510



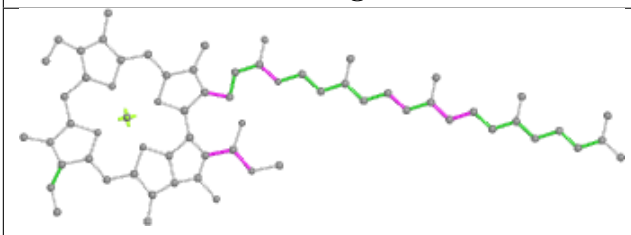
Ligand CLA b 605



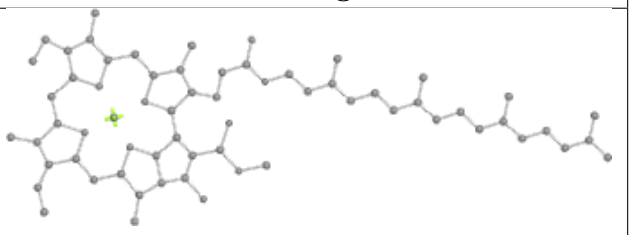
Bond lengths



Bond angles

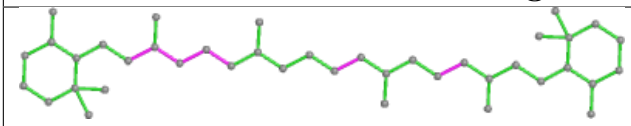


Torsions

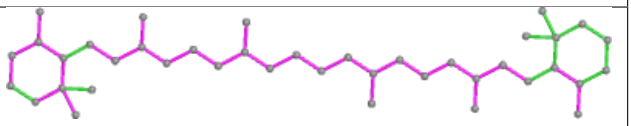


Rings

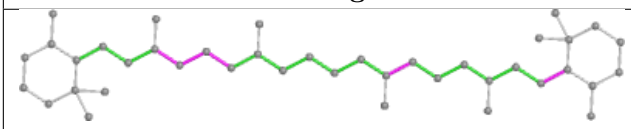
Ligand BCR k 103



Bond lengths



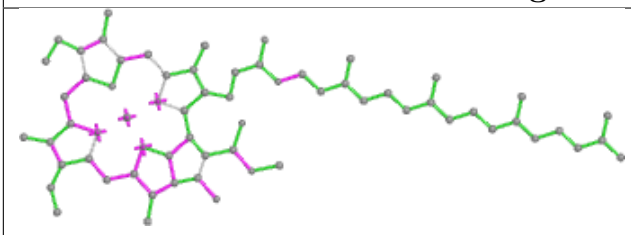
Bond angles



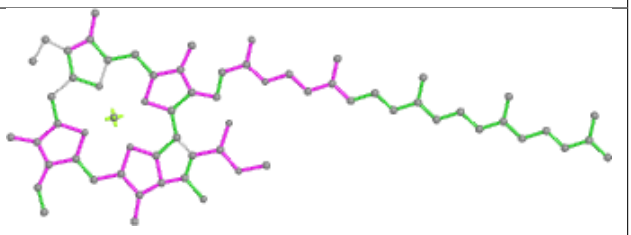
Torsions

Rings

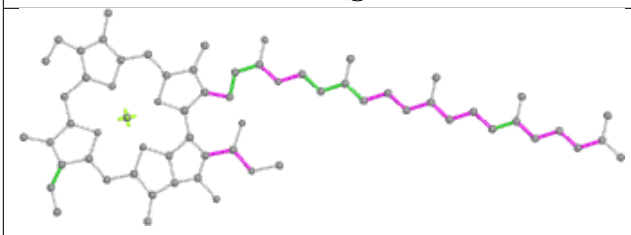
Ligand CLA c 512



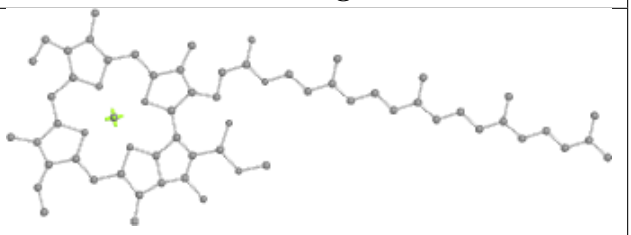
Bond lengths



Bond angles

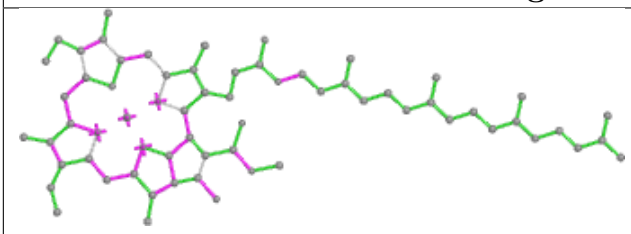


Torsions

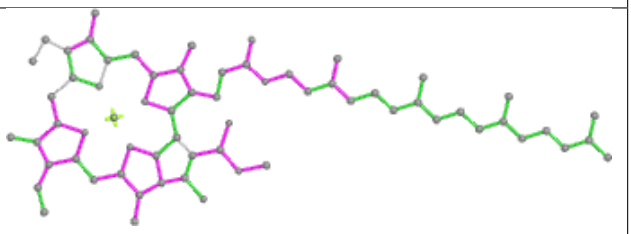


Rings

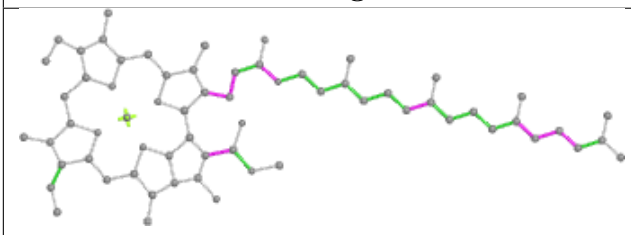
Ligand CLA b 607



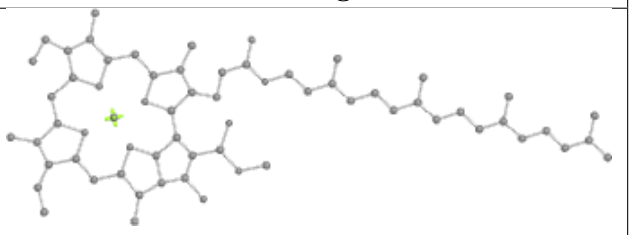
Bond lengths



Bond angles

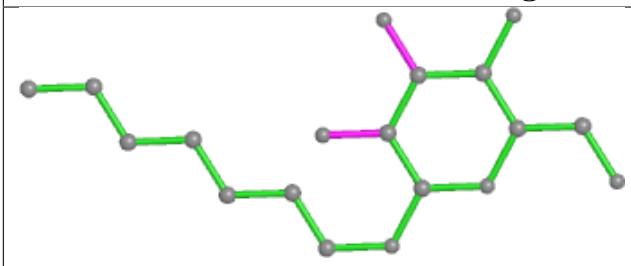


Torsions

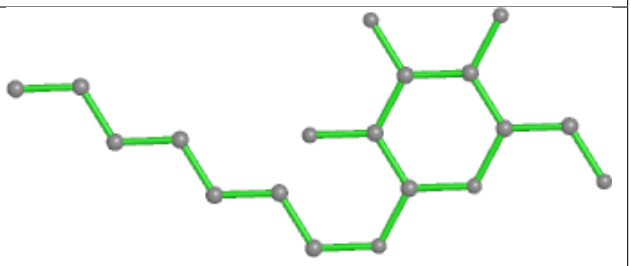


Rings

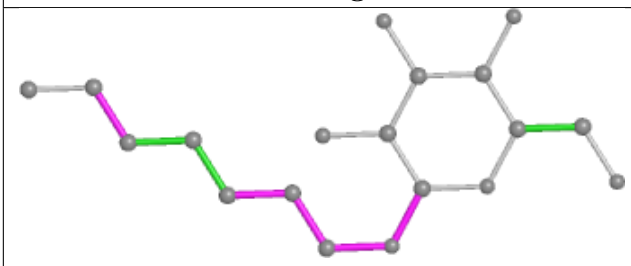
Ligand LMT X 105



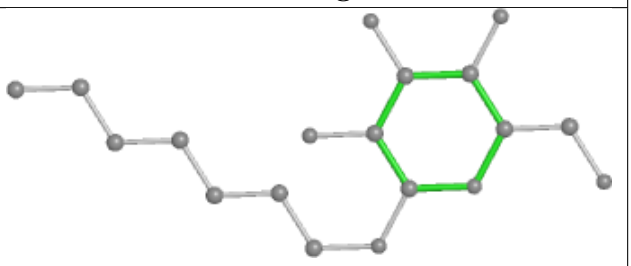
Bond lengths



Bond angles

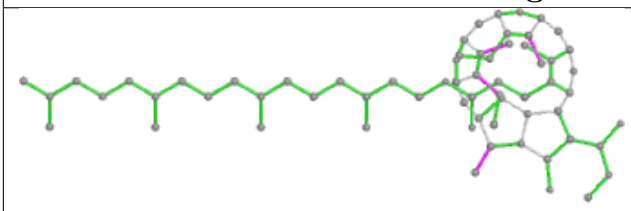


Torsions

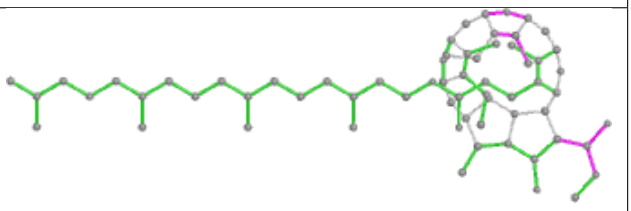


Rings

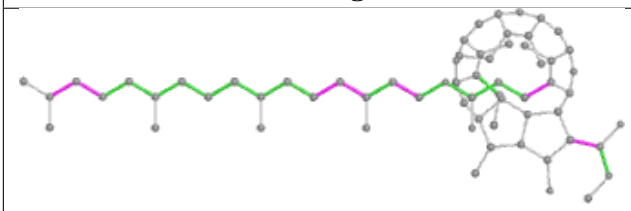
Ligand PHO a 407



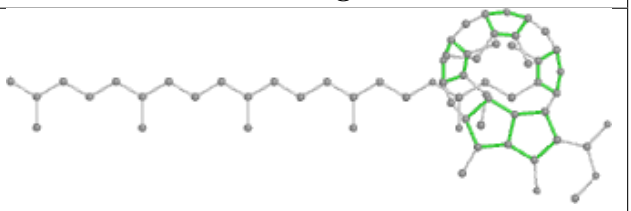
Bond lengths



Bond angles

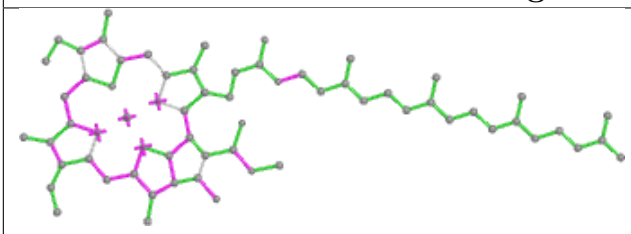


Torsions

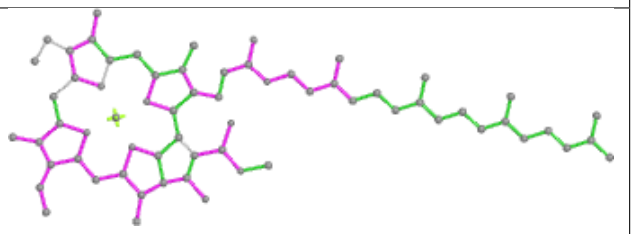


Rings

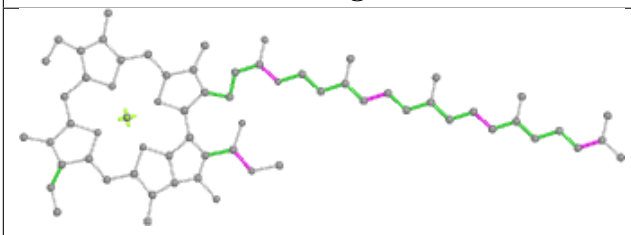
Ligand CLA b 613



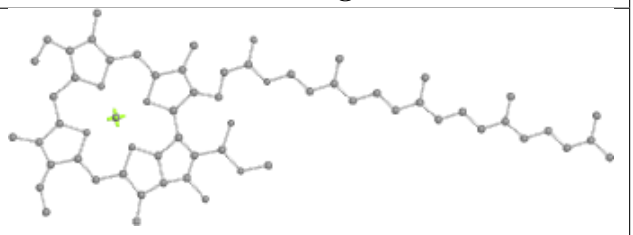
Bond lengths



Bond angles

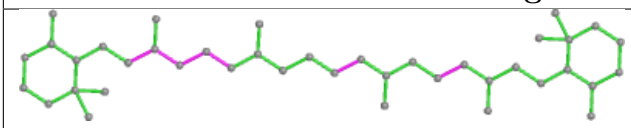


Torsions

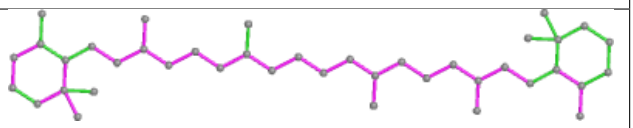


Rings

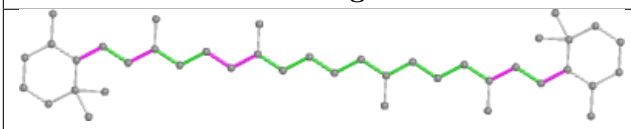
Ligand BCR Z 101



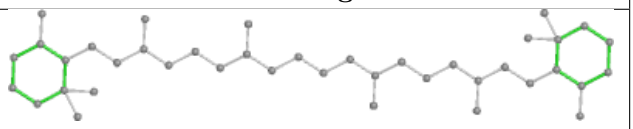
Bond lengths



Bond angles

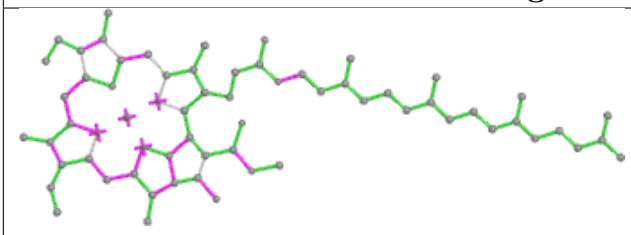


Torsions

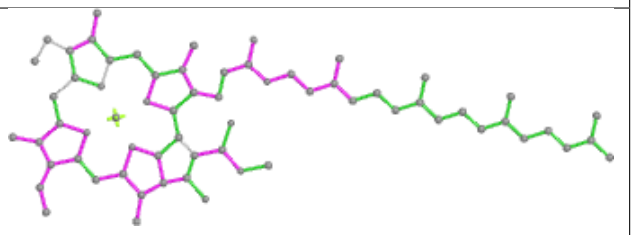


Rings

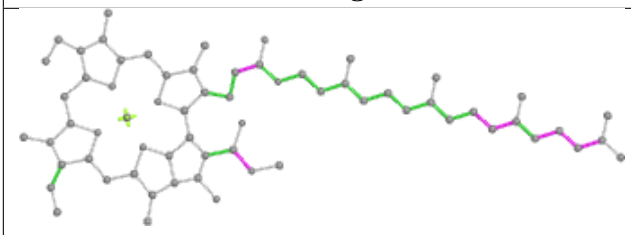
Ligand CLA d 403



Bond lengths



Bond angles



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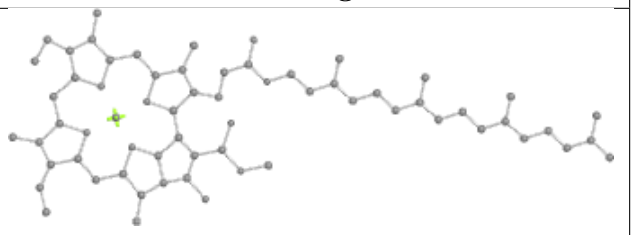
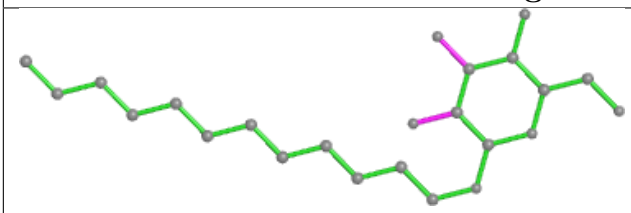
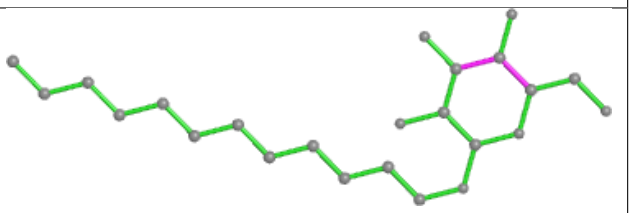


Rings

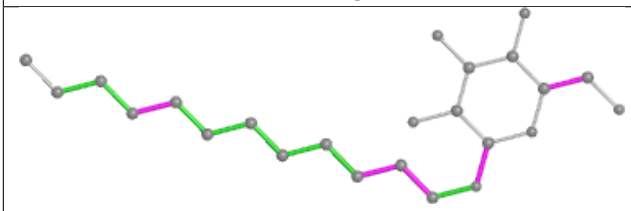
Ligand LMT x 101



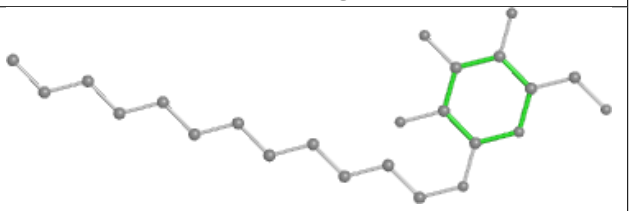
Bond lengths



Bond angles

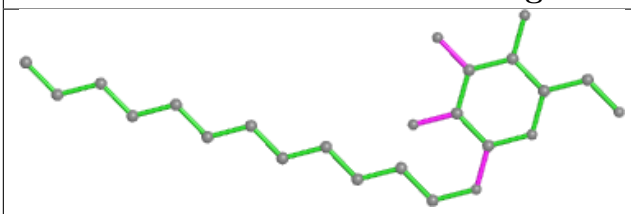


Torsions

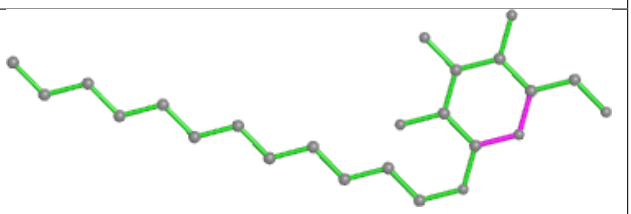


Rings

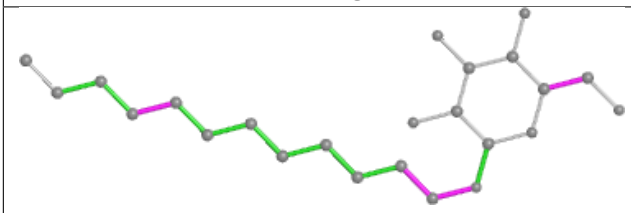
Ligand LMT a 416



Bond lengths



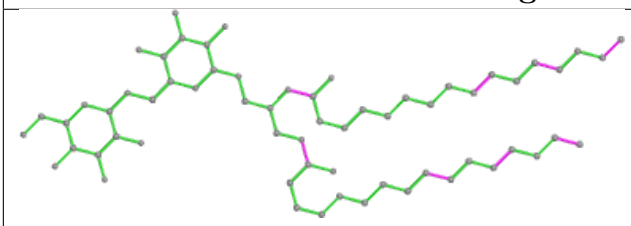
Bond angles



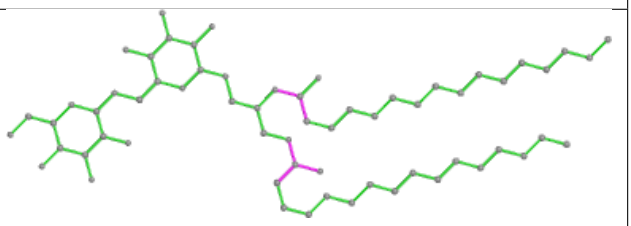
Torsions

Rings

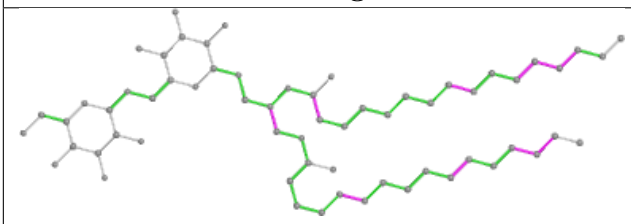
Ligand DGD H 104



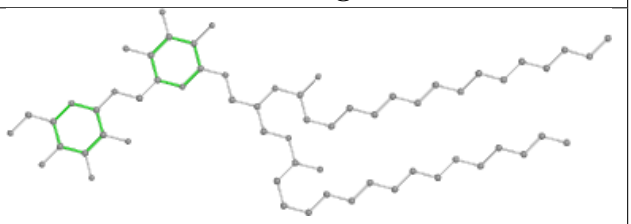
Bond lengths



Bond angles

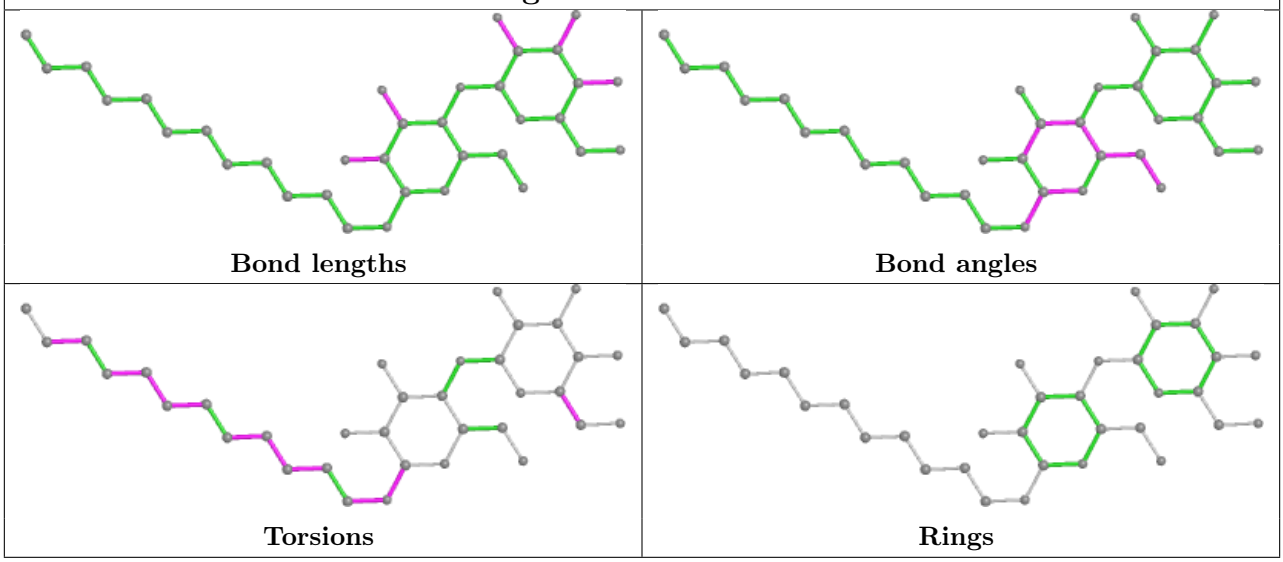


Torsions

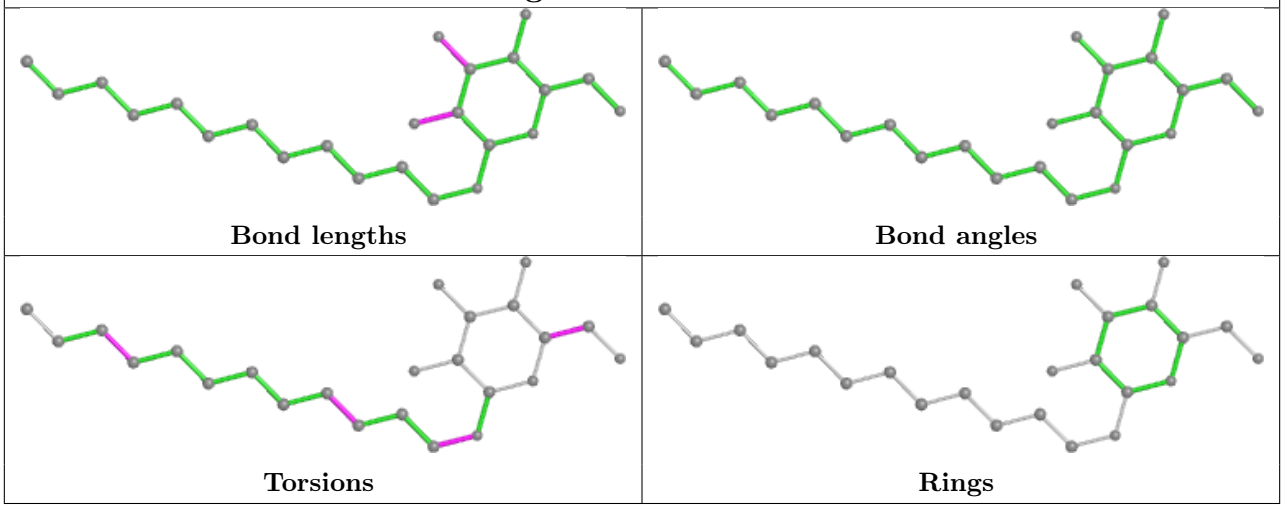


Rings

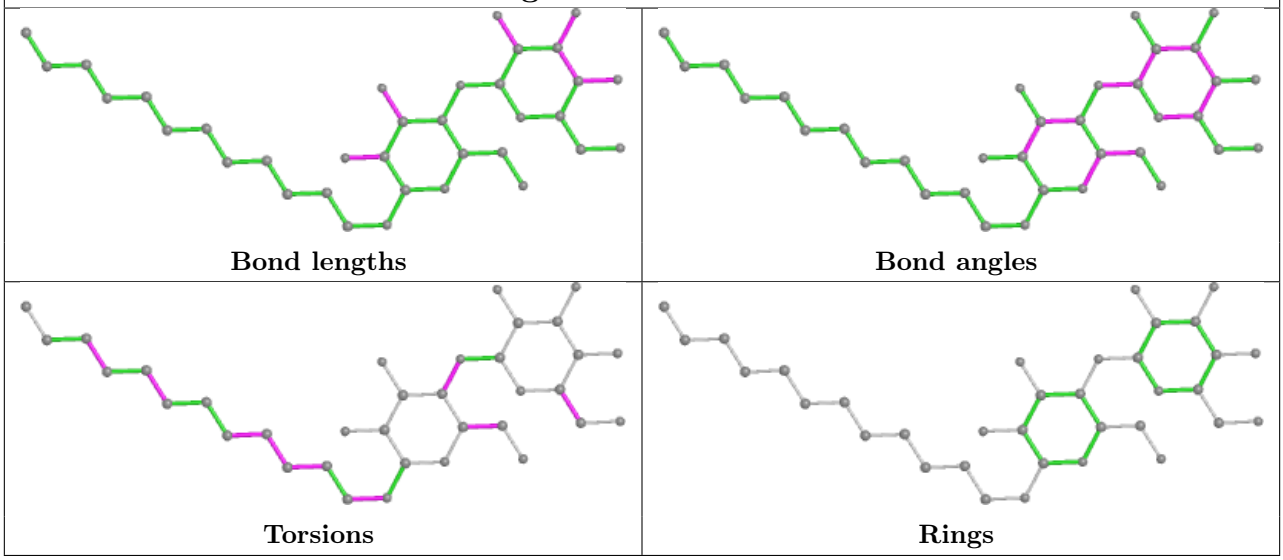
Ligand LMT B 623



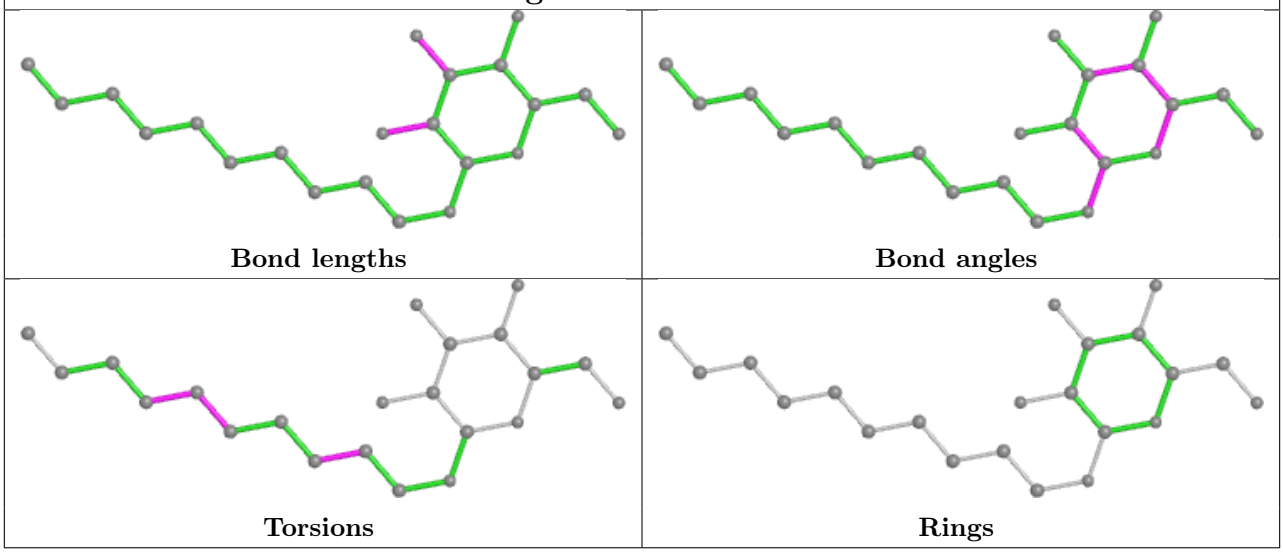
Ligand LMT b 626



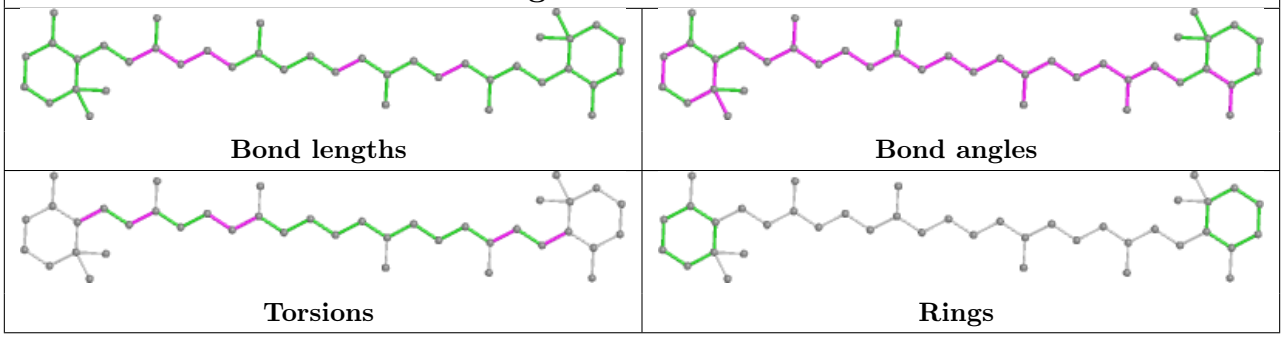
Ligand LMT K 105



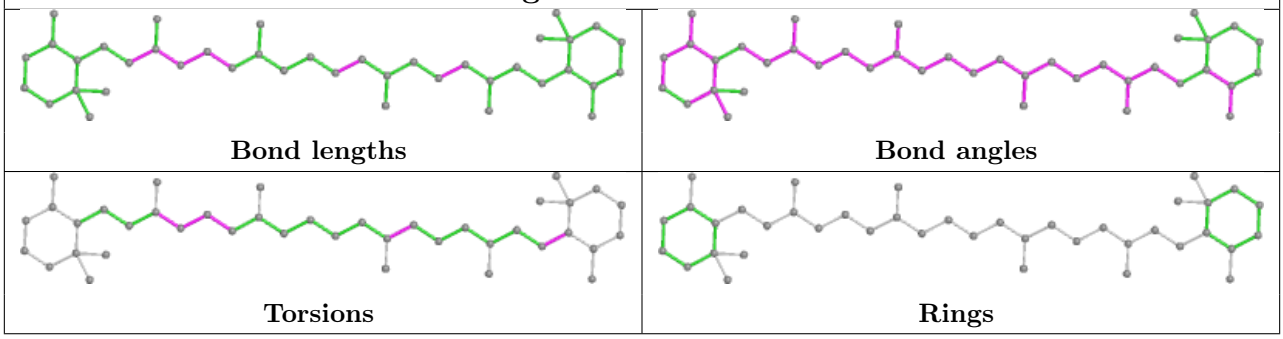
Ligand LMT x 103



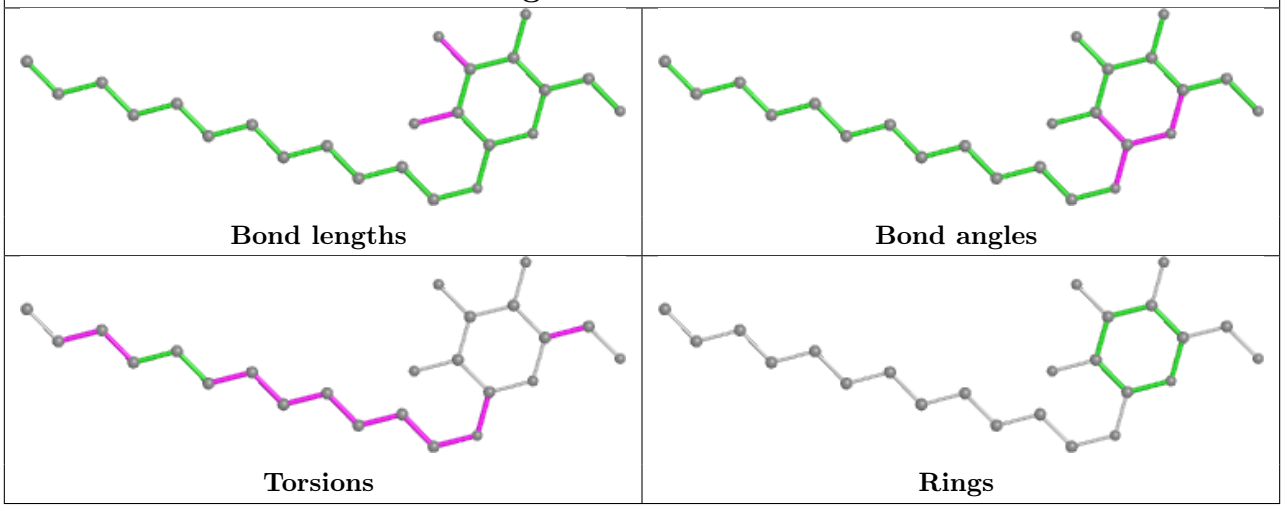
Ligand BCR z 101



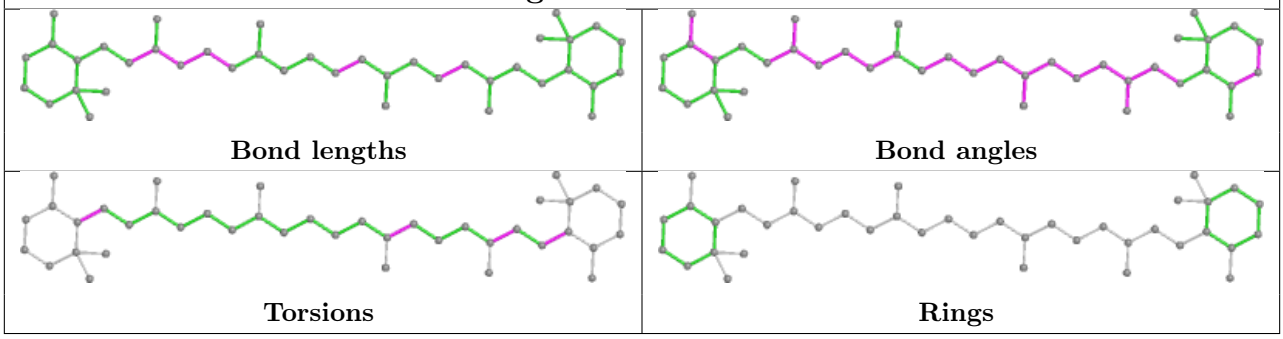
Ligand BCR K 103



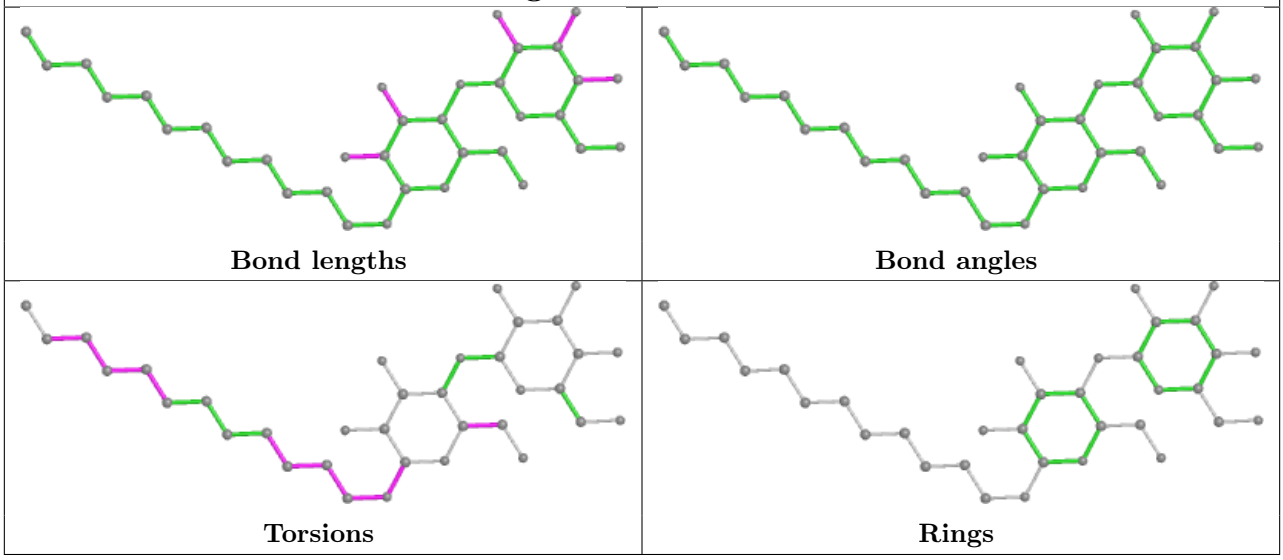
Ligand LMT T 101



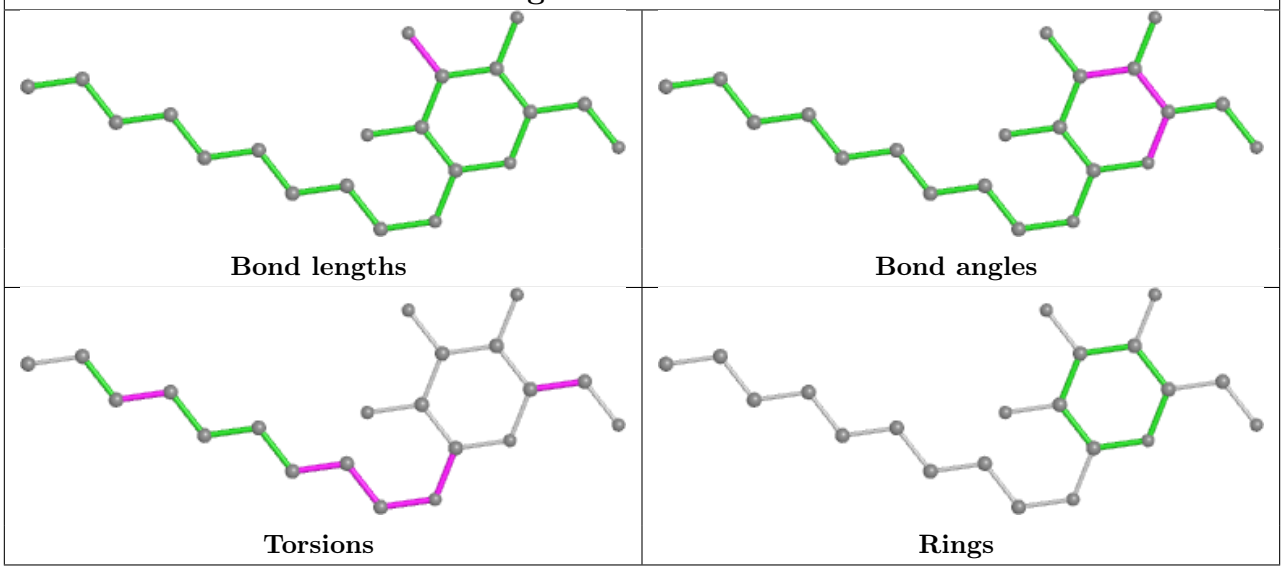
Ligand BCR b 617



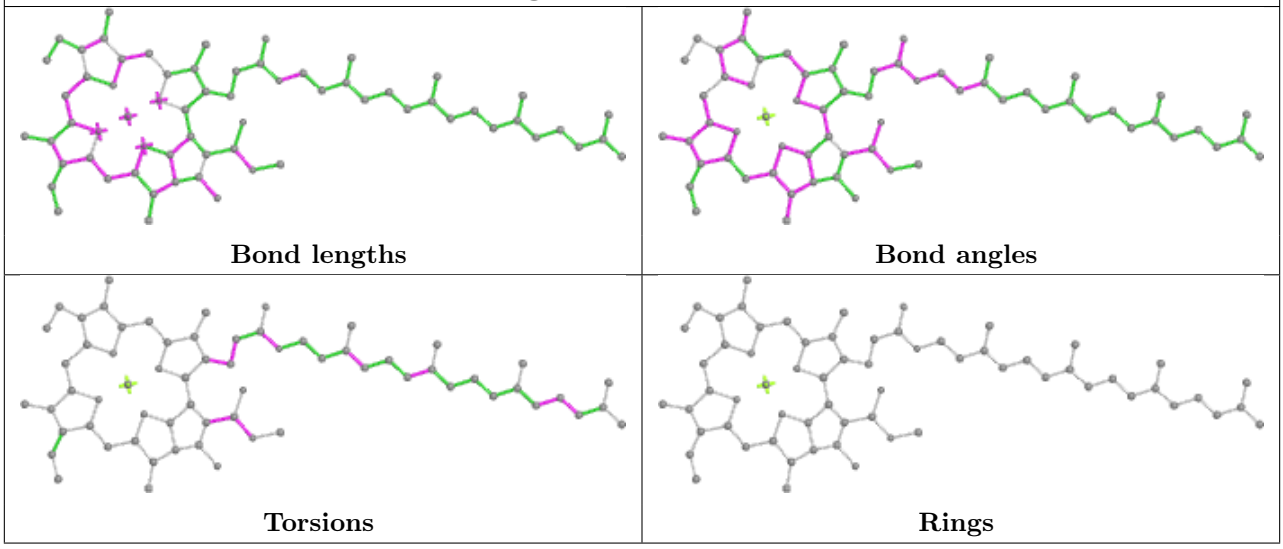
Ligand LMT d 411



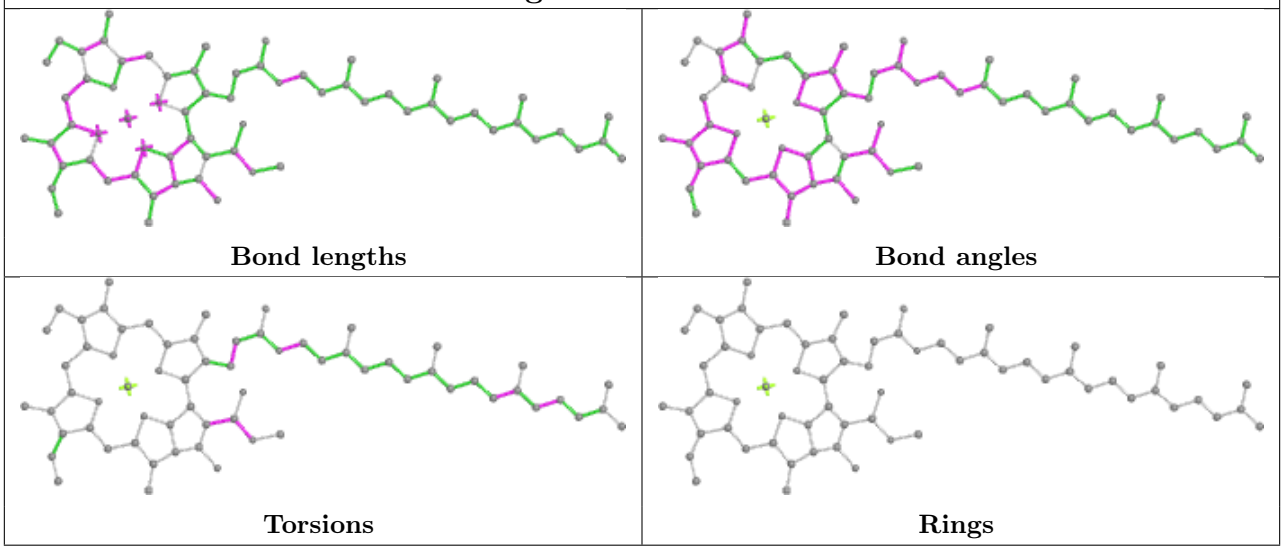
Ligand LMT c 525

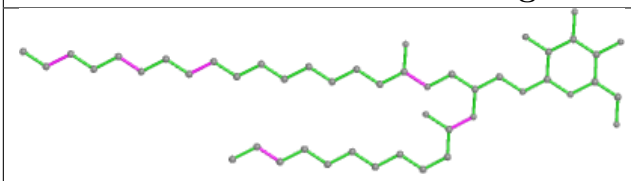
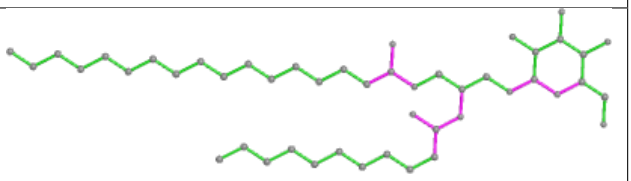
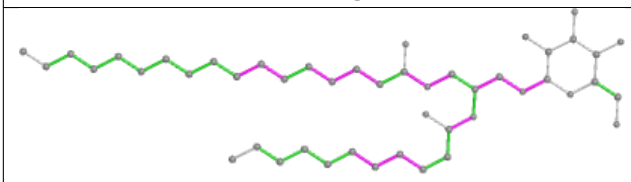
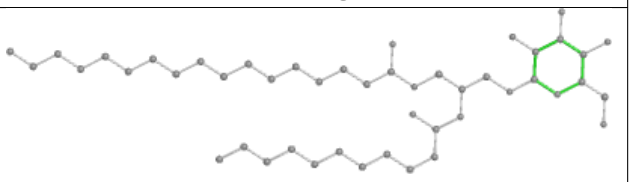


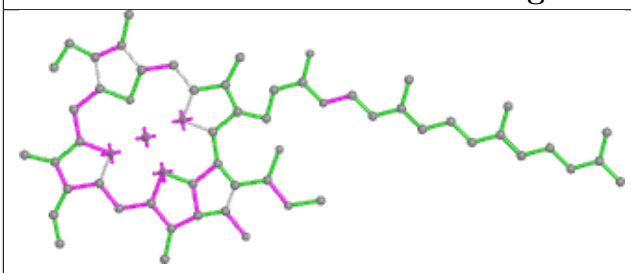
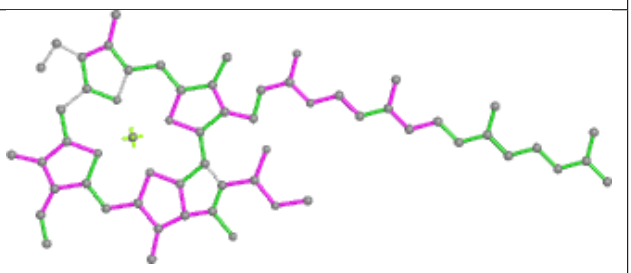
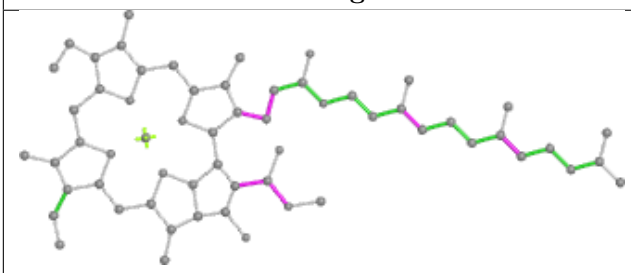
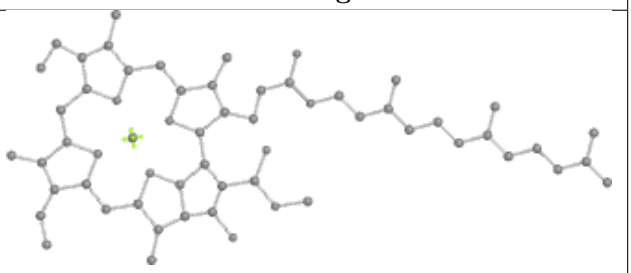
Ligand CLA B 609



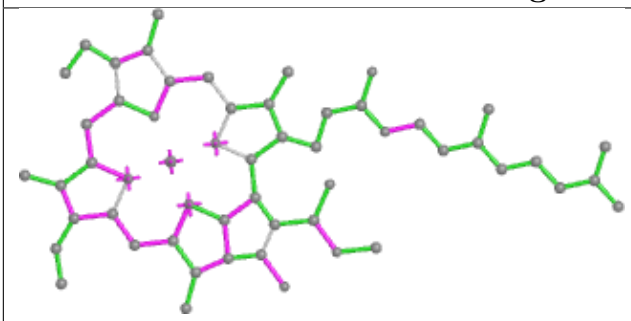
Ligand CLA C 503



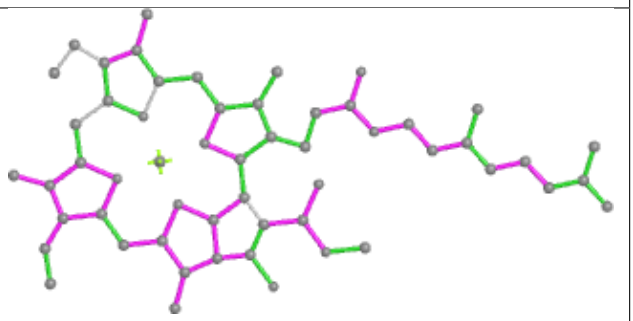
Ligand LMG H 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

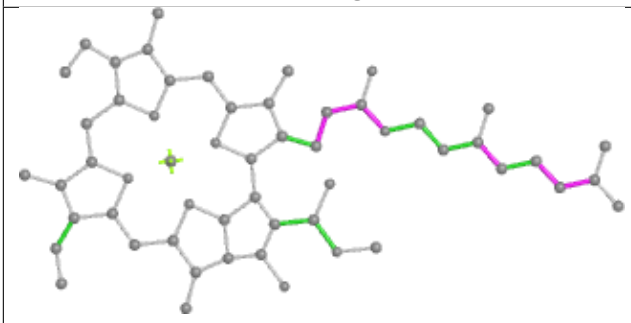
Ligand CLA c 506



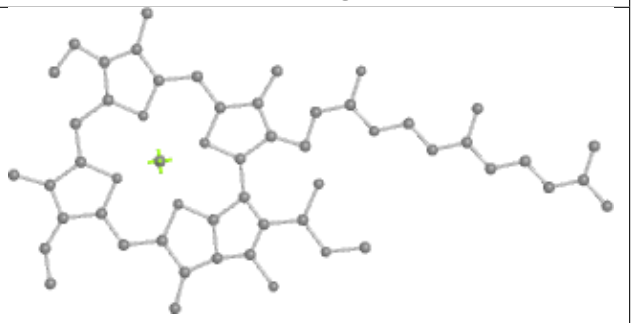
Bond lengths



Bond angles

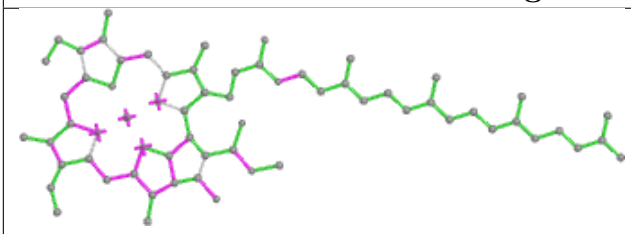


Torsions

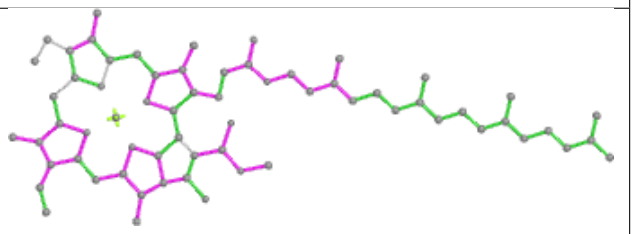


Rings

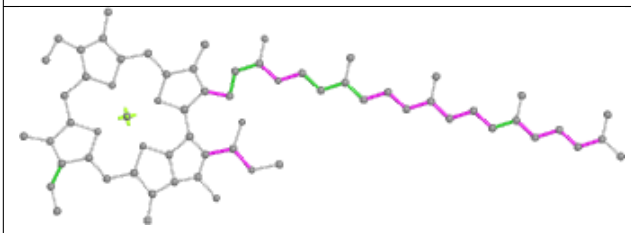
Ligand CLA C 512



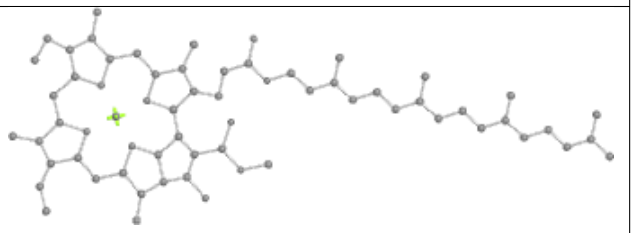
Bond lengths



Bond angles

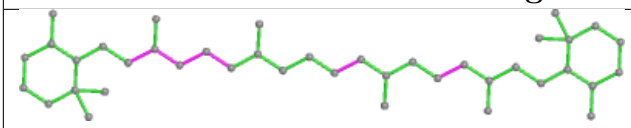


Torsions

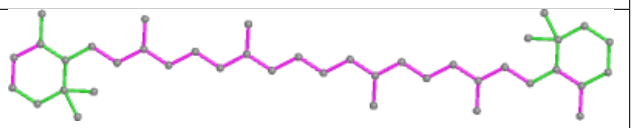


Rings

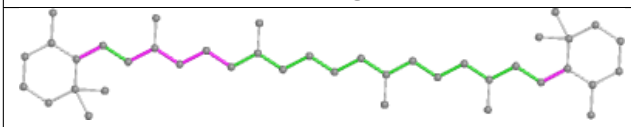
Ligand BCR b 618



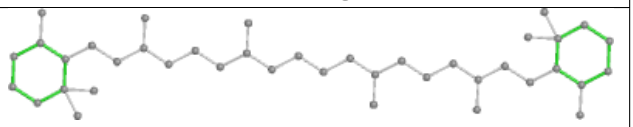
Bond lengths



Bond angles

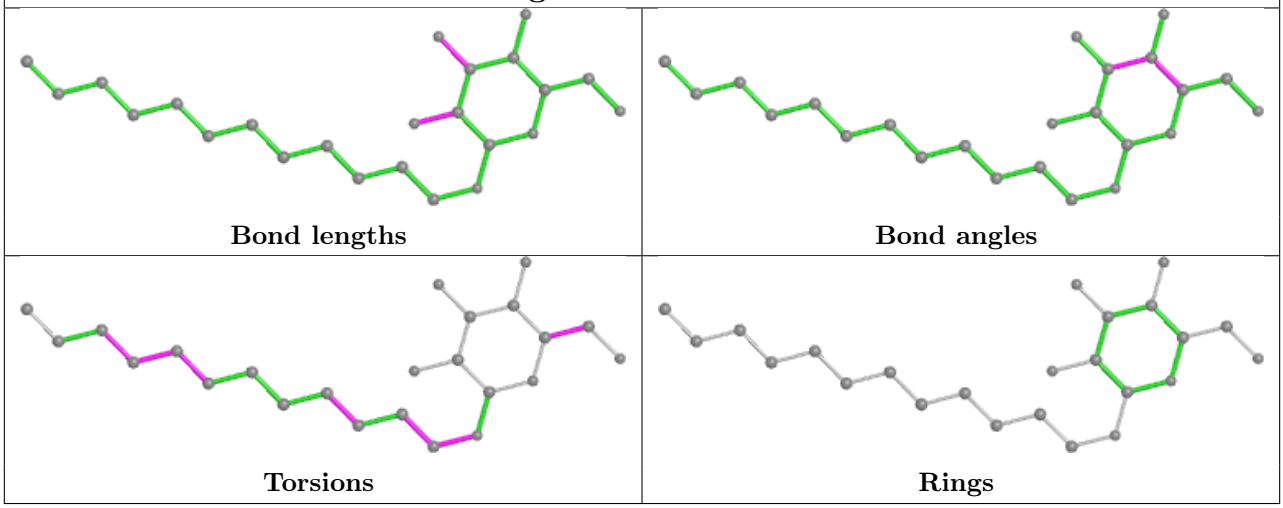


Torsions

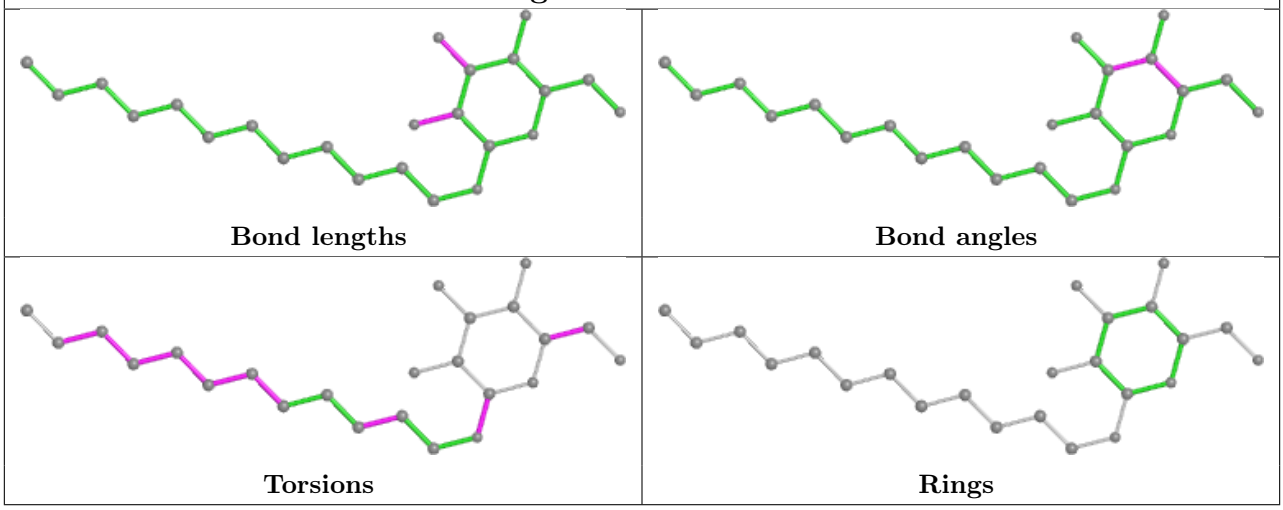


Rings

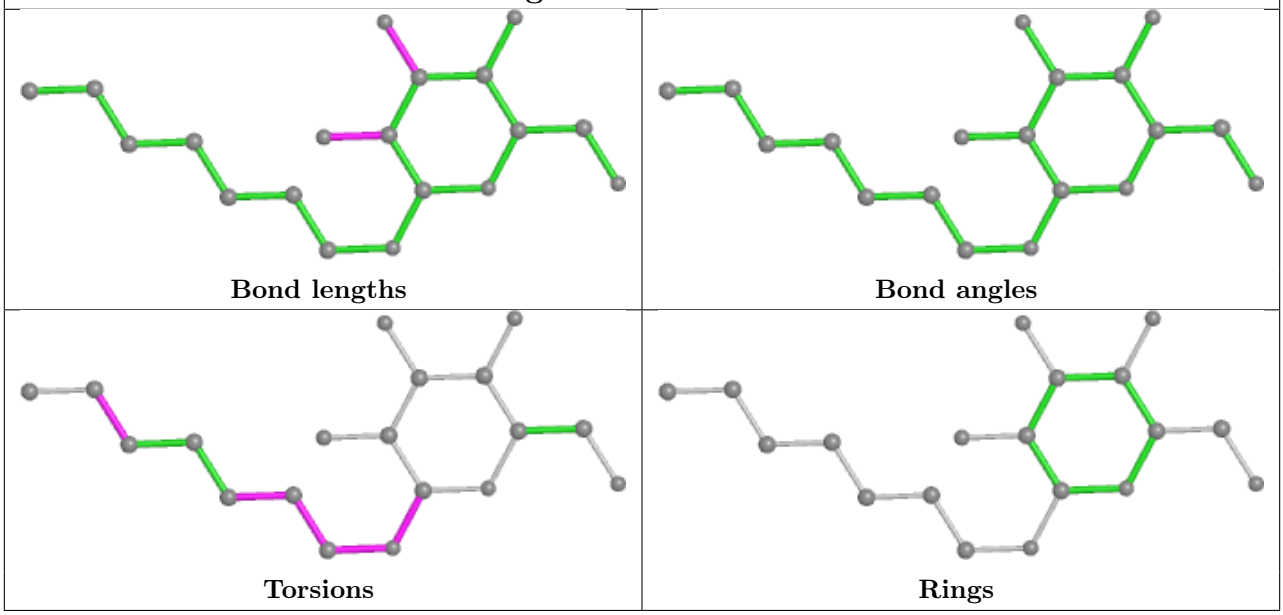
Ligand LMT I 102



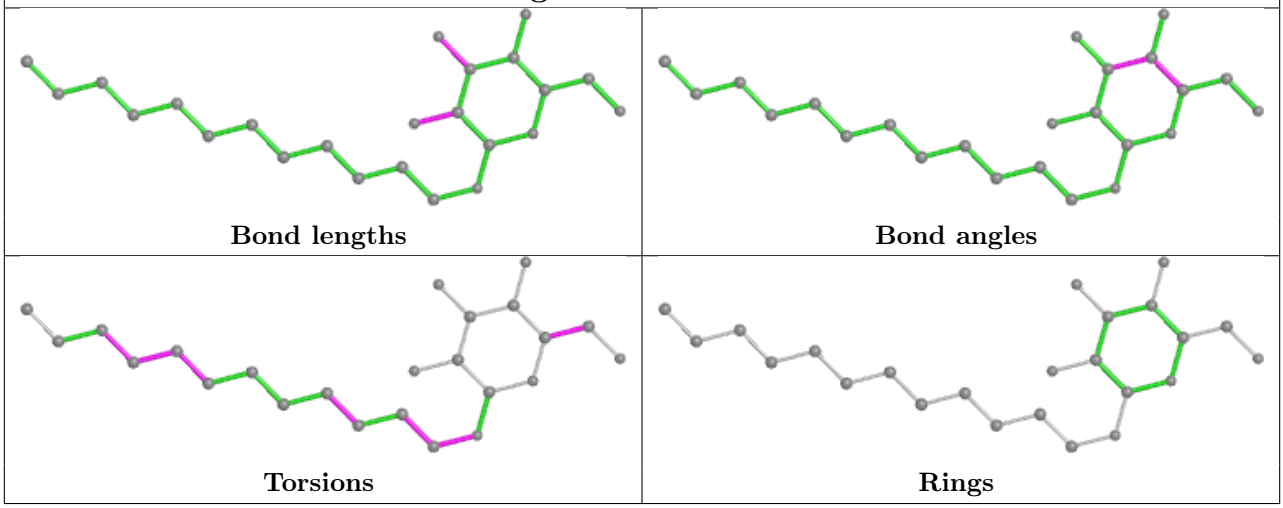
Ligand LMT i 101



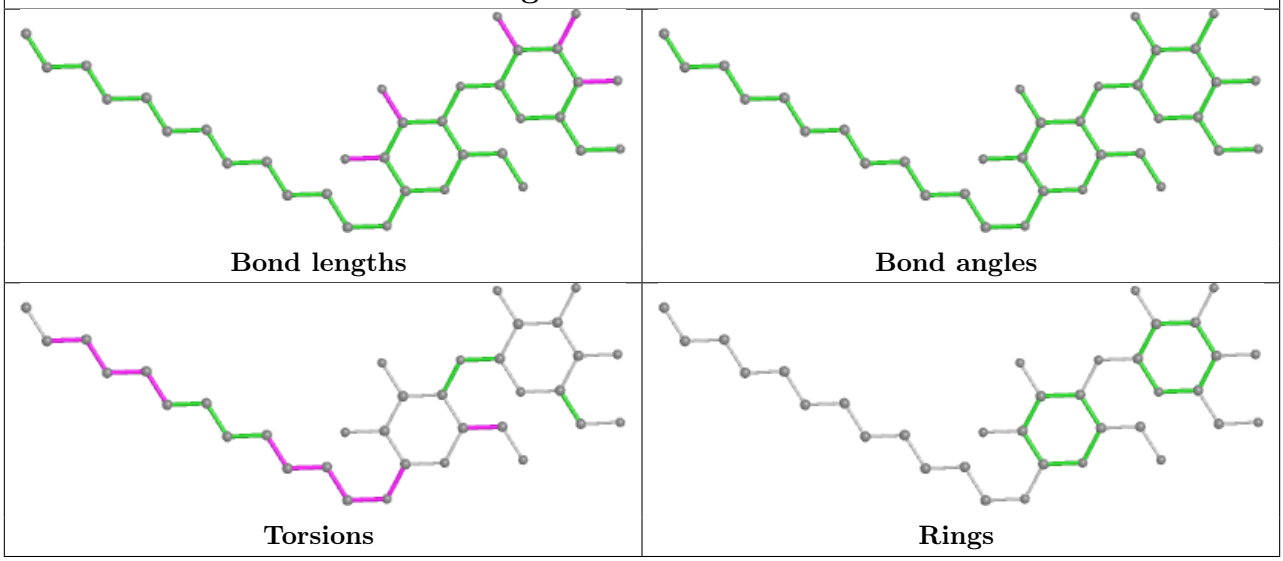
Ligand LMT x 105



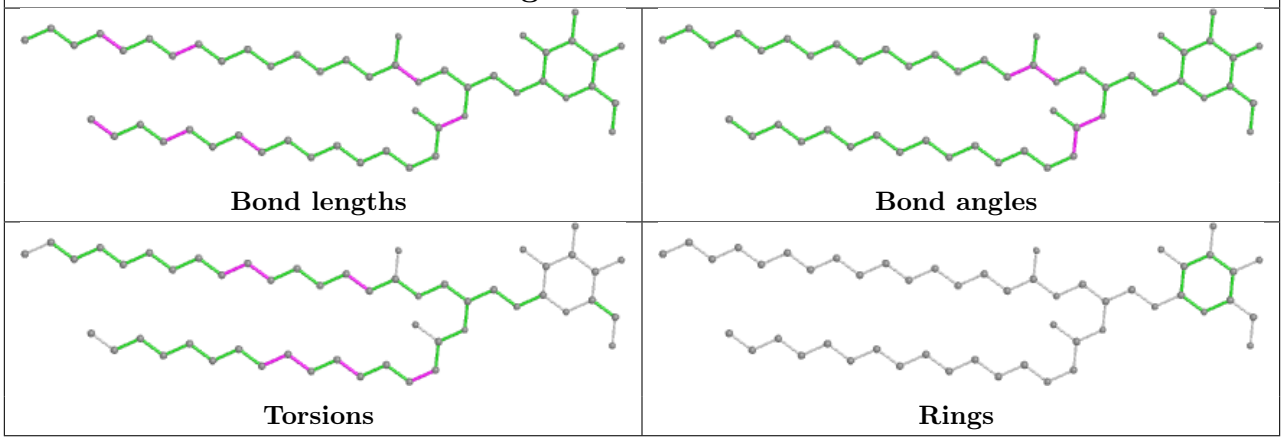
Ligand LMT i 102



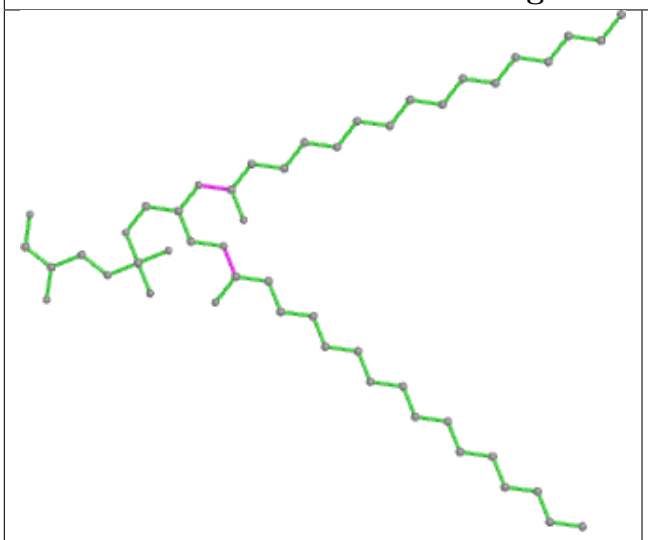
Ligand LMT D 411



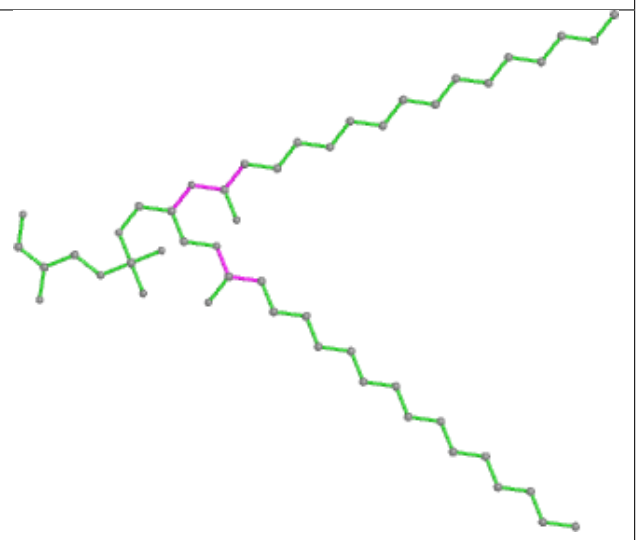
Ligand LMG B 621



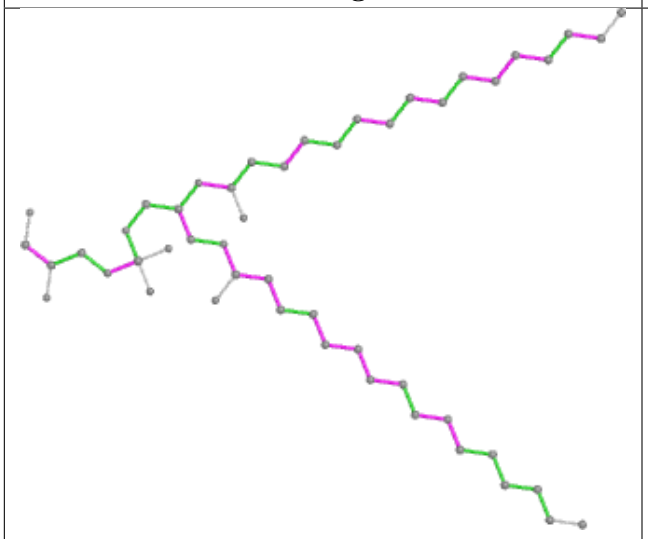
Ligand LHG d 406



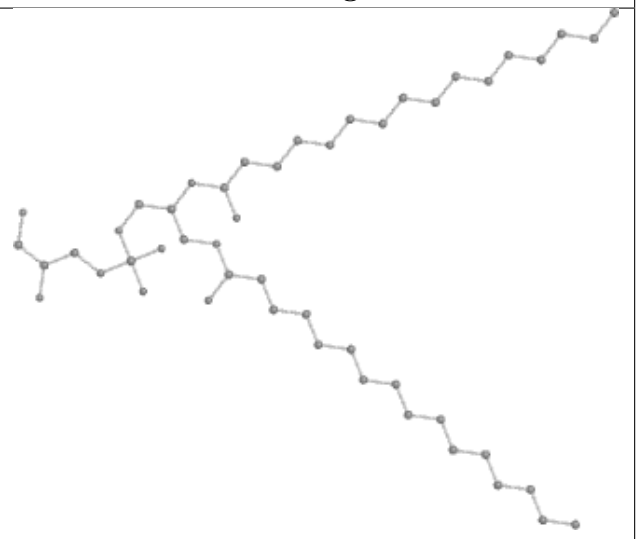
Bond lengths



Bond angles

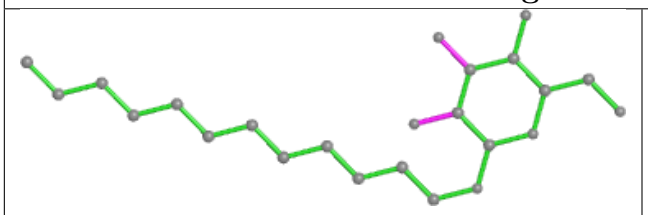


Torsions

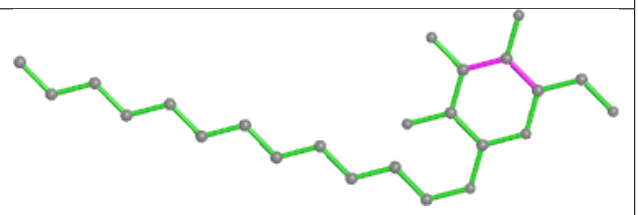


Rings

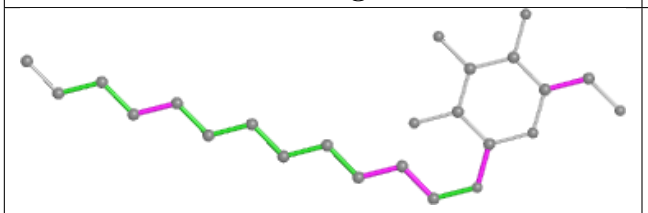
Ligand LMT X 101



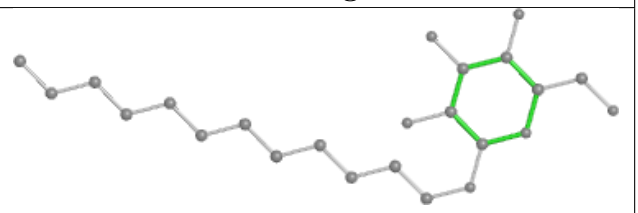
Bond lengths



Bond angles

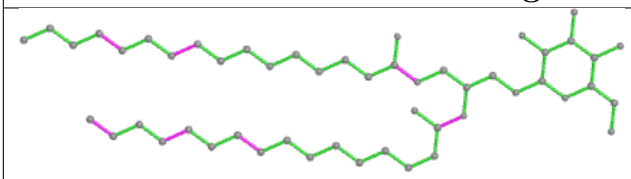


Torsions

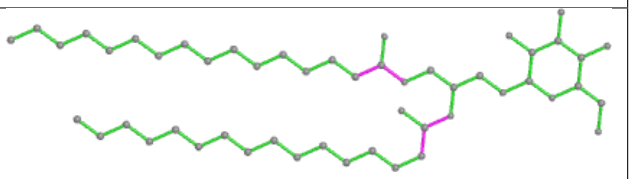


Rings

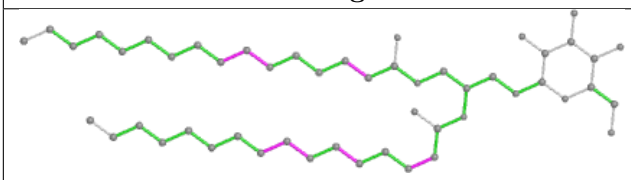
Ligand LMG b 621



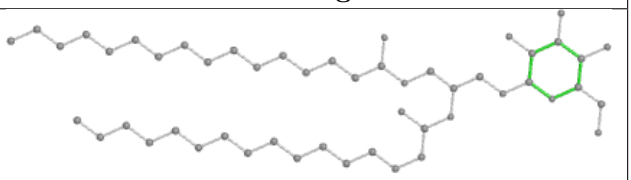
Bond lengths



Bond angles

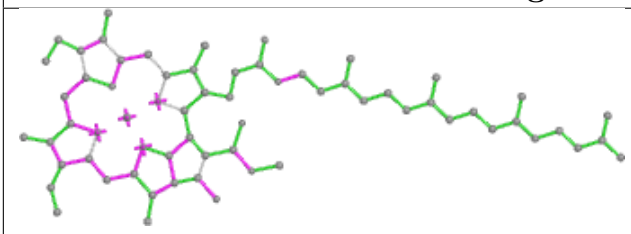


Torsions

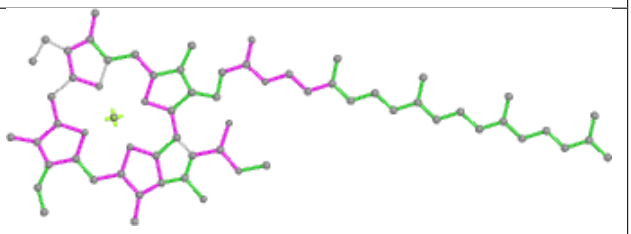


Rings

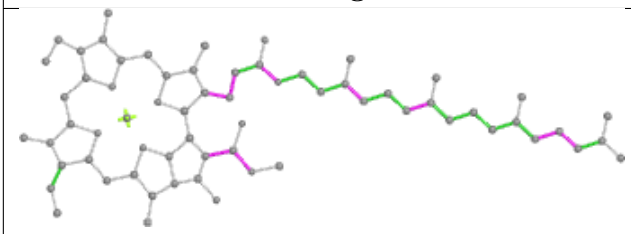
Ligand CLA b 609



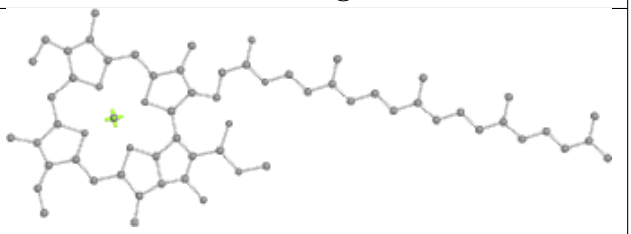
Bond lengths



Bond angles

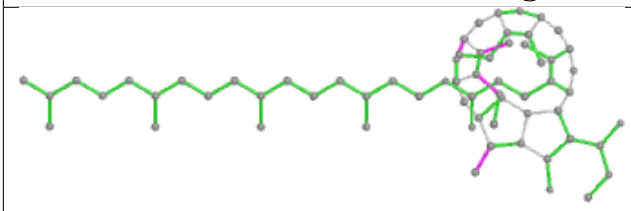


Torsions

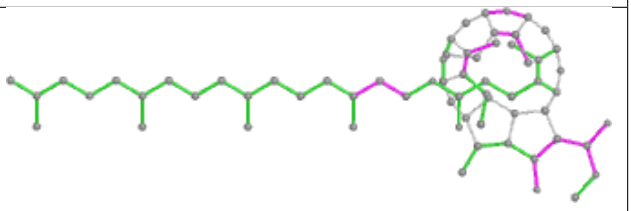


Rings

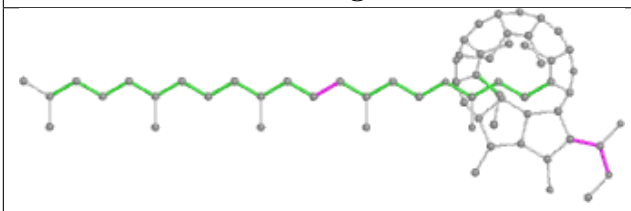
Ligand PHO D 402



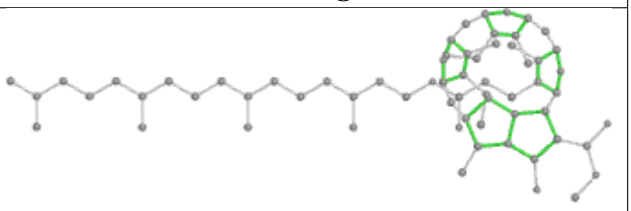
Bond lengths



Bond angles

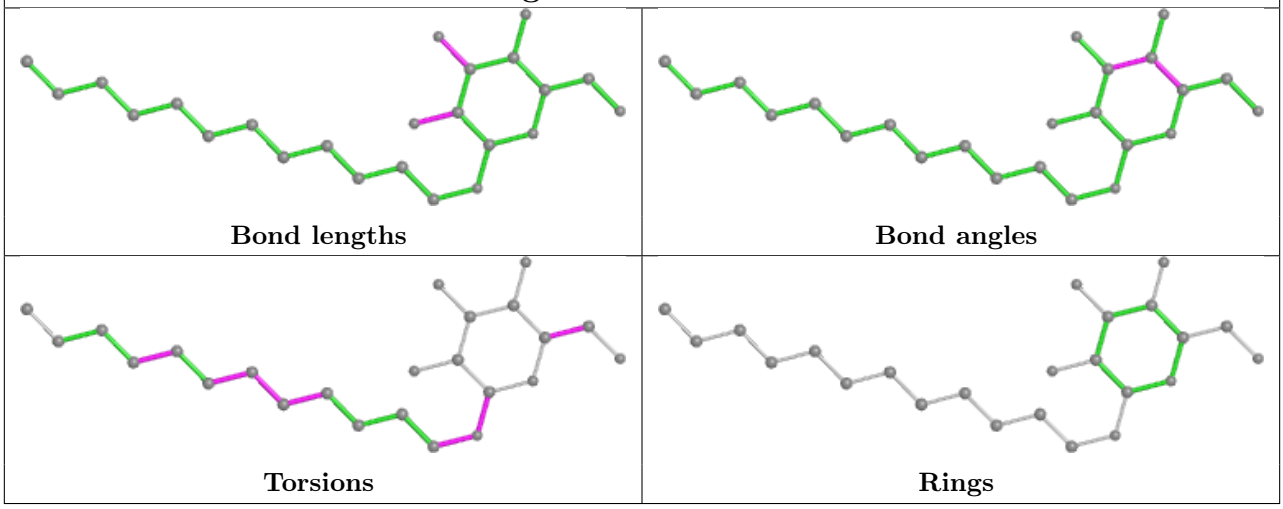


Torsions

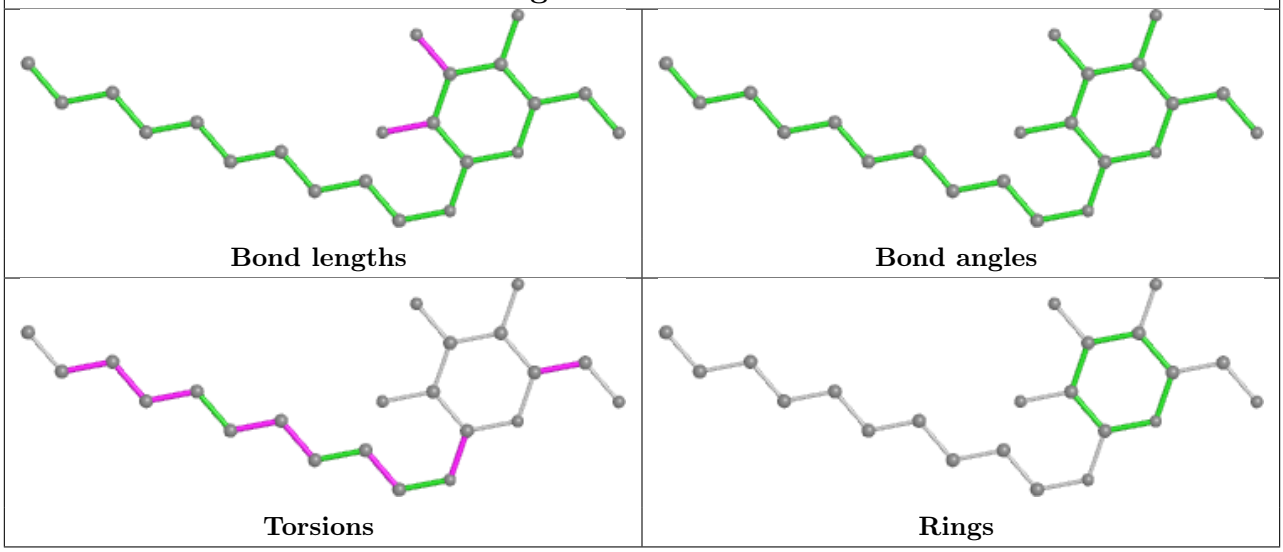


Rings

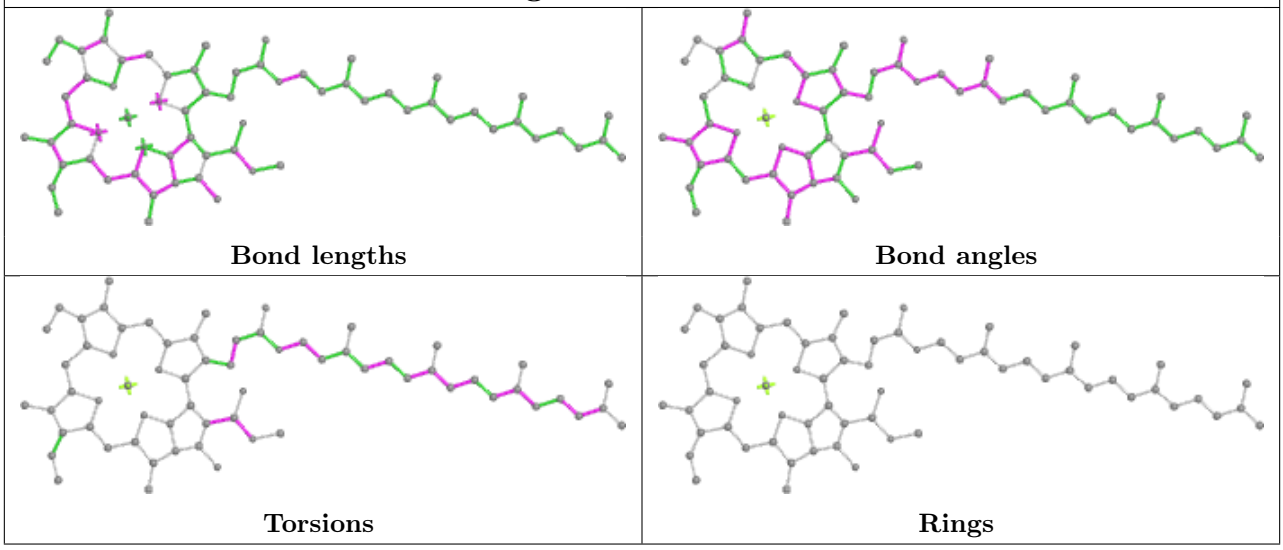
Ligand LMT B 624



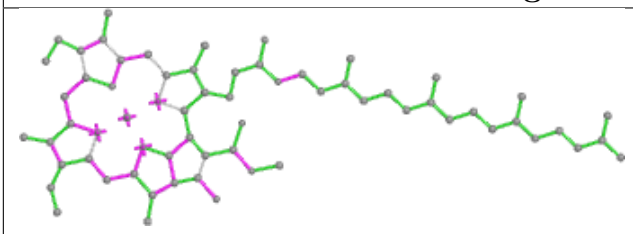
Ligand LMT i 104



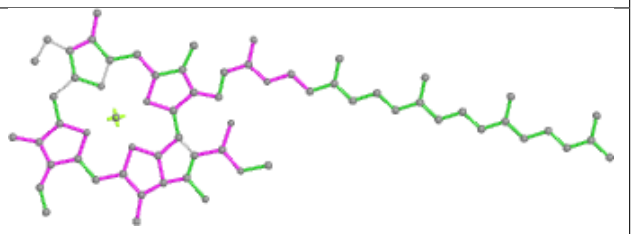
Ligand CLA B 602



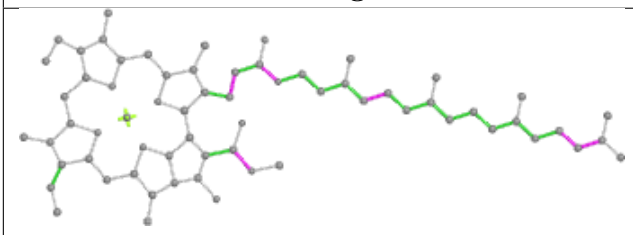
Ligand CLA A 405



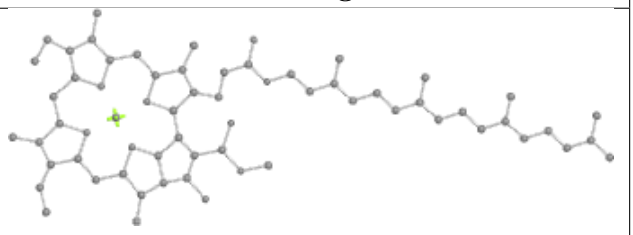
Bond lengths



Bond angles

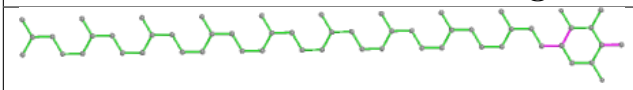


Torsions

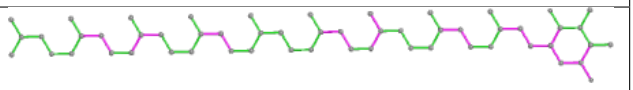


Rings

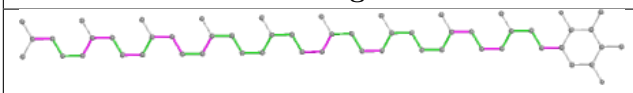
Ligand PL9 A 411



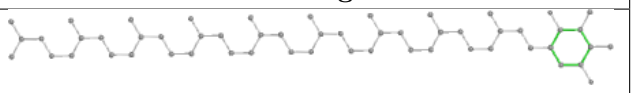
Bond lengths



Bond angles

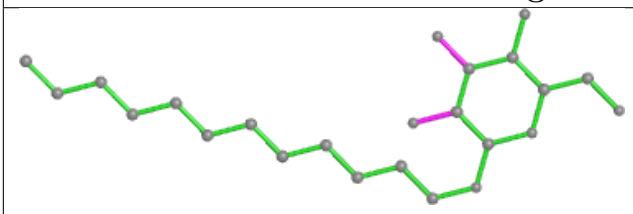


Torsions

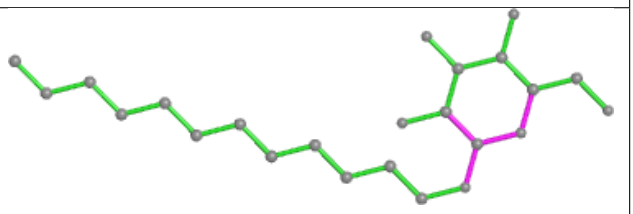


Rings

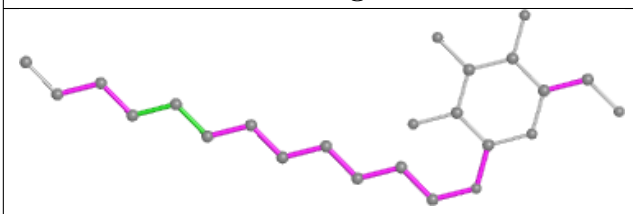
Ligand LMT t 101



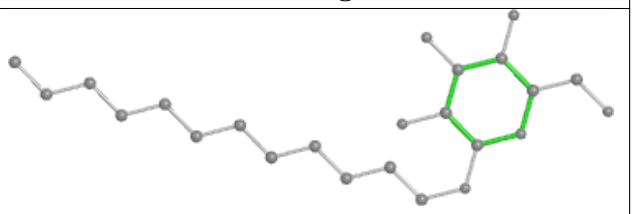
Bond lengths



Bond angles

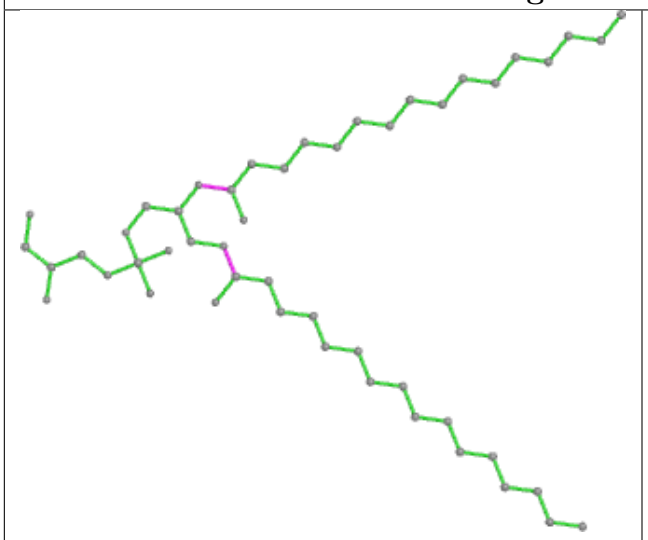


Torsions

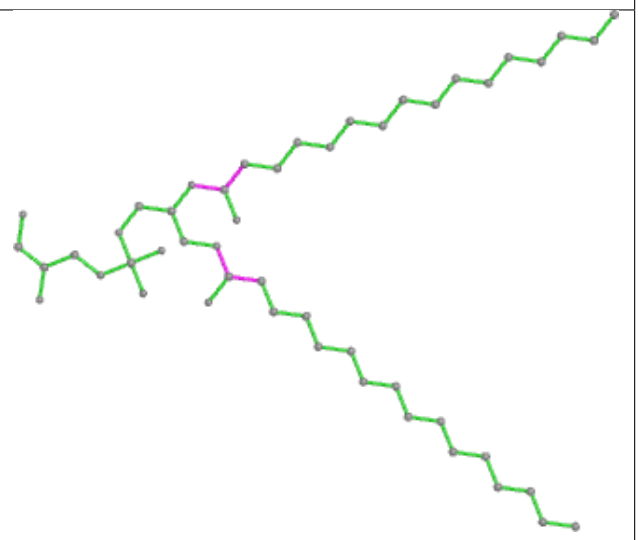


Rings

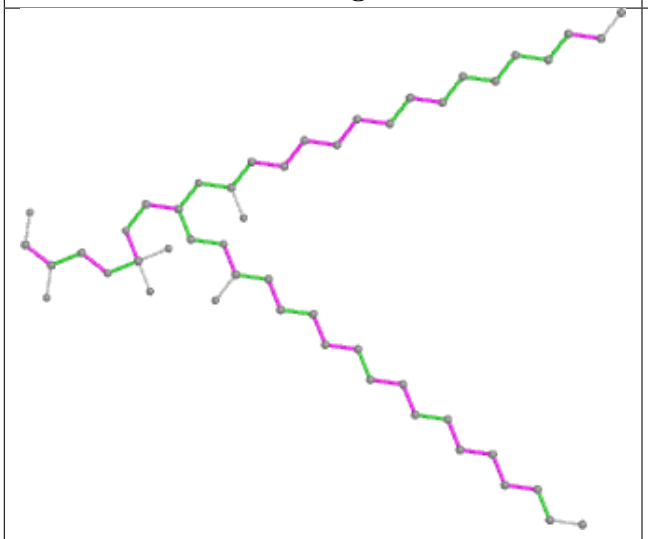
Ligand LHG d 408



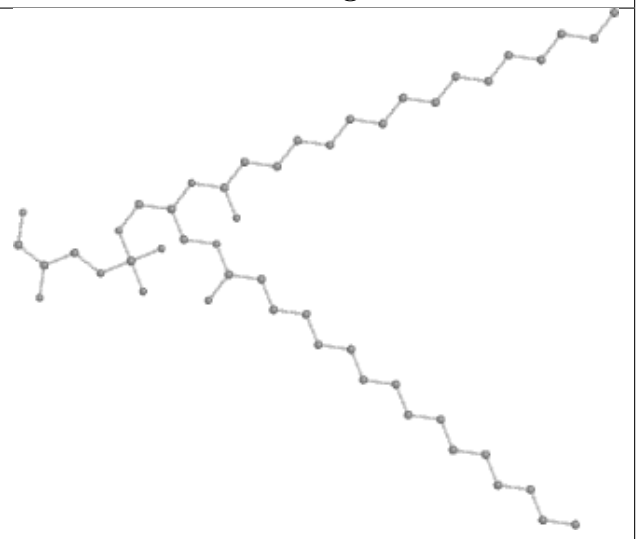
Bond lengths



Bond angles

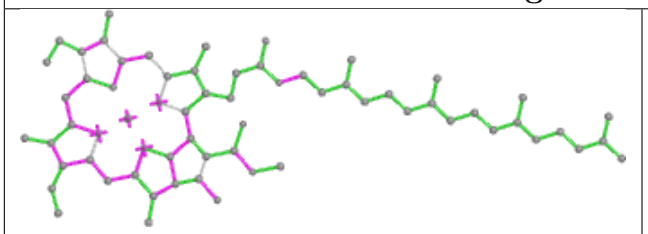


Torsions

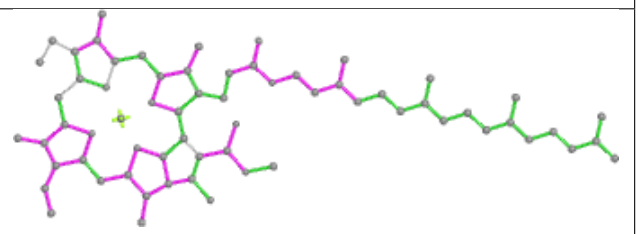


Rings

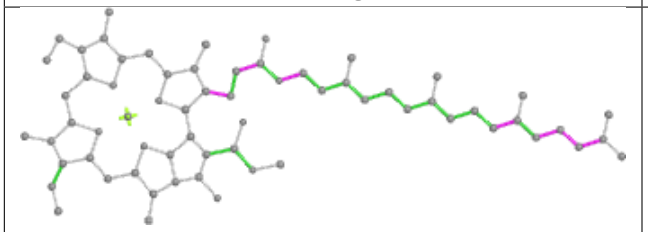
Ligand CLA B 608



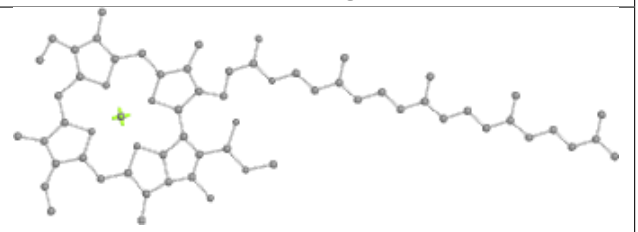
Bond lengths



Bond angles

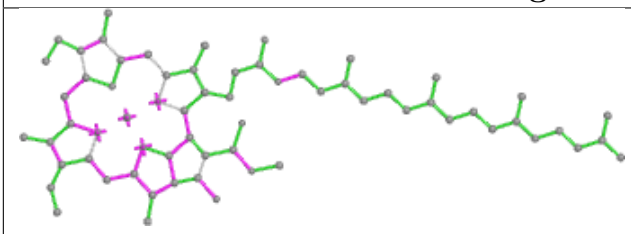


Torsions

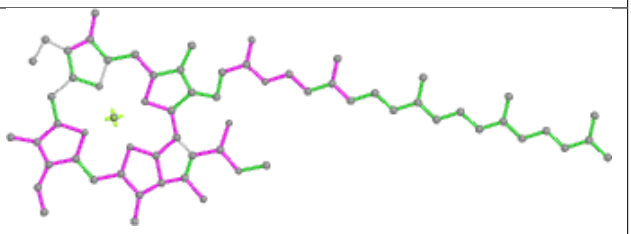


Rings

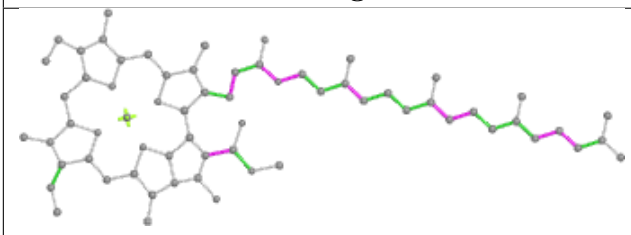
Ligand CLA c 508



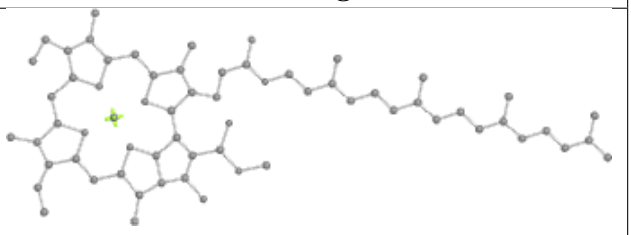
Bond lengths



Bond angles

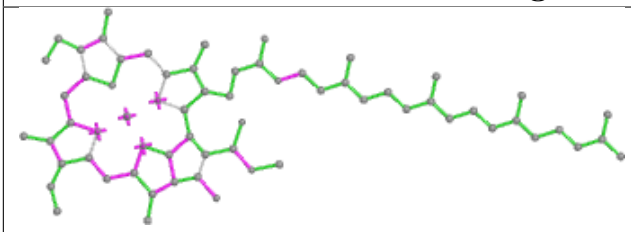


Torsions

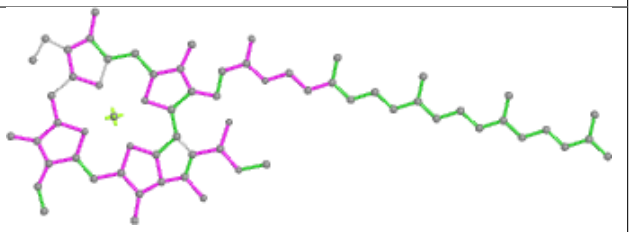


Rings

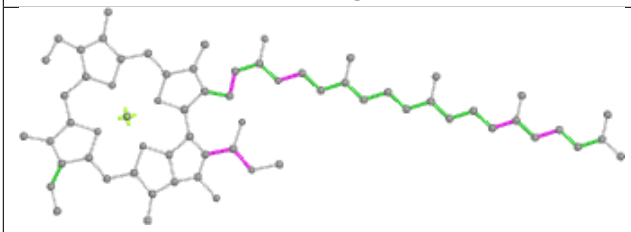
Ligand CLA c 503



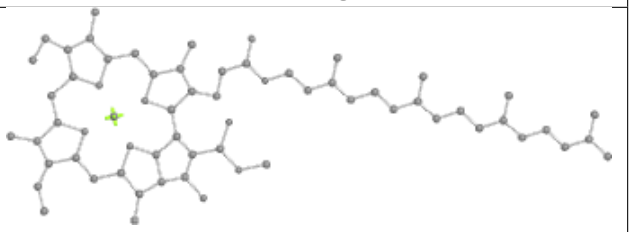
Bond lengths



Bond angles

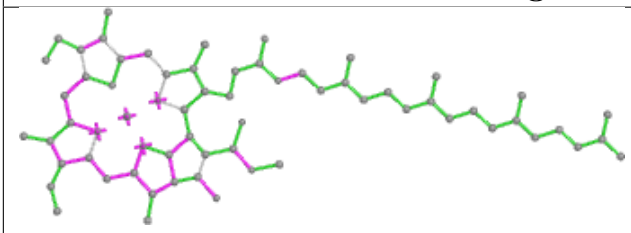


Torsions

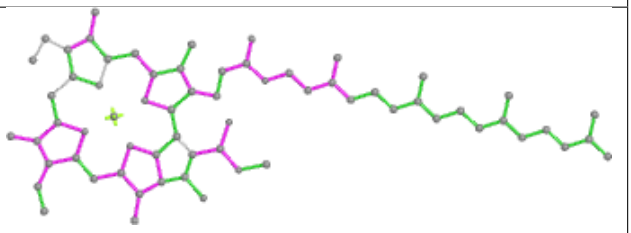


Rings

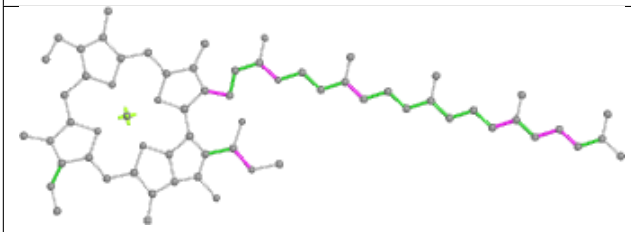
Ligand CLA d 404



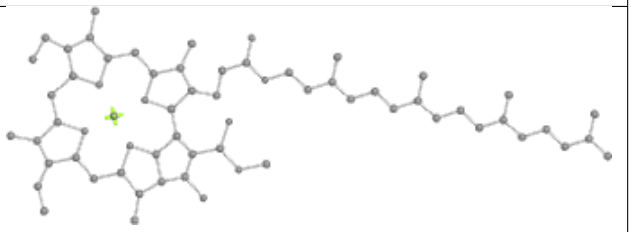
Bond lengths



Bond angles

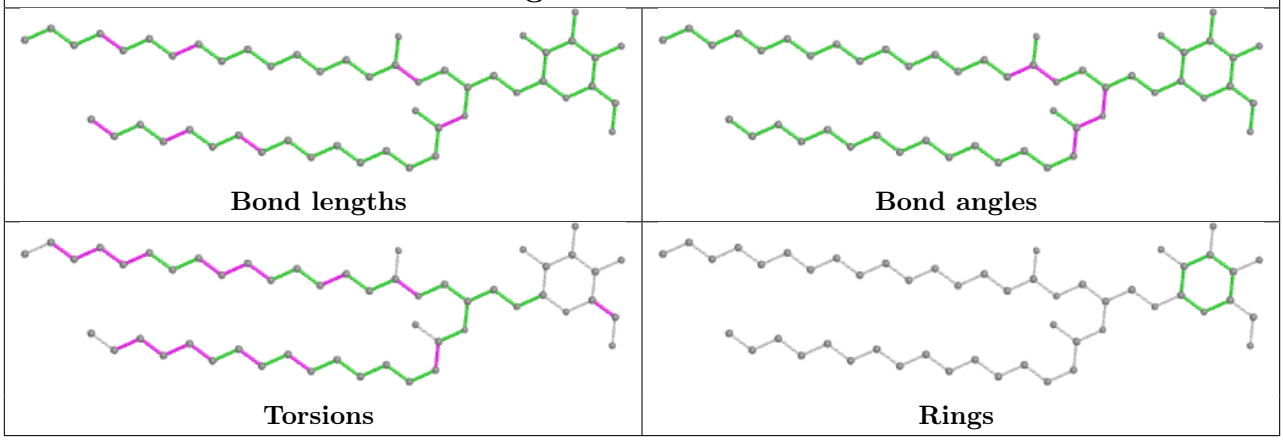


Torsions

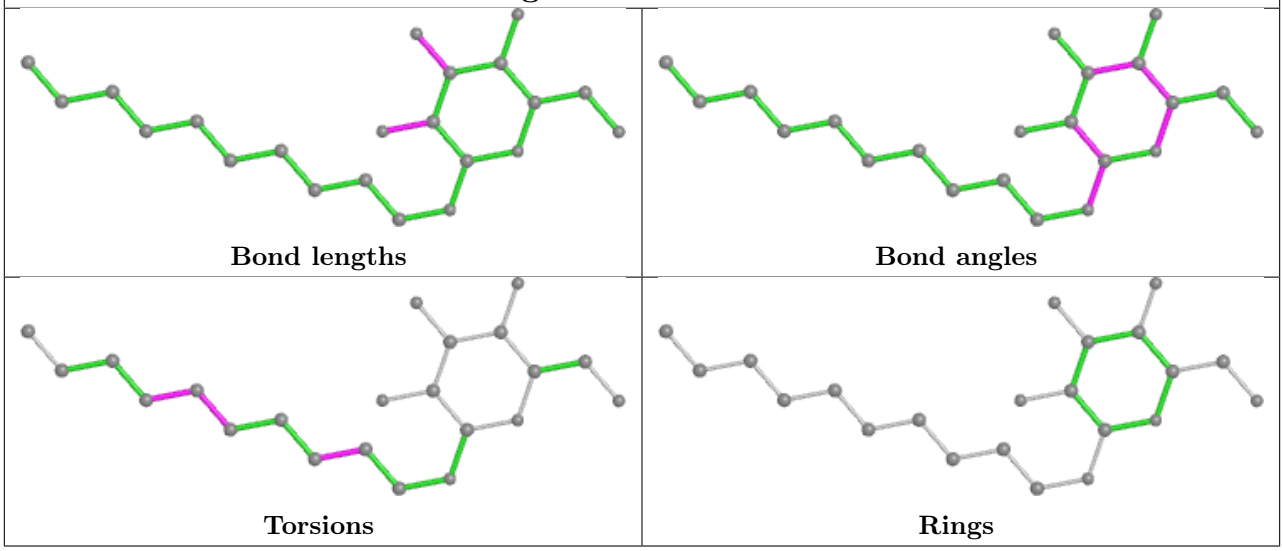


Rings

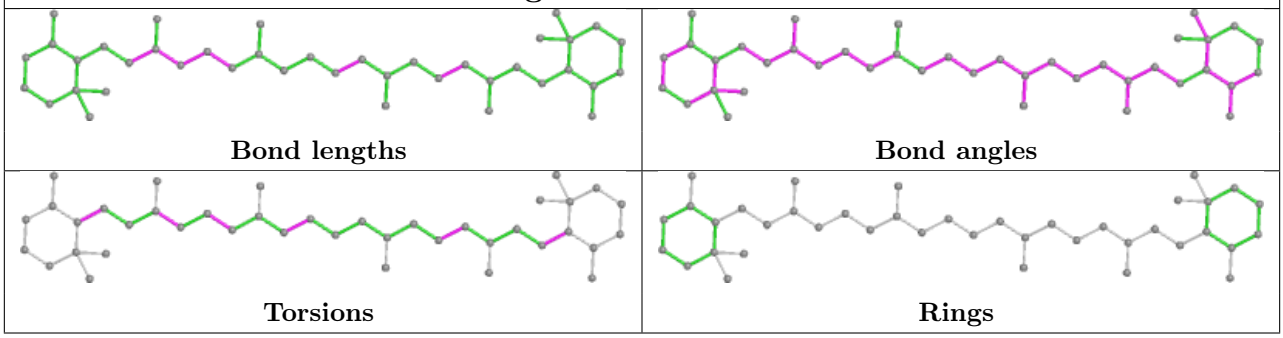
Ligand LMG c 519



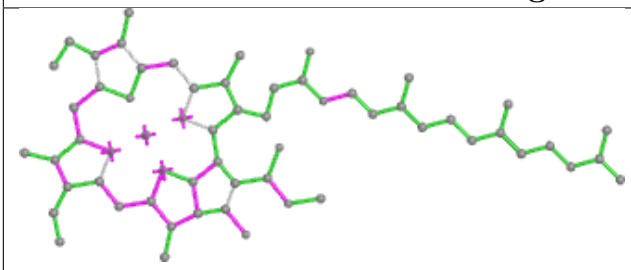
Ligand LMT X 103



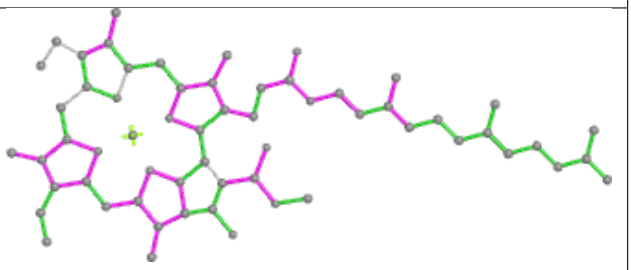
Ligand BCR F 101



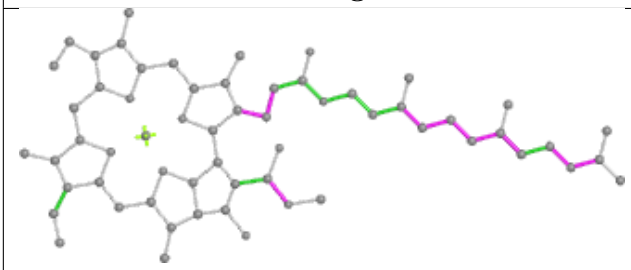
Ligand CLA a 408



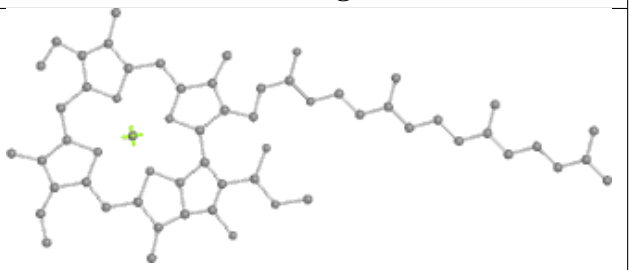
Bond lengths



Bond angles

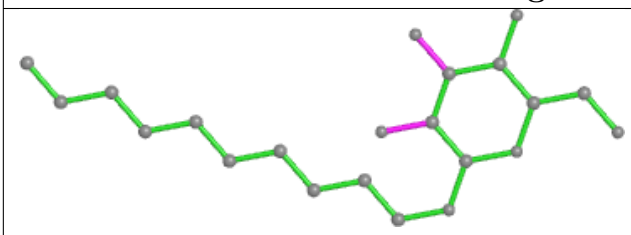


Torsions

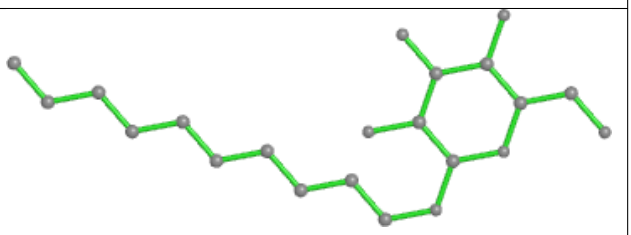


Rings

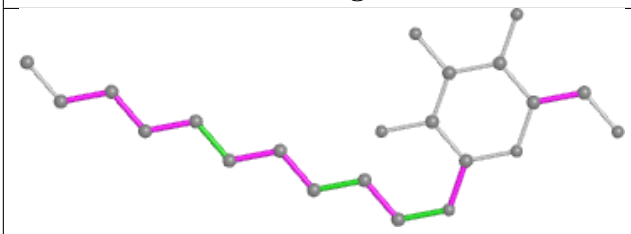
Ligand LMT I 104



Bond lengths



Bond angles



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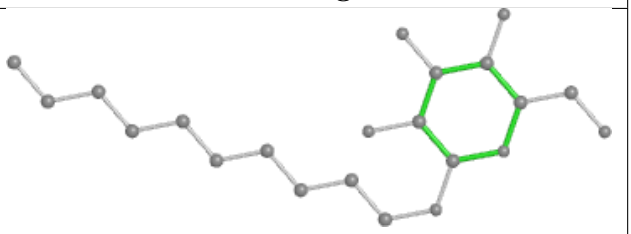
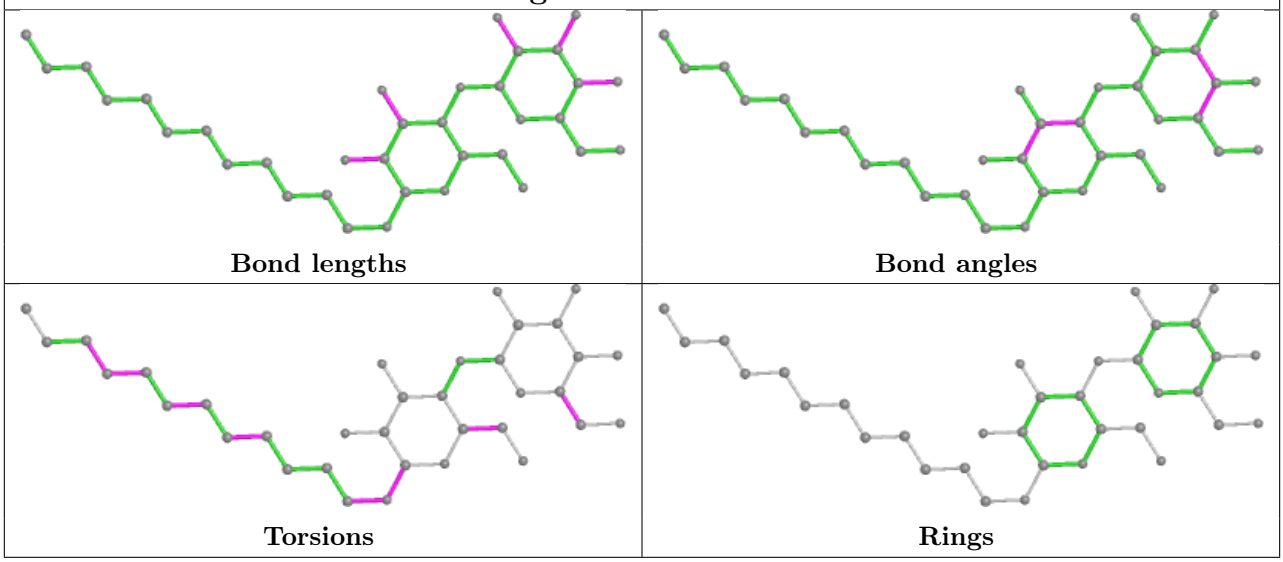
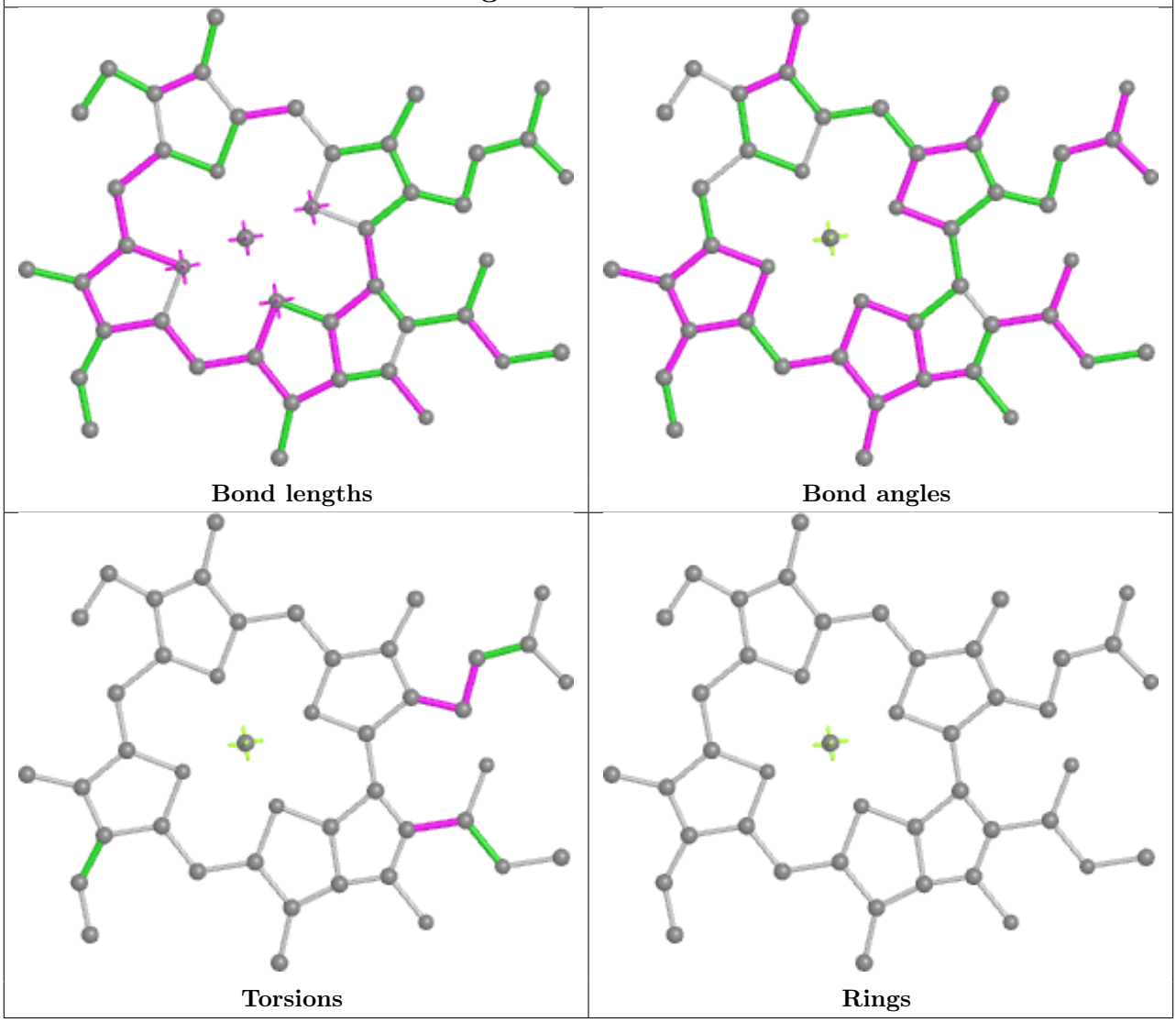


Rings

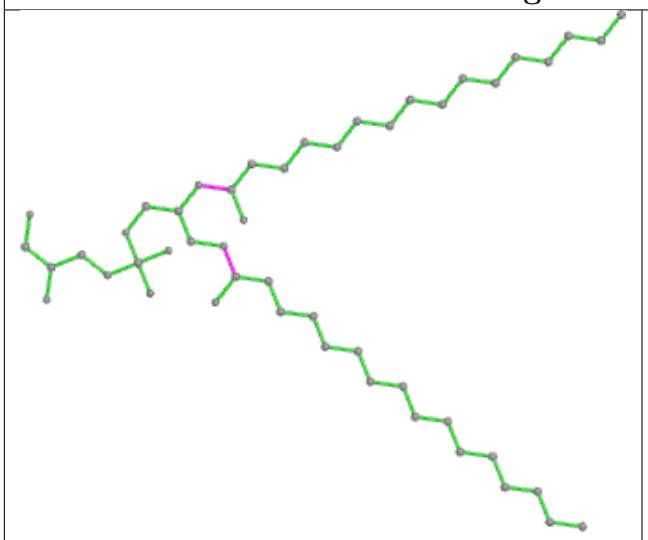
Ligand LMT f 103



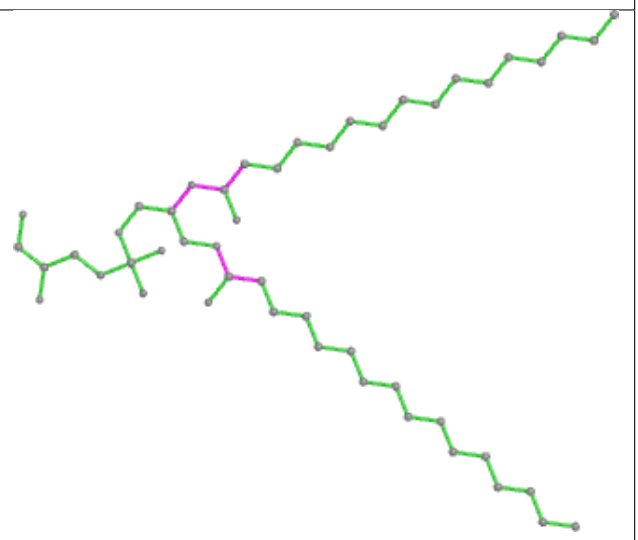
Ligand CLA B 601



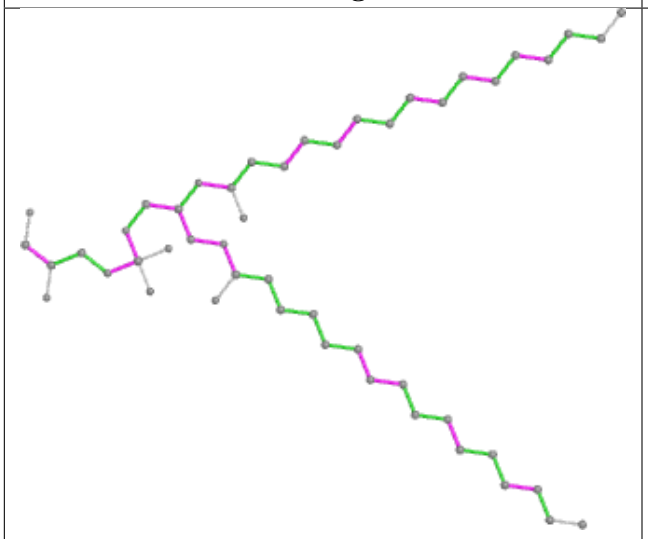
Ligand LHG B 628



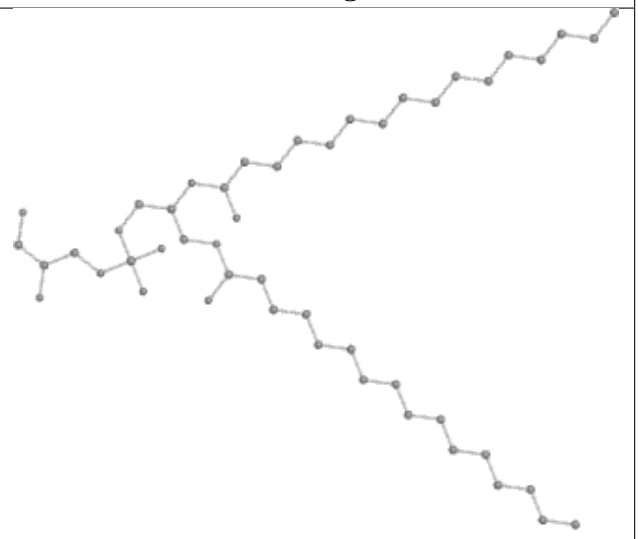
Bond lengths



Bond angles

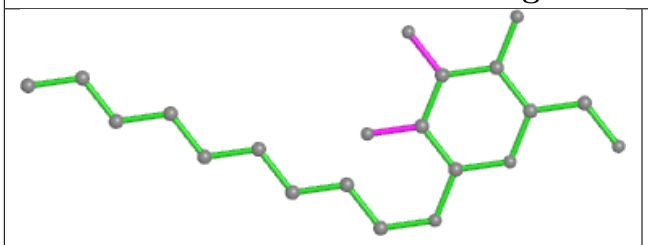


Torsions

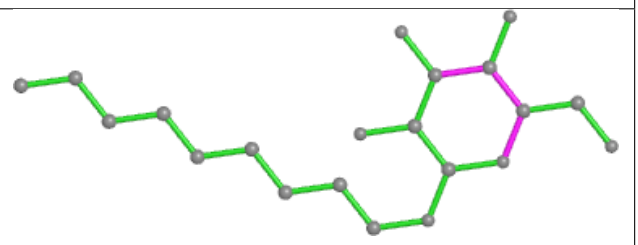


Rings

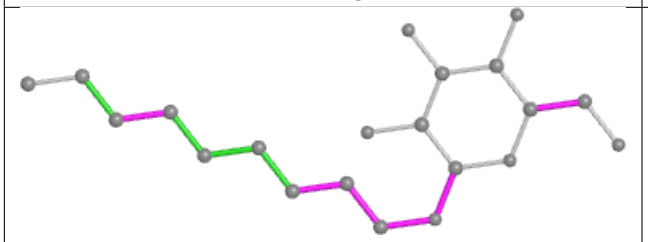
Ligand LMT C 525



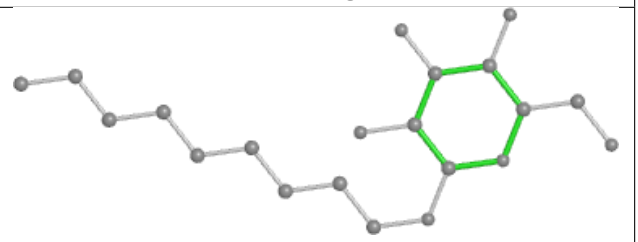
Bond lengths



Bond angles

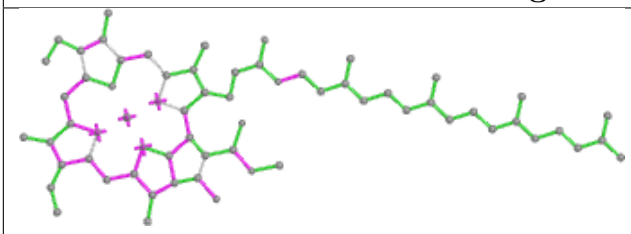


Torsions

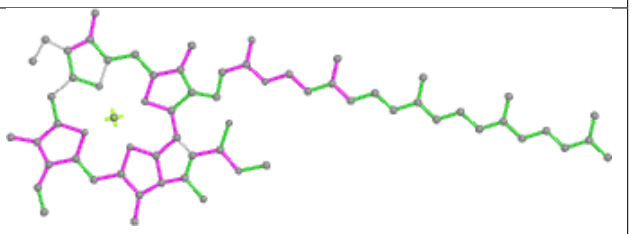


Rings

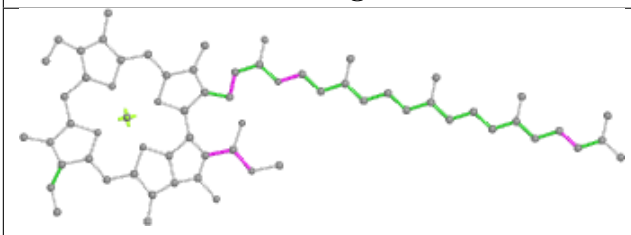
Ligand CLA c 504



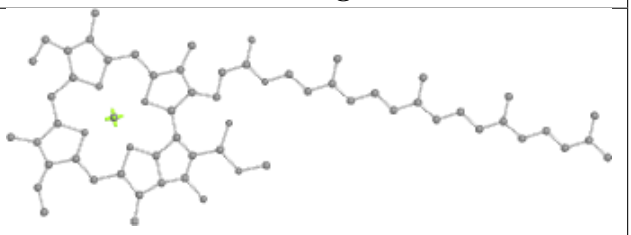
Bond lengths



Bond angles

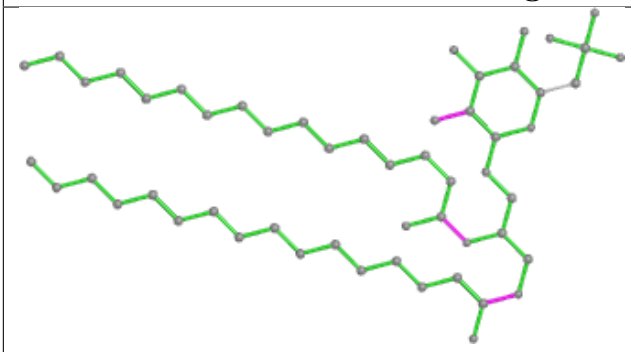


Torsions

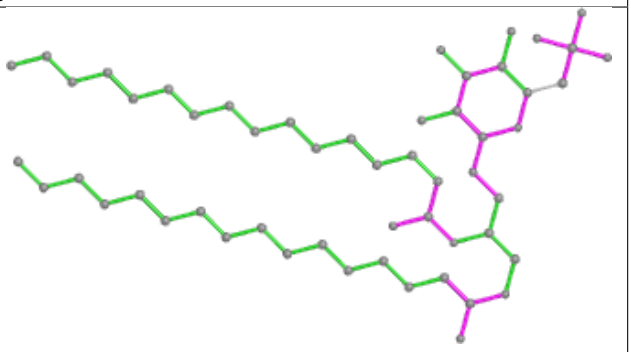


Rings

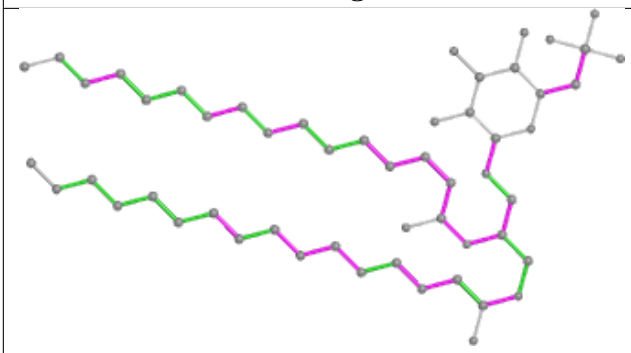
Ligand SQD A 412



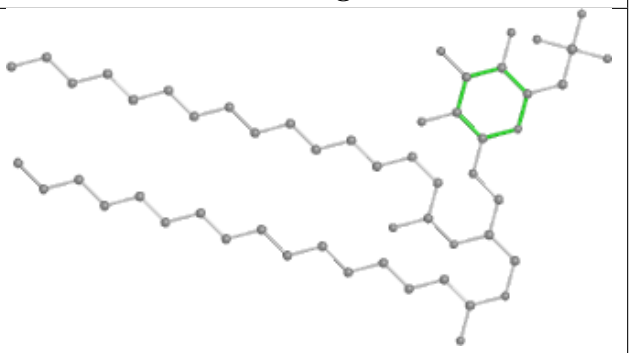
Bond lengths



Bond angles

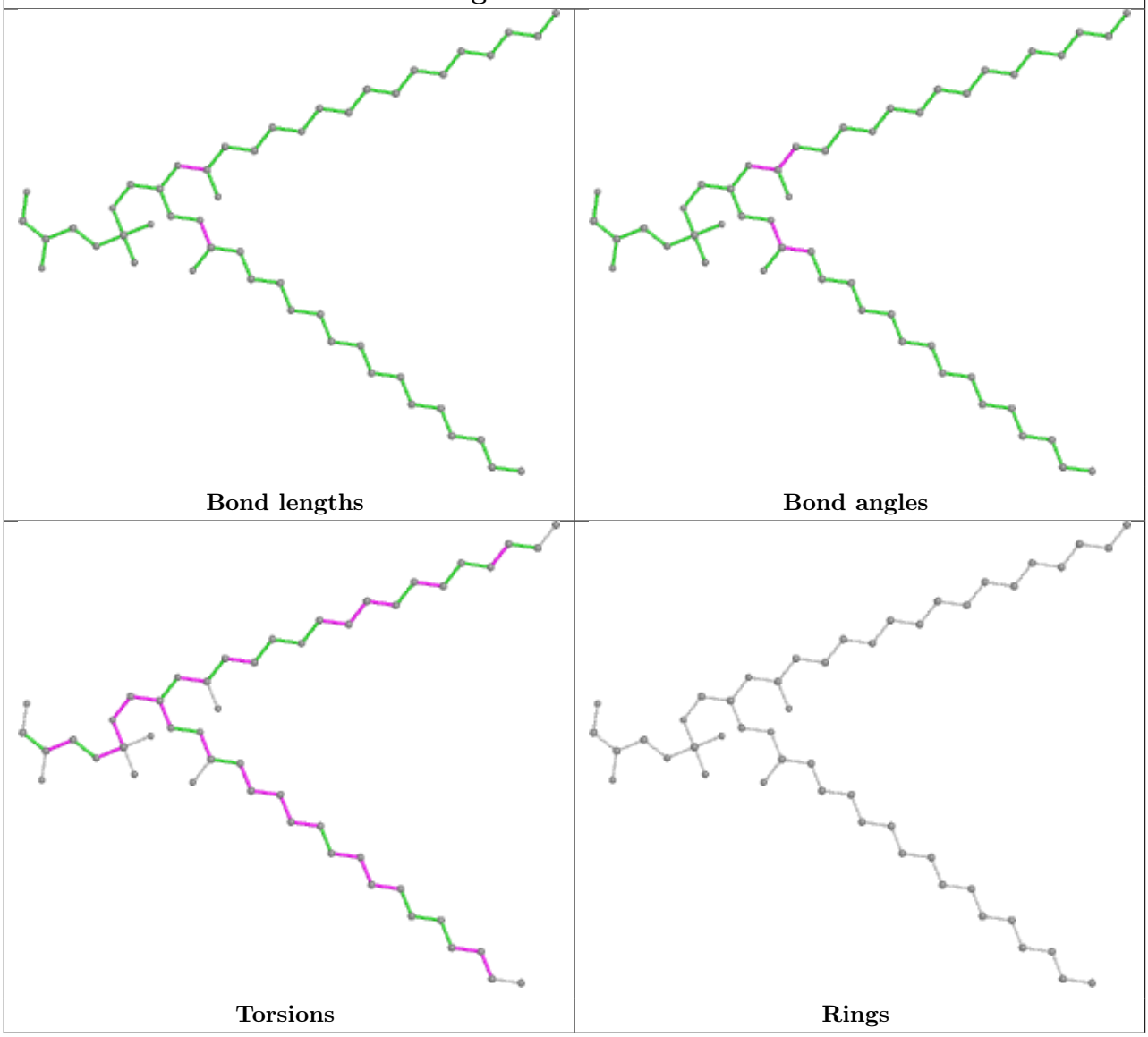


Torsions

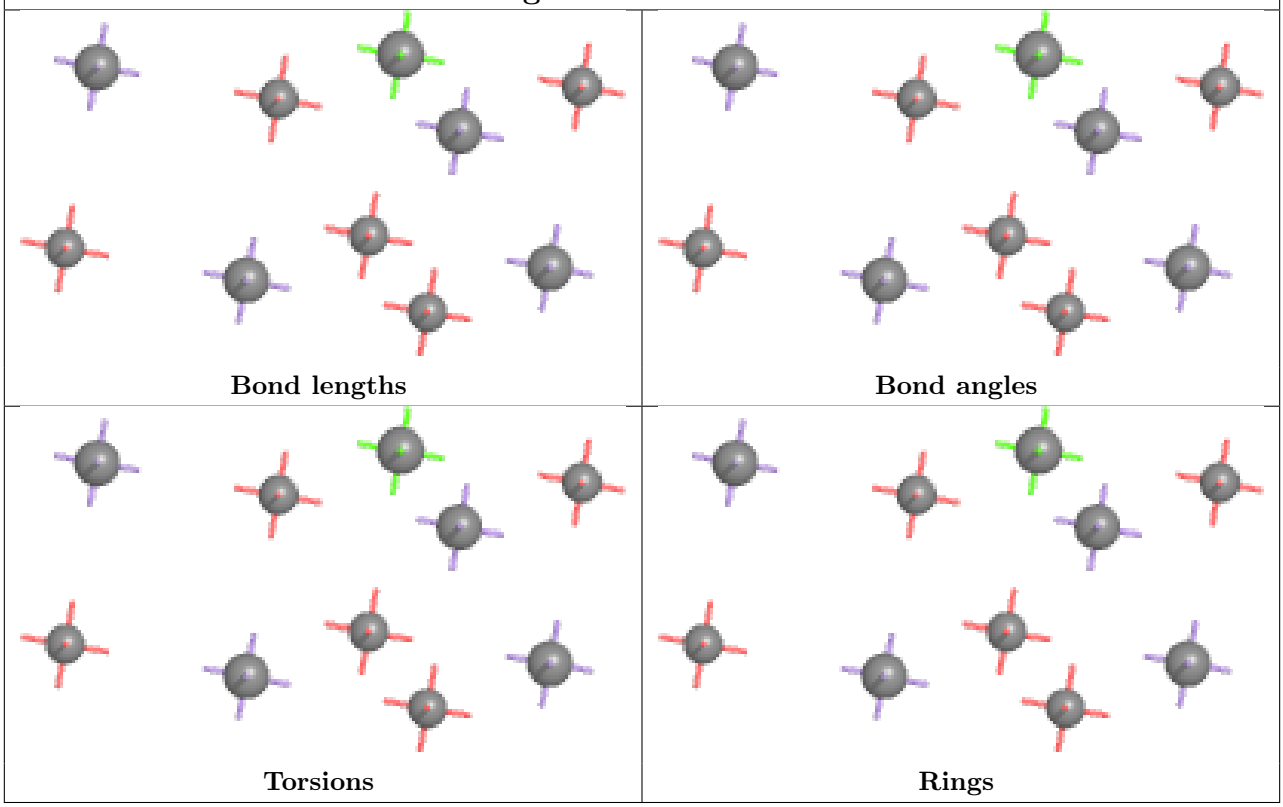


Rings

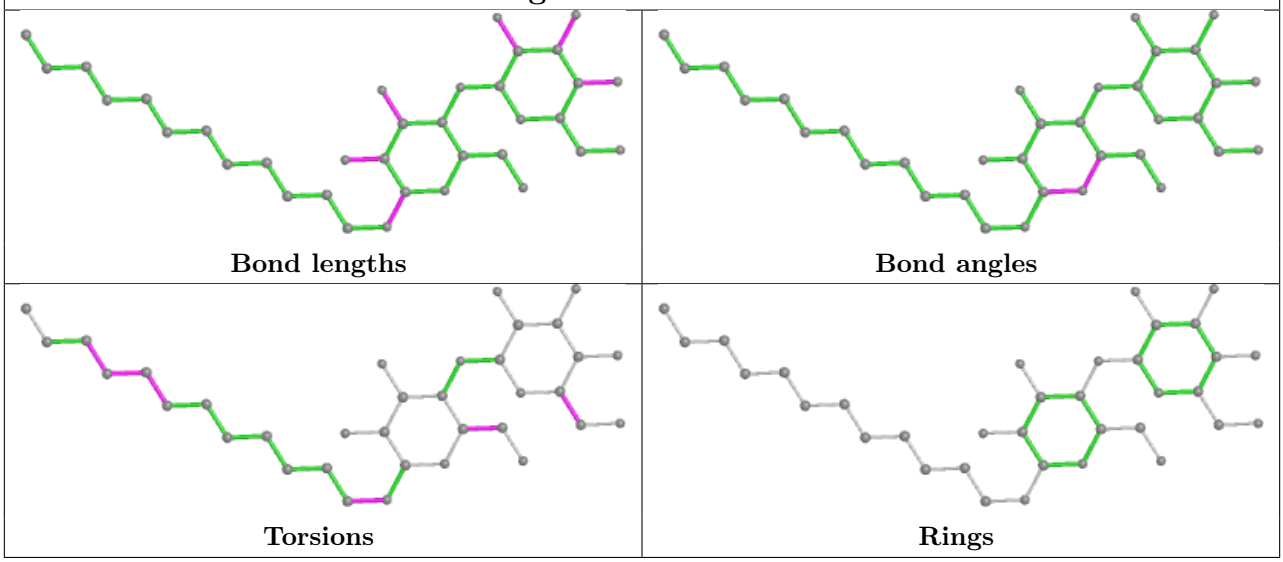
Ligand LHG b 627



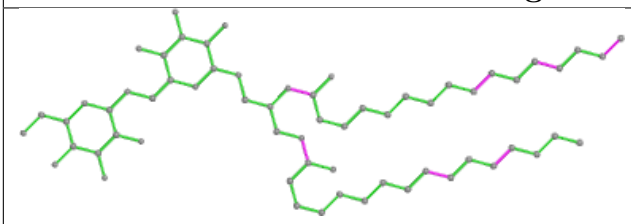
Ligand OEX A 401



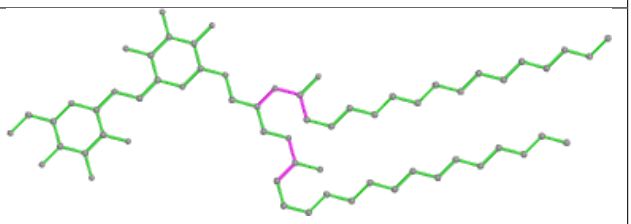
Ligand LMT I 103



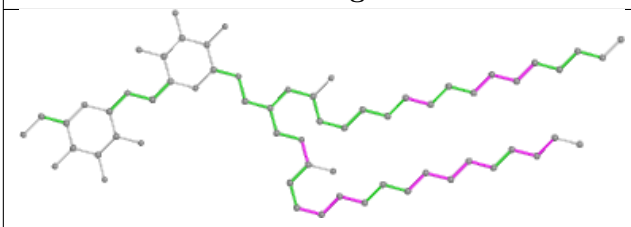
Ligand DGD c 518



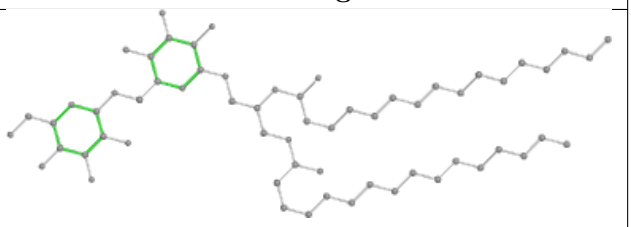
Bond lengths



Bond angles

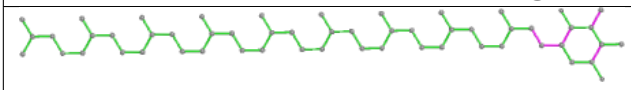


Torsions

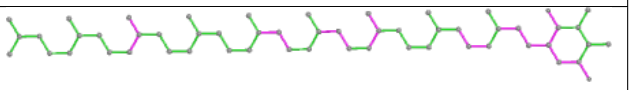


Rings

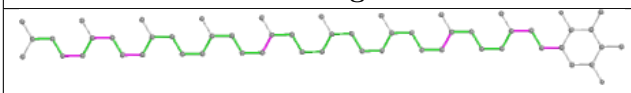
Ligand PL9 D 405



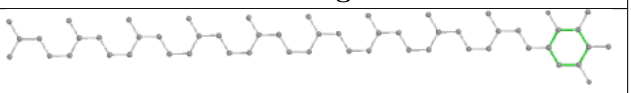
Bond lengths



Bond angles

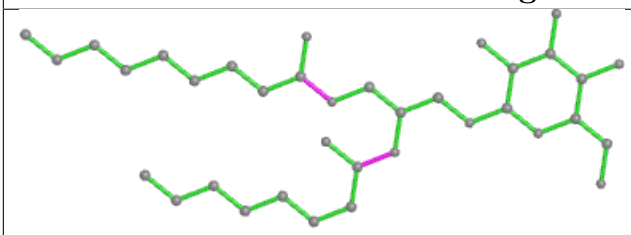


Torsions

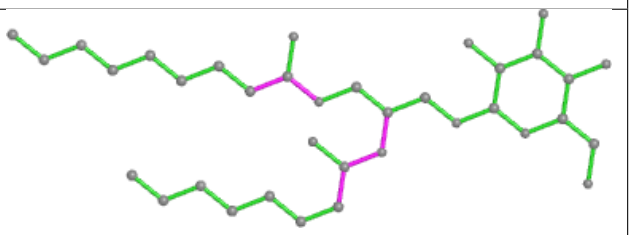


Rings

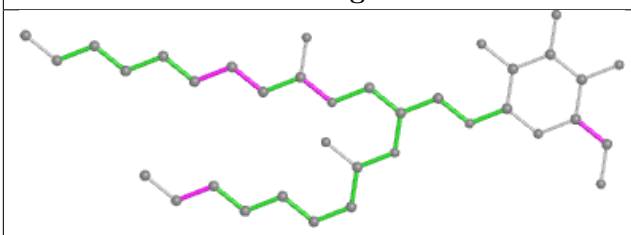
Ligand LMG A 414



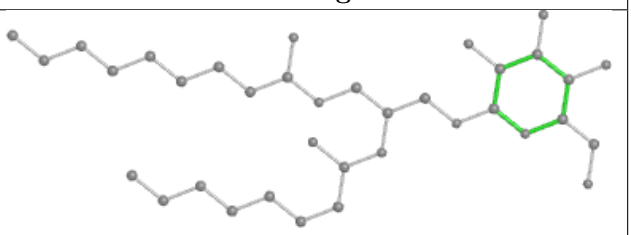
Bond lengths



Bond angles

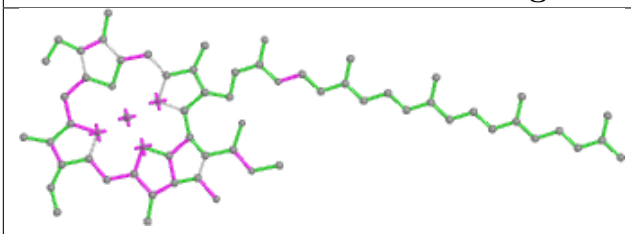


Torsions

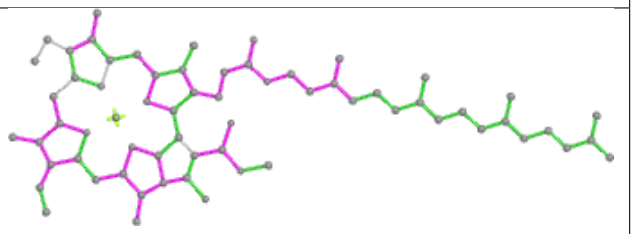


Rings

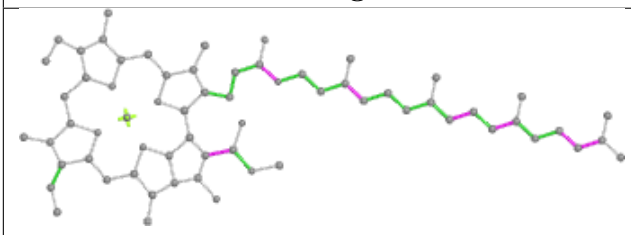
Ligand CLA c 505



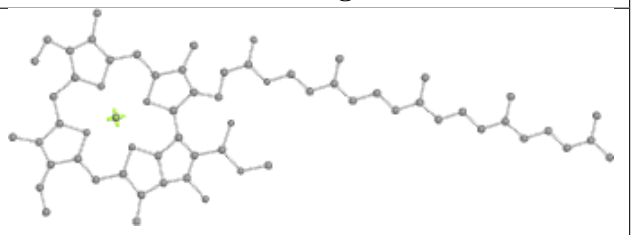
Bond lengths



Bond angles

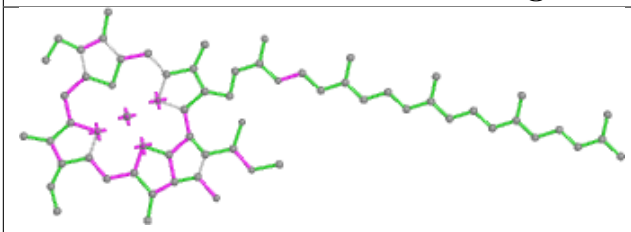


Torsions

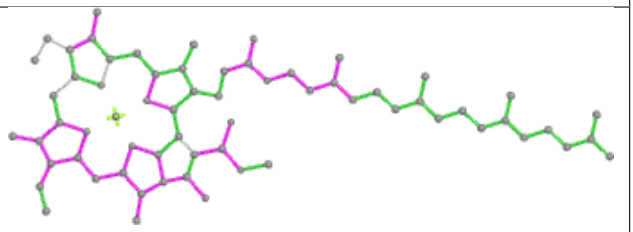


Rings

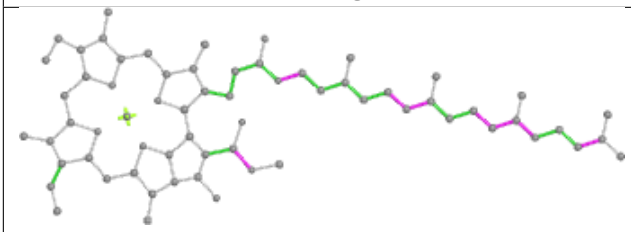
Ligand CLA b 615



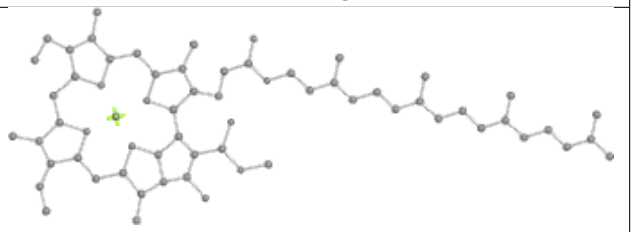
Bond lengths



Bond angles

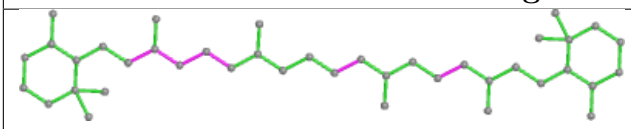


Torsions

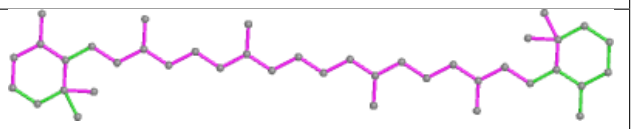


Rings

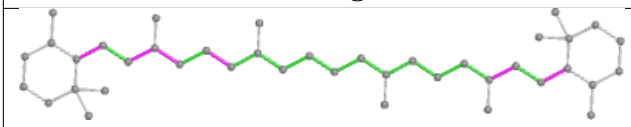
Ligand BCR B 619



Bond lengths



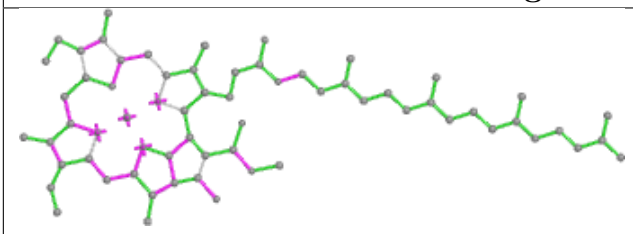
Bond angles



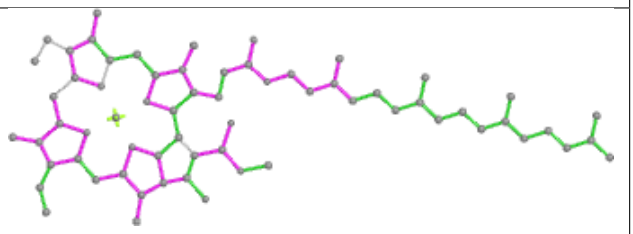
Torsions

Rings

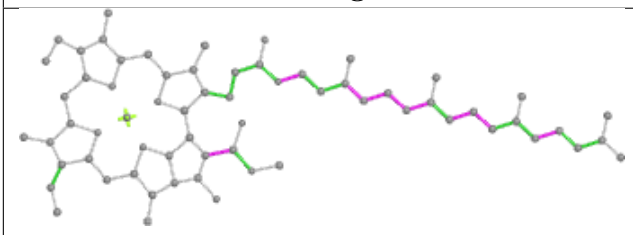
Ligand CLA B 604



Bond lengths



Bond angles



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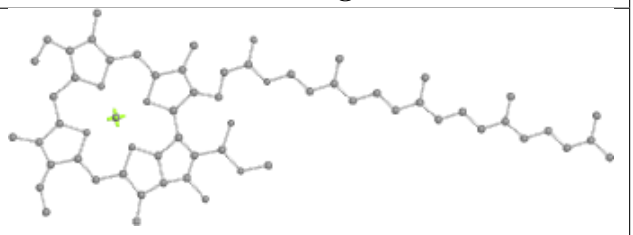
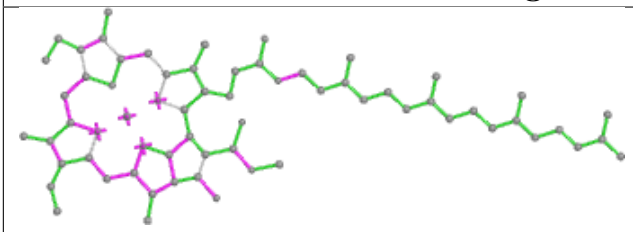
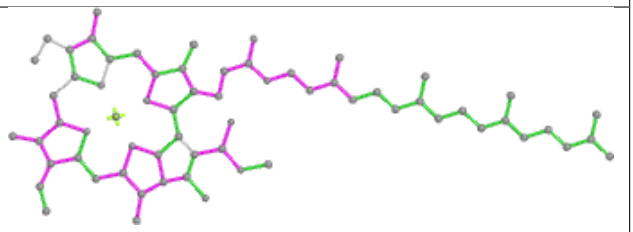


Rings

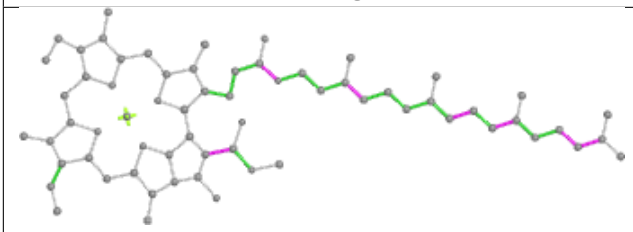
Ligand CLA C 505



Bond lengths



Bond angles



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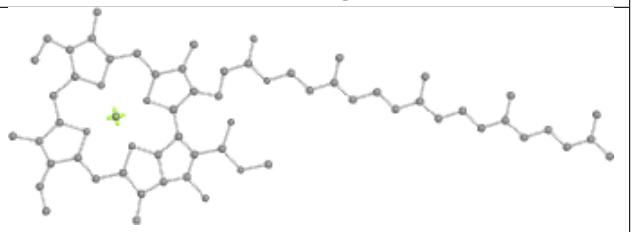
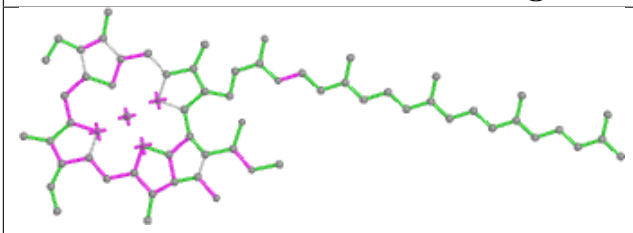


Rings

Ligand CLA b 610



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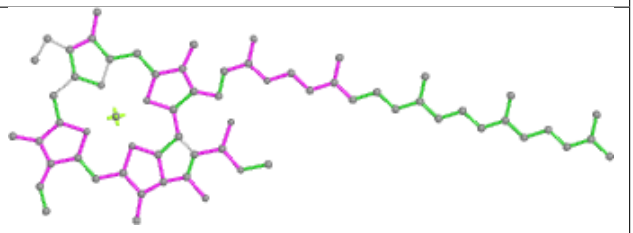
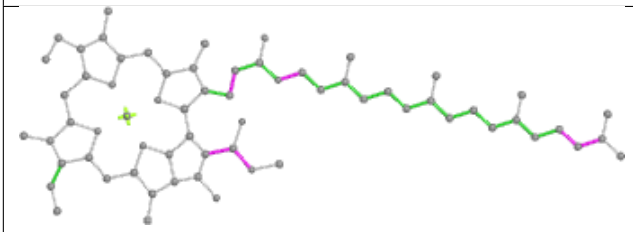


Bond angles



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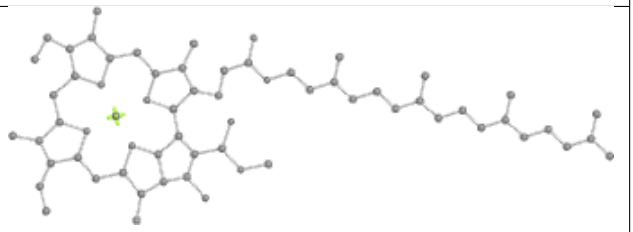
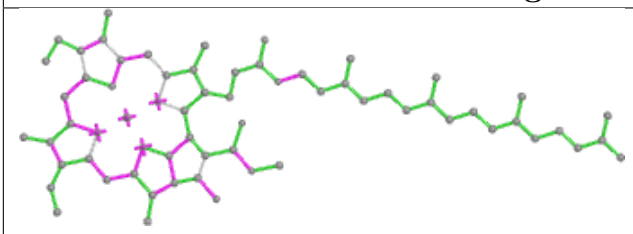
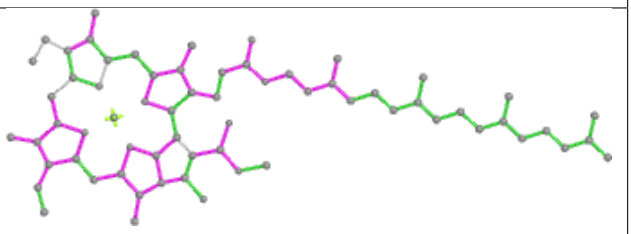


Rings

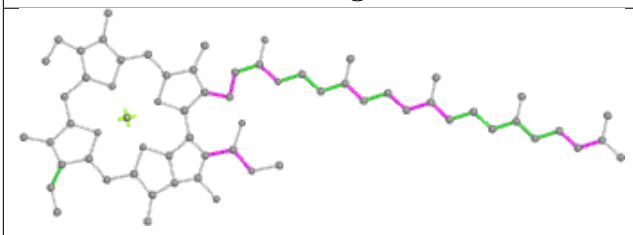
Ligand CLA B 603



Bond lengths



Bond angles



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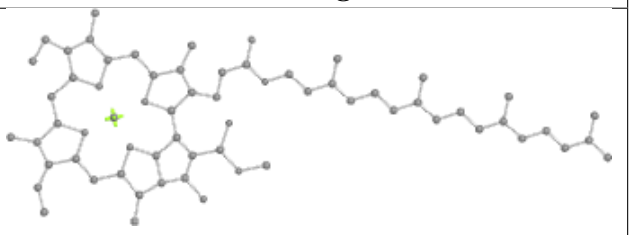
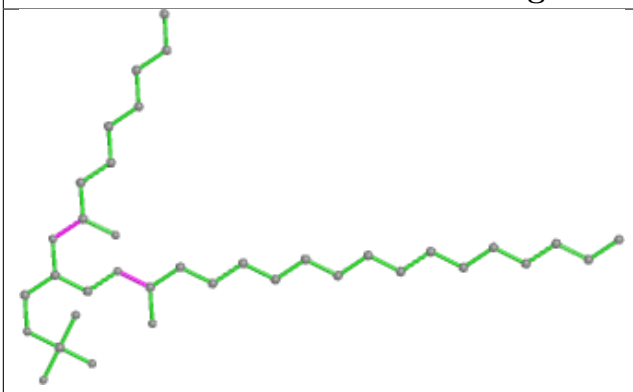
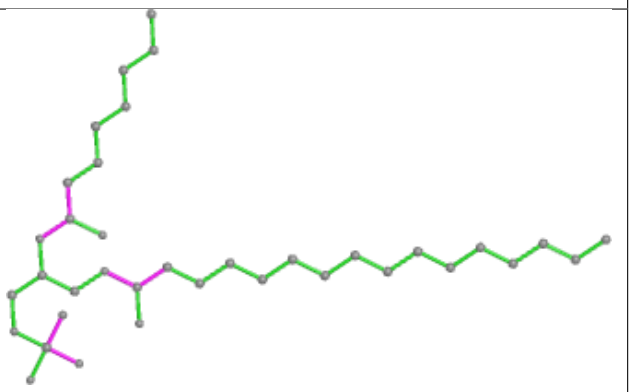


Rings

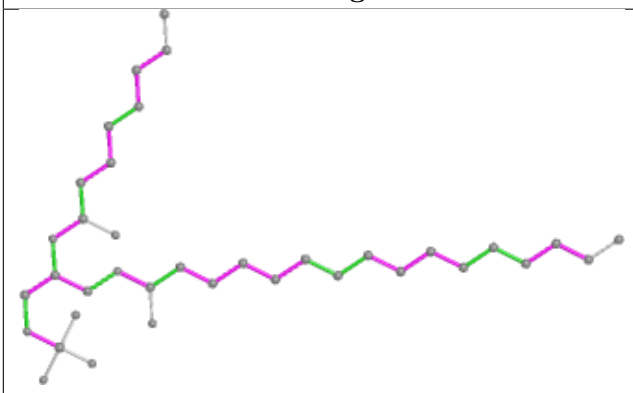
Ligand LHG z 102



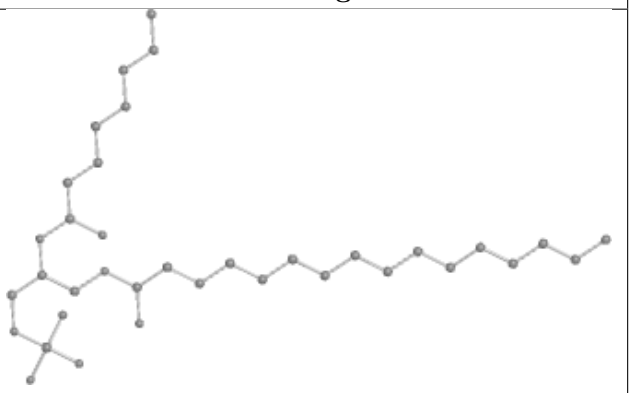
Bond lengths



Bond angles

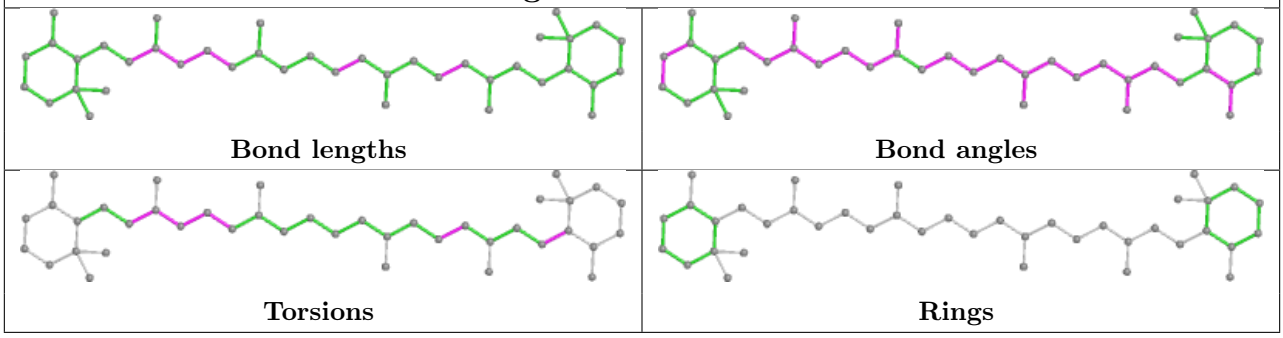


Torsions

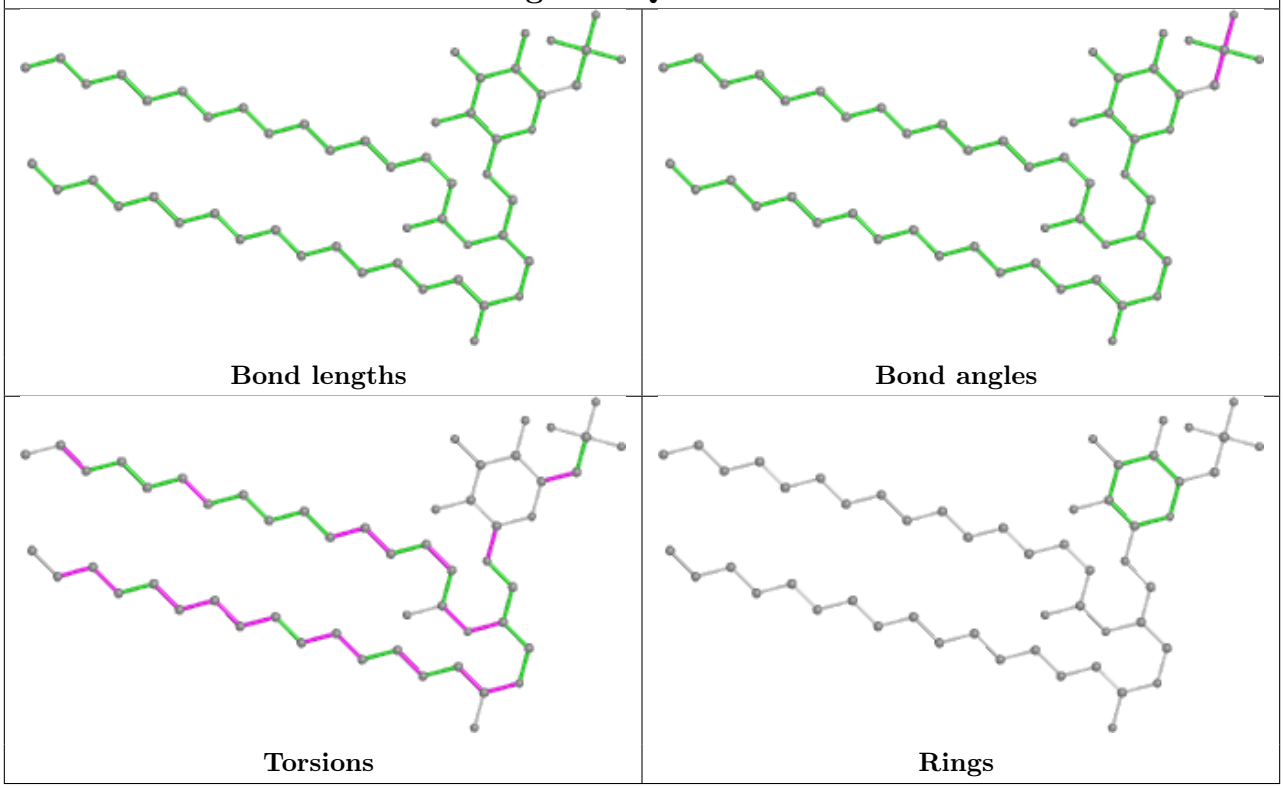


Rings

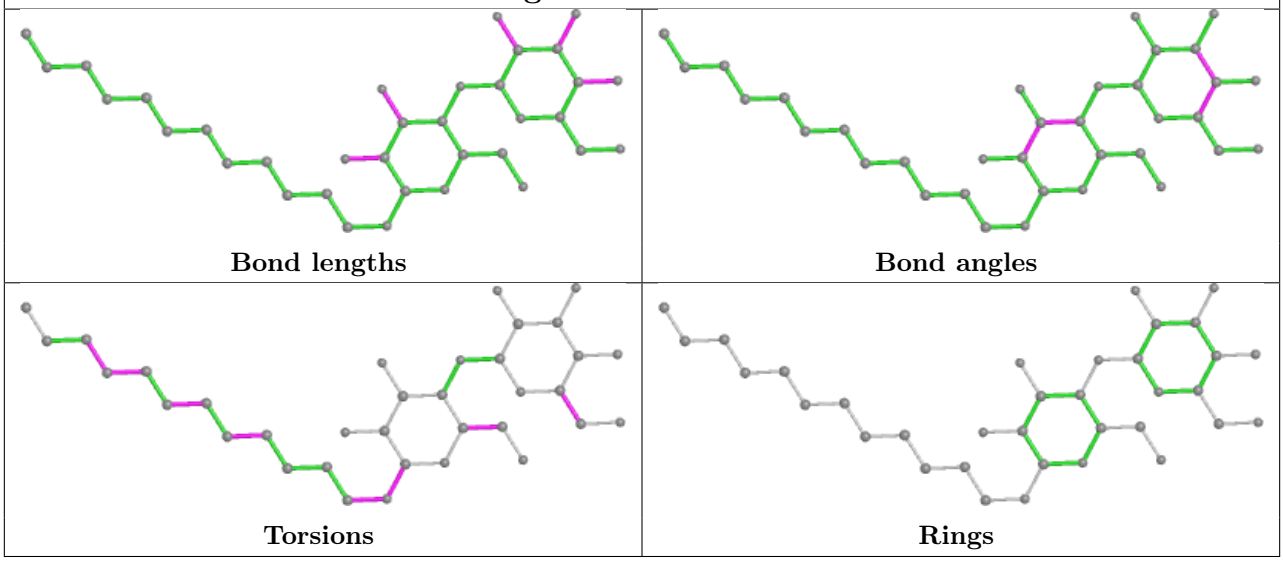
Ligand BCR C 515

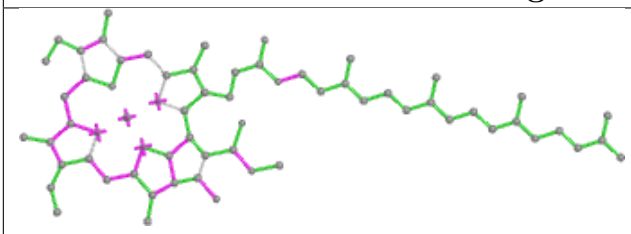
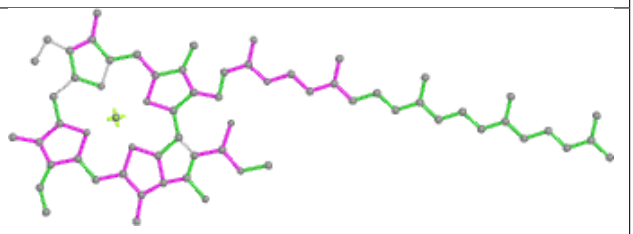
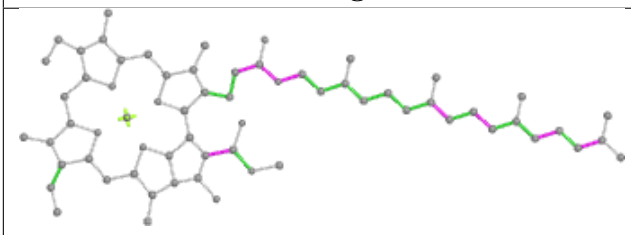
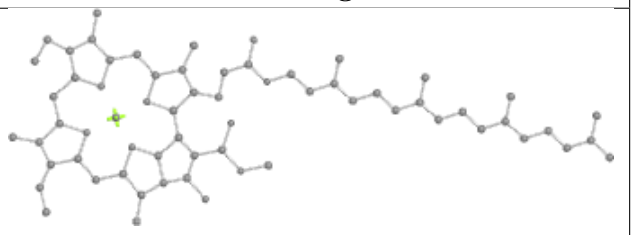


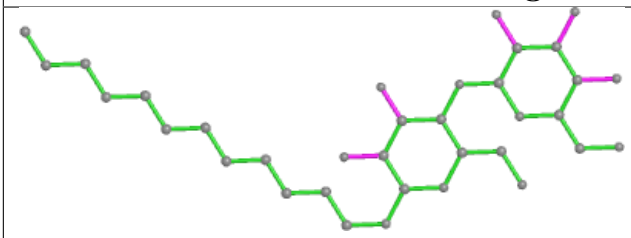
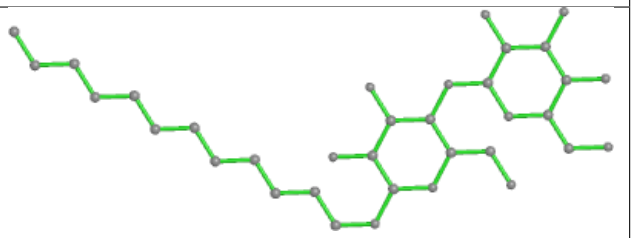
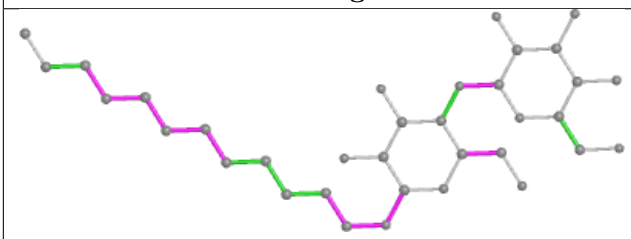
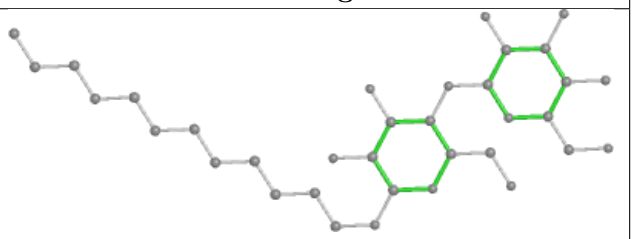
Ligand SQD B 620



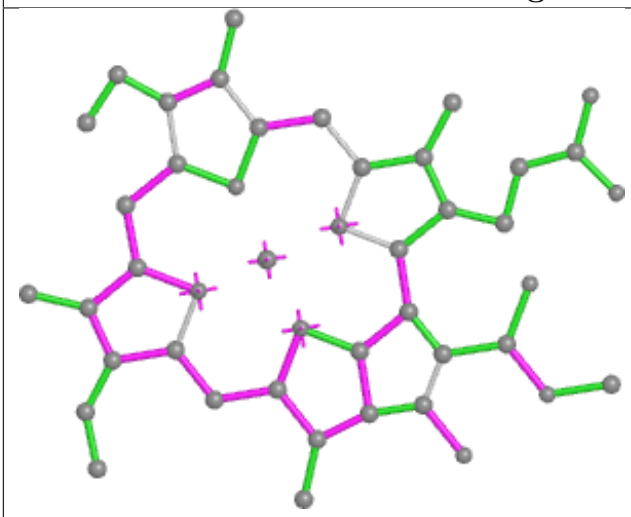
Ligand LMT F 103



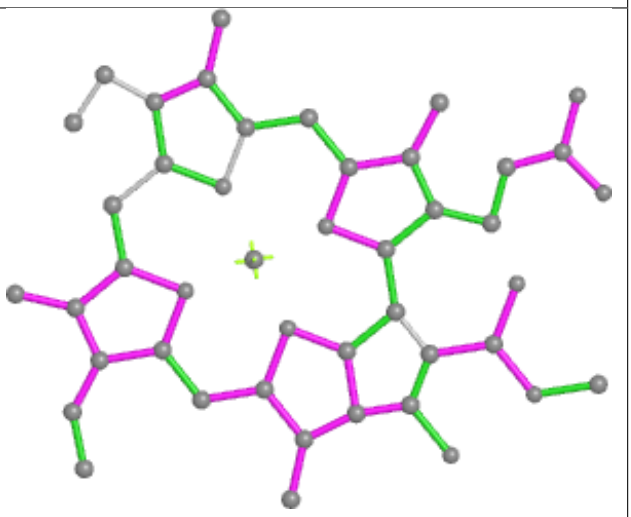
Ligand CLA b 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT b 629	
 Bond lengths	 Bond angles
 Torsions	 Rings

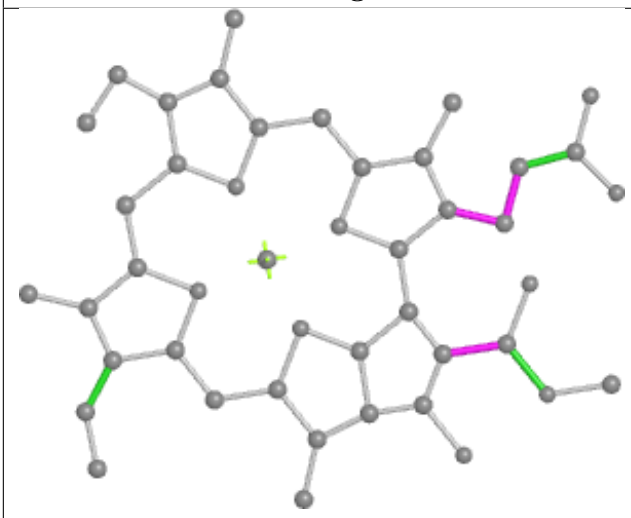
Ligand CLA b 601



Bond lengths



Bond angles



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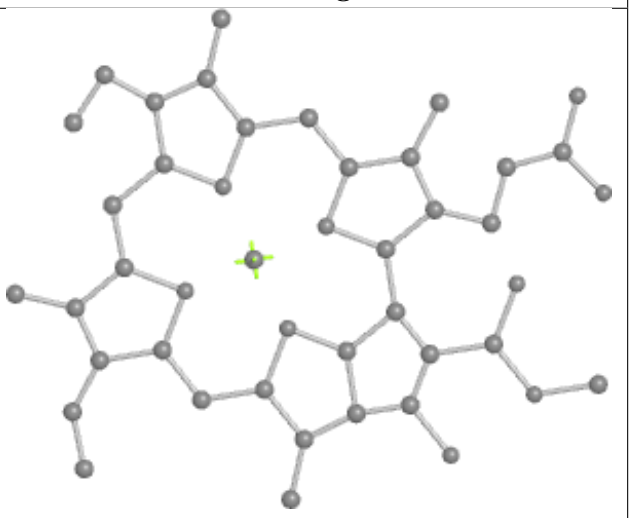
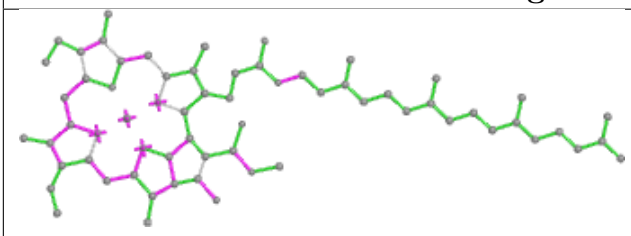
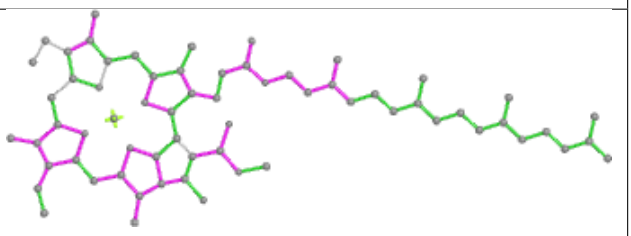


Rings

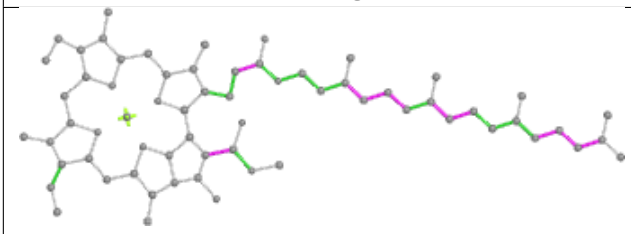
Ligand CLA b 614



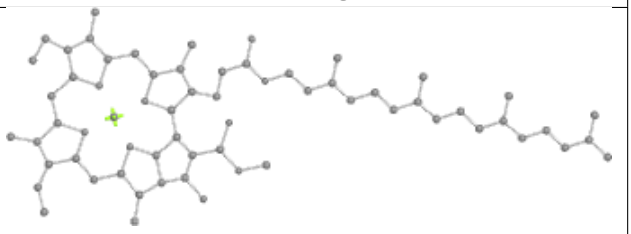
Bond lengths



Bond angles

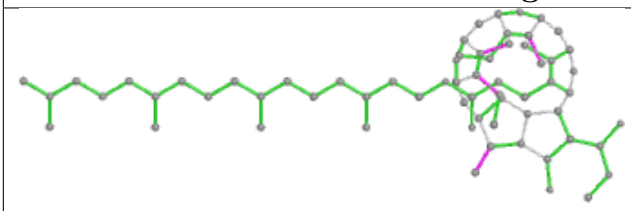


Torsions



Rings

Ligand PHO A 407



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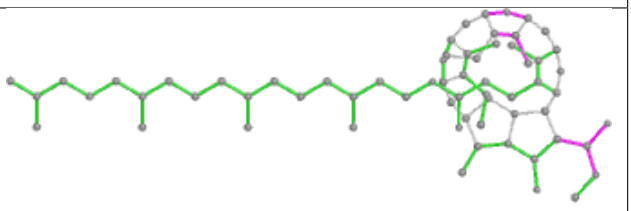
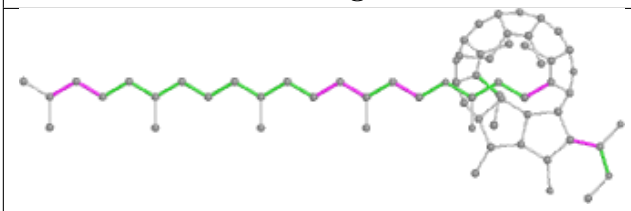


Bond angles



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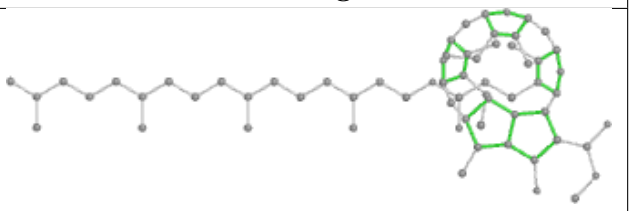
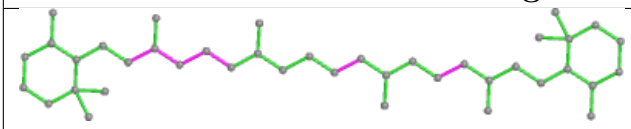
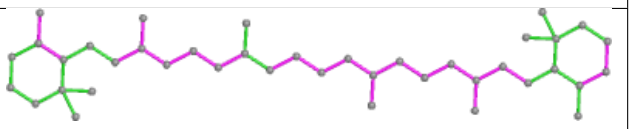


Rings

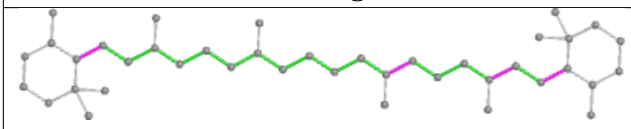
Ligand BCR B 617



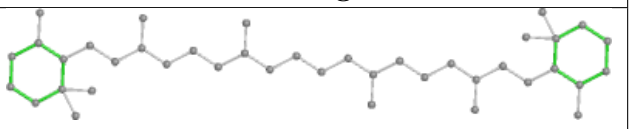
Bond lengths



Bond angles

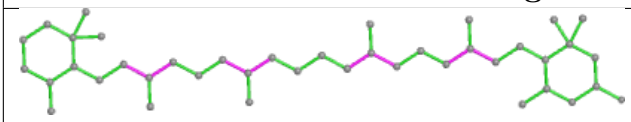


Torsions

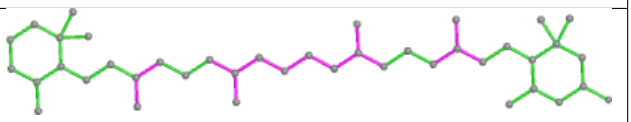


Rings

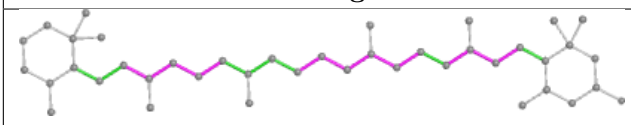
Ligand RRX h 101



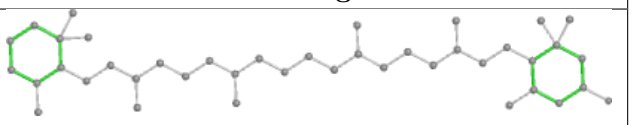
Bond lengths



Bond angles

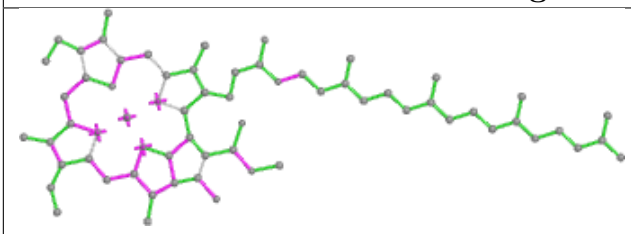


Torsions

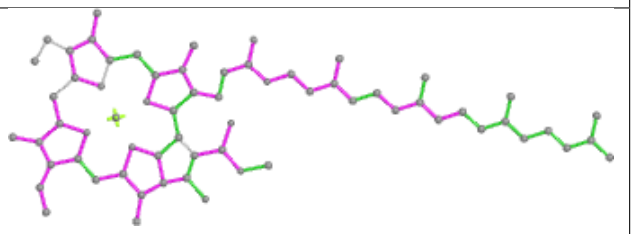


Rings

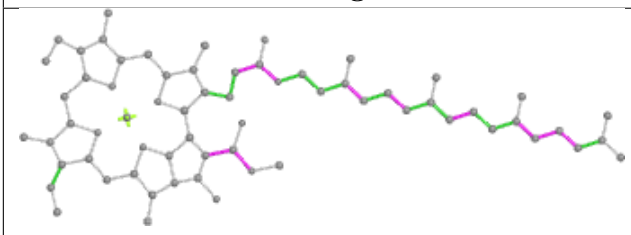
Ligand CLA c 511



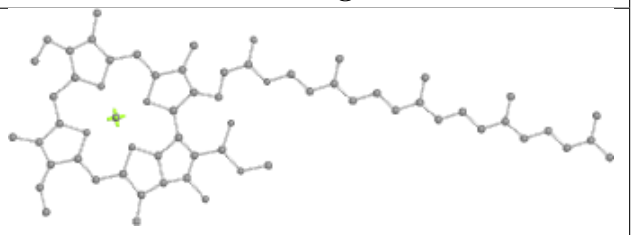
Bond lengths



Bond angles

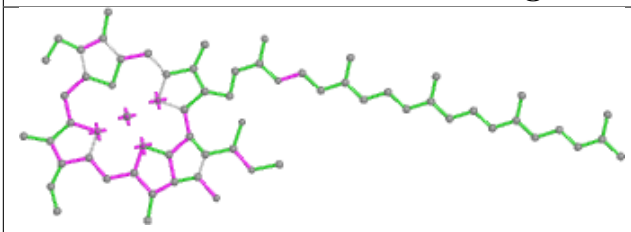


Torsions

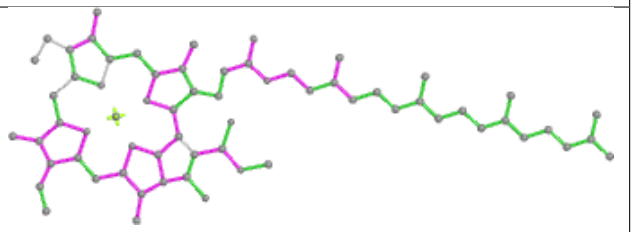


Rings

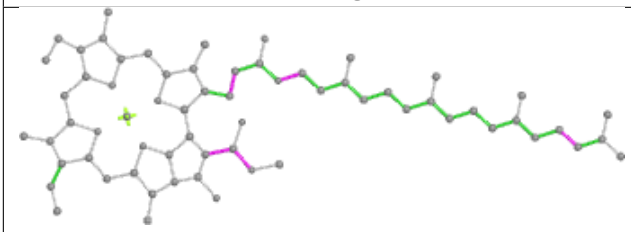
Ligand CLA C 504



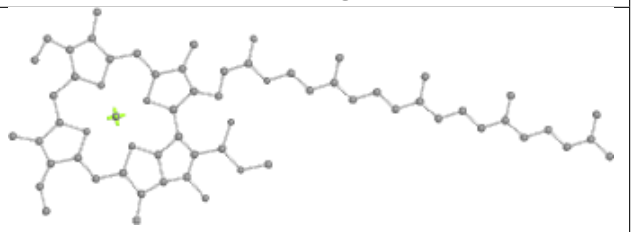
Bond lengths



Bond angles

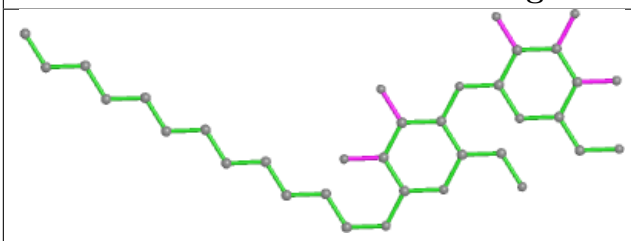


Torsions

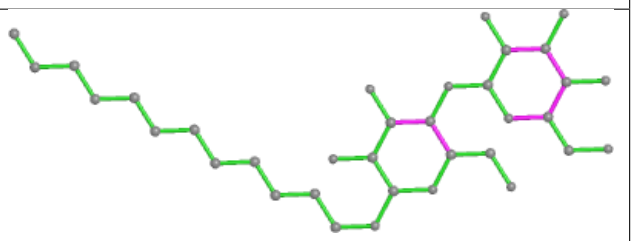


Rings

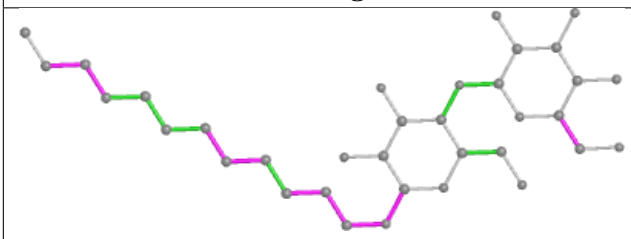
Ligand LMT c 524



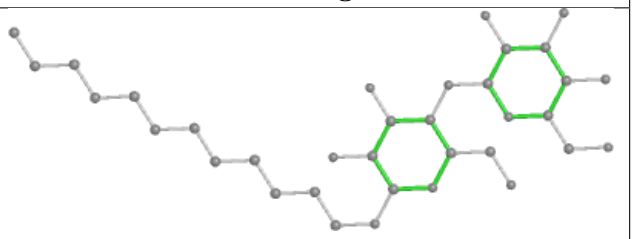
Bond lengths



Bond angles

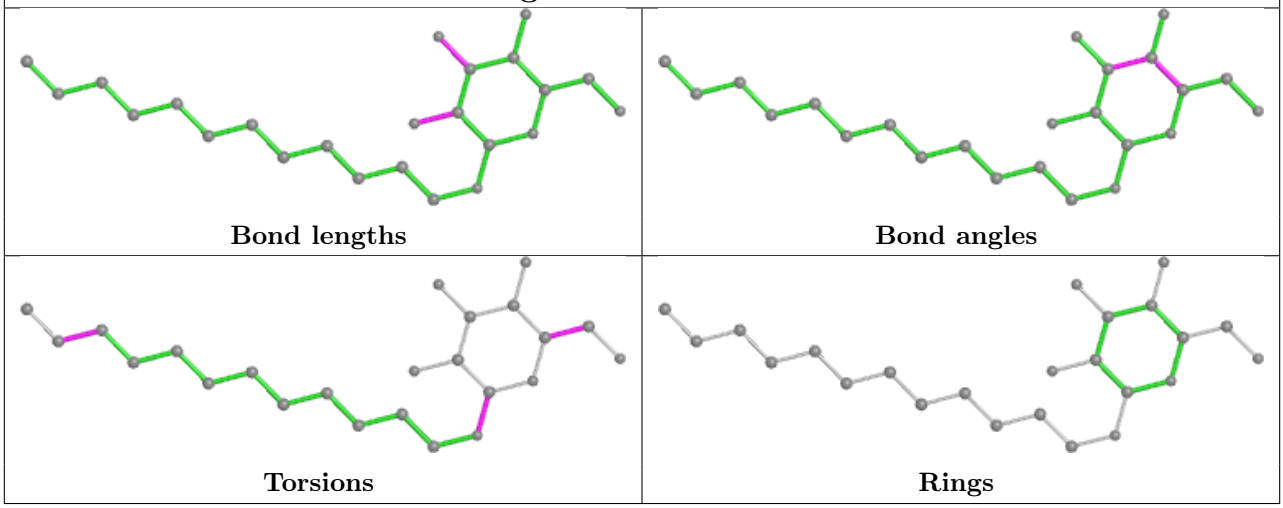


Torsions

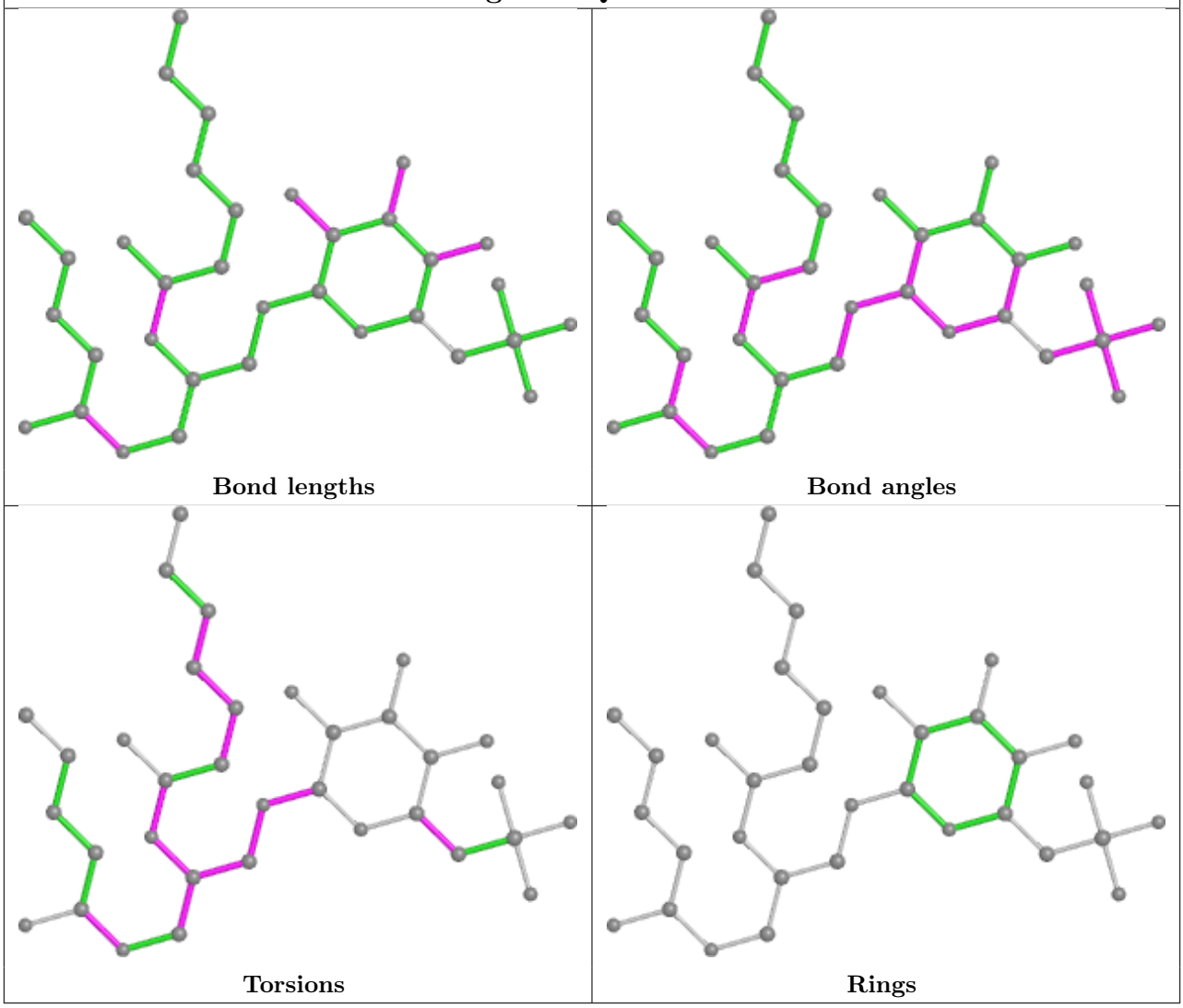


Rings

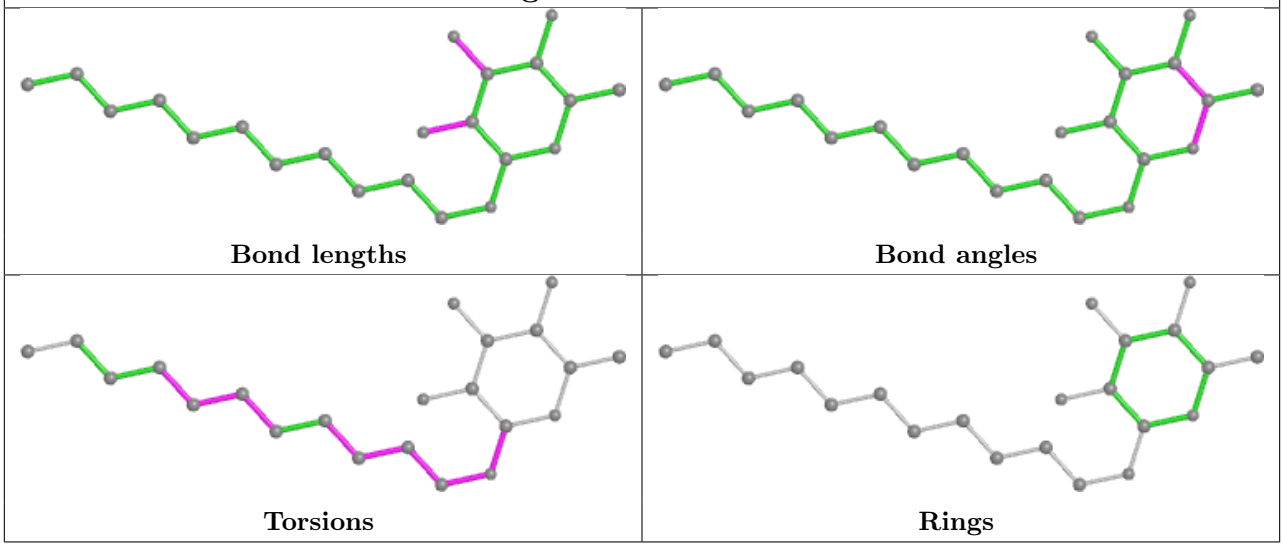
Ligand LMT m 102



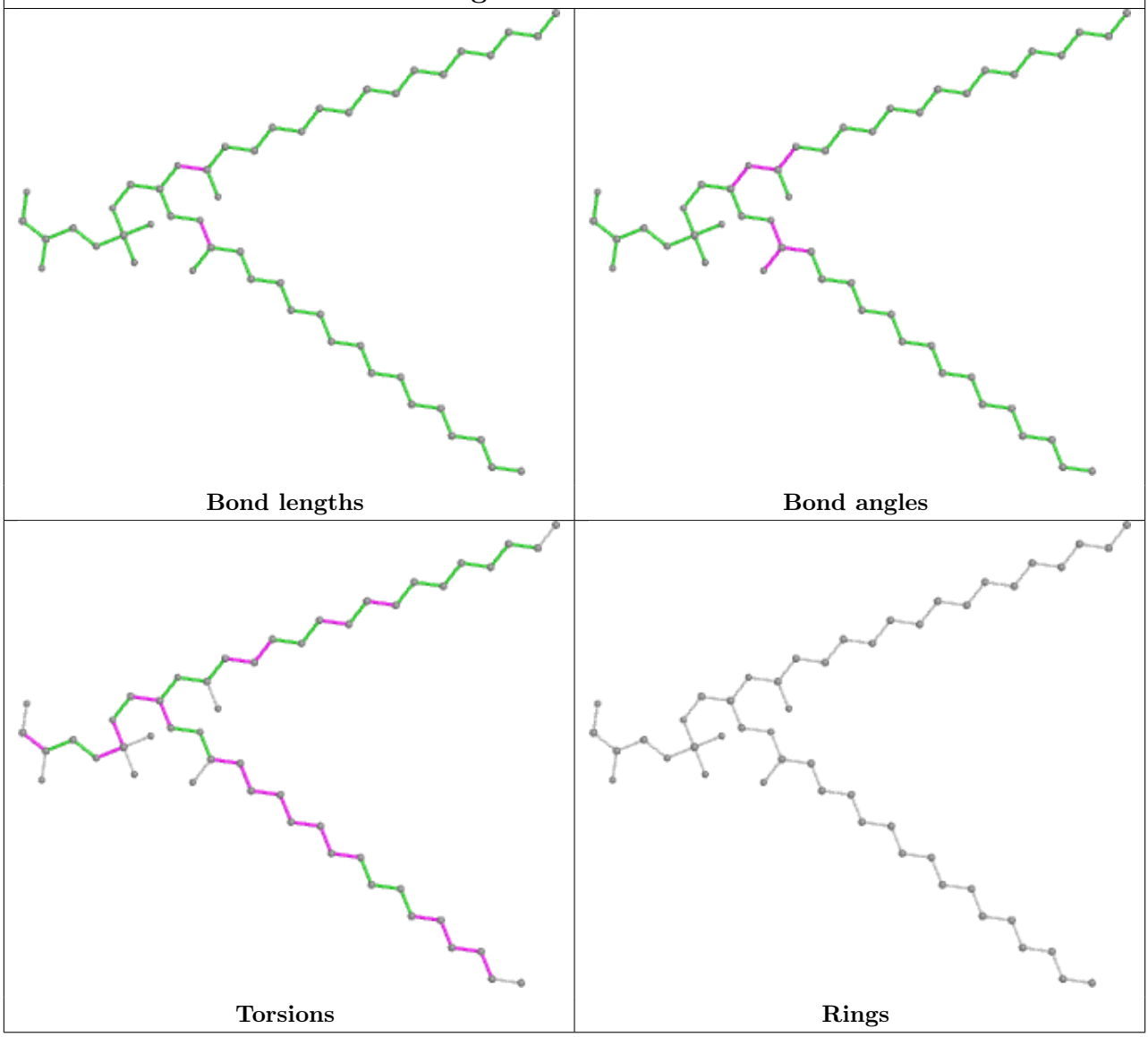
Ligand SQD F 102



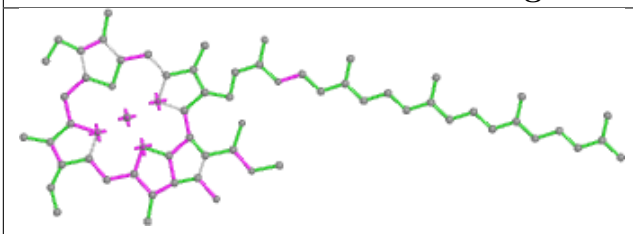
Ligand LMT X 102



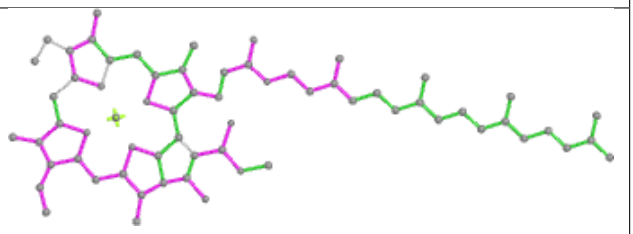
Ligand LHG d 407



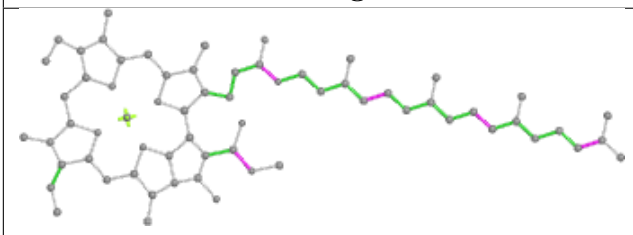
Ligand CLA B 613



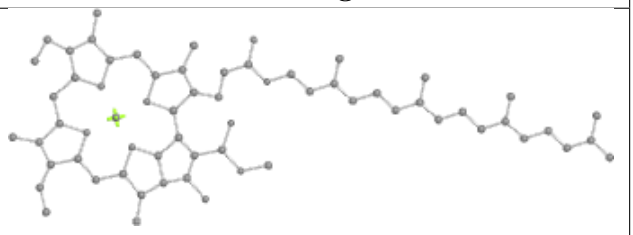
Bond lengths



Bond angles

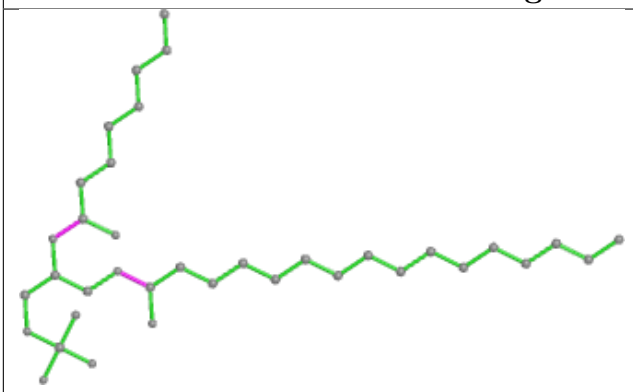


Torsions



Rings

Ligand LHG Z 102



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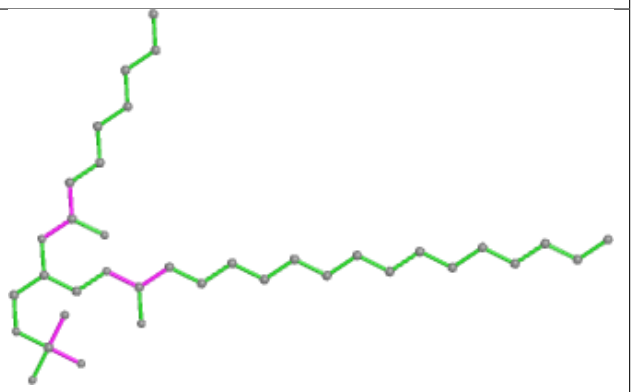
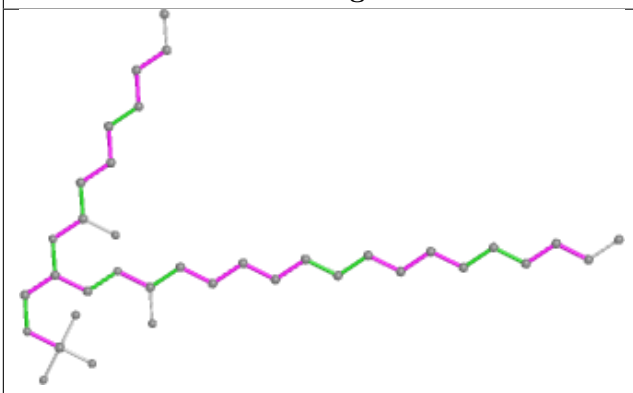
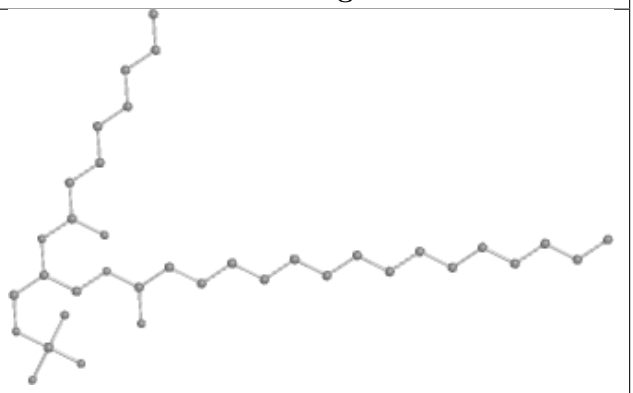


Bond angles

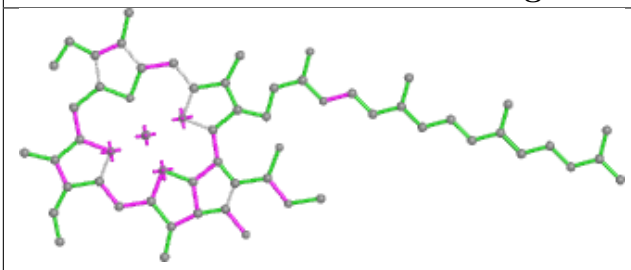


Torsions

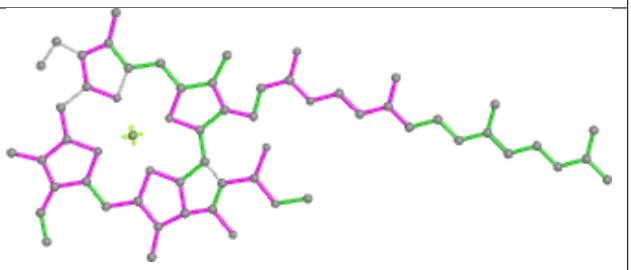


Rings

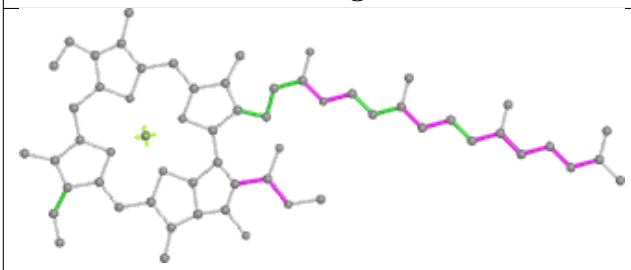
Ligand CLA B 616



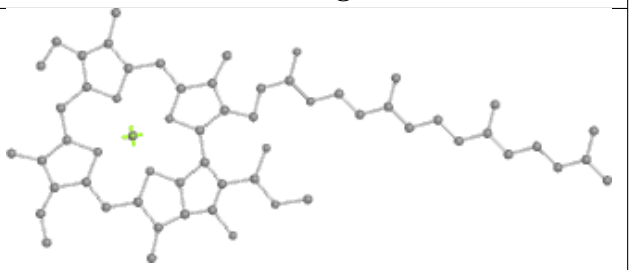
Bond lengths



Bond angles

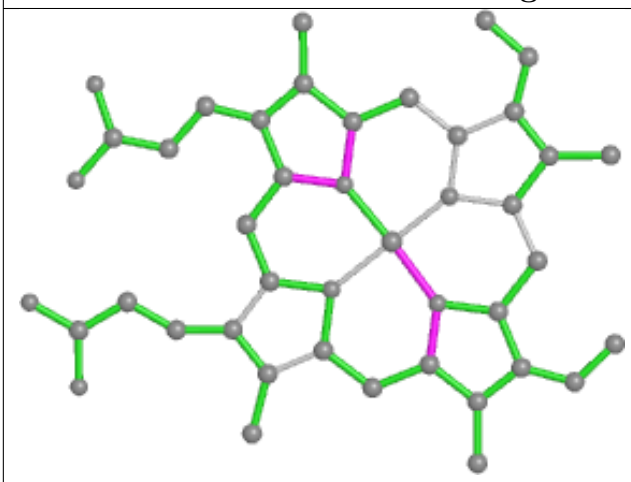


Torsions

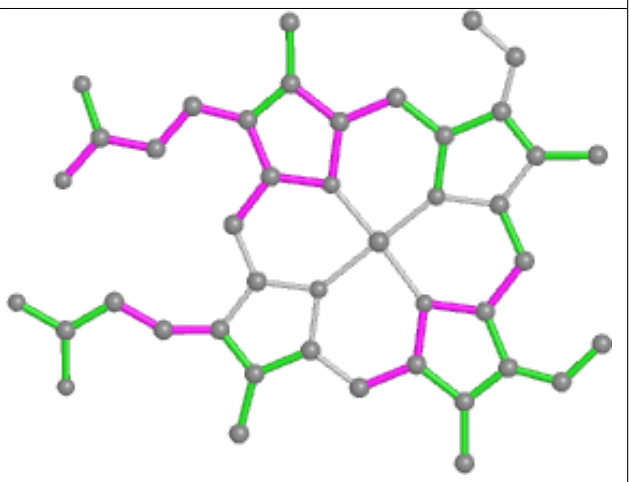


Rings

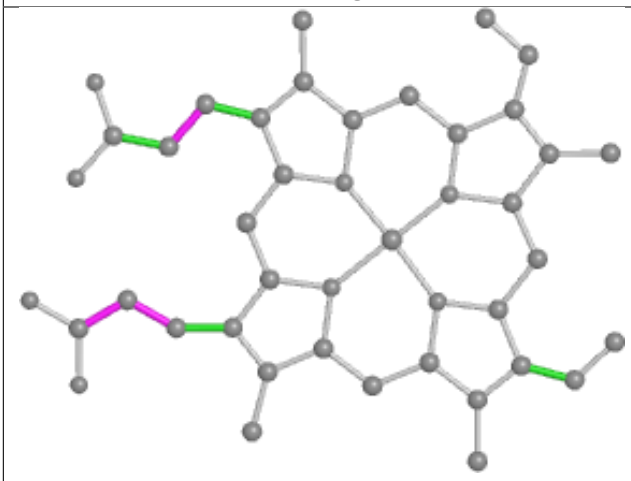
Ligand HEM E 104



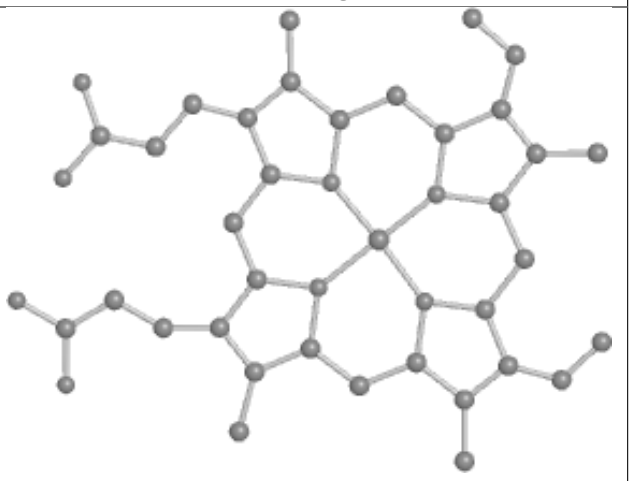
Bond lengths



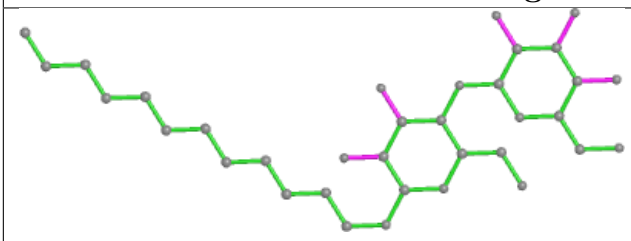
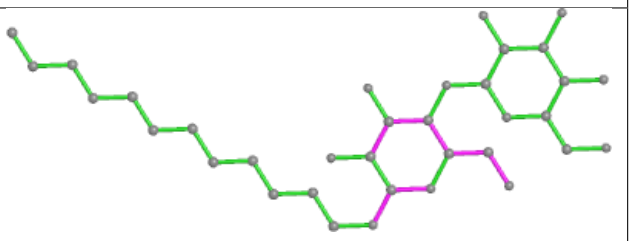
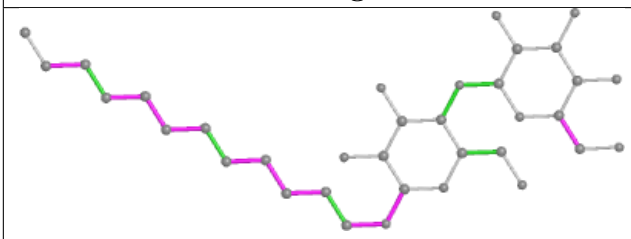
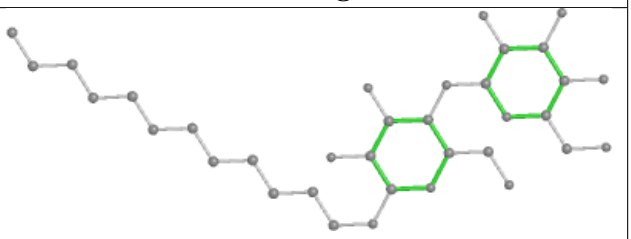
Bond angles

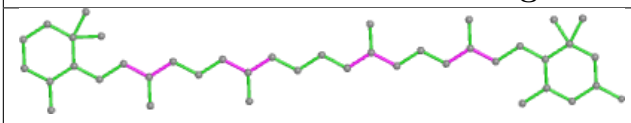
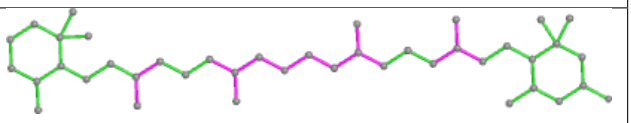
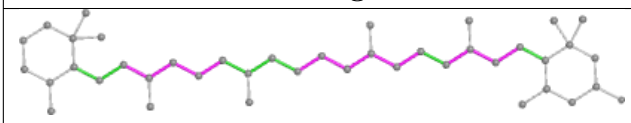
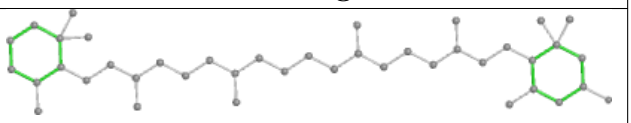


Torsions

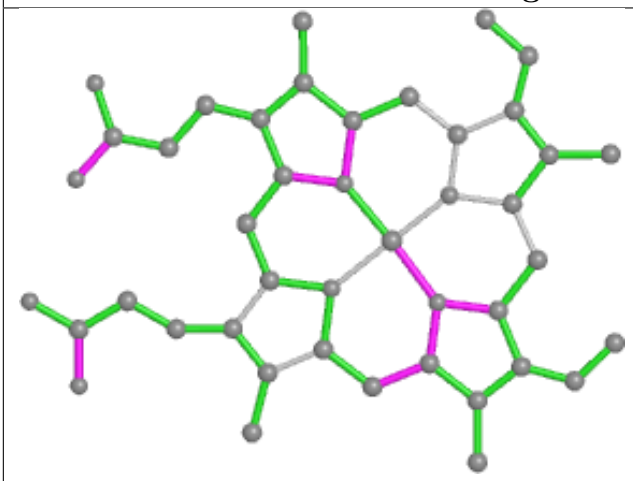


Rings

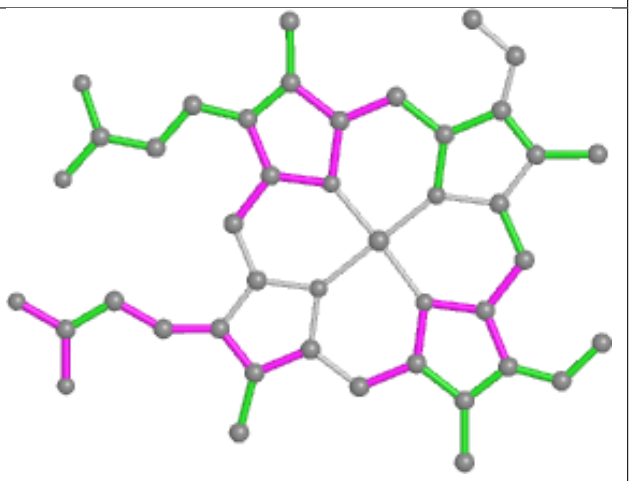
Ligand LMT b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand RRX H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

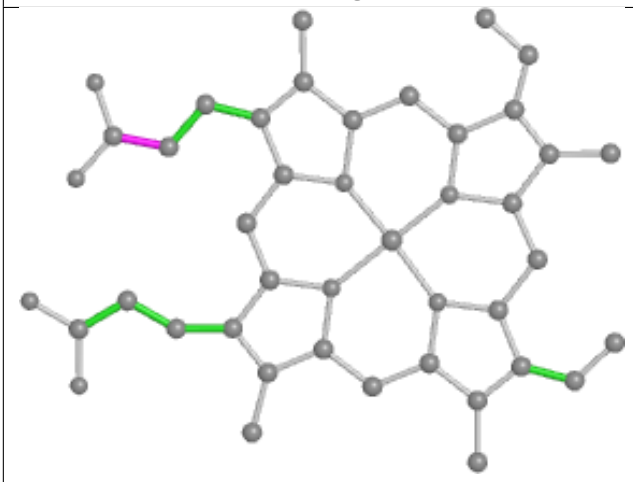
Ligand HEM v 201



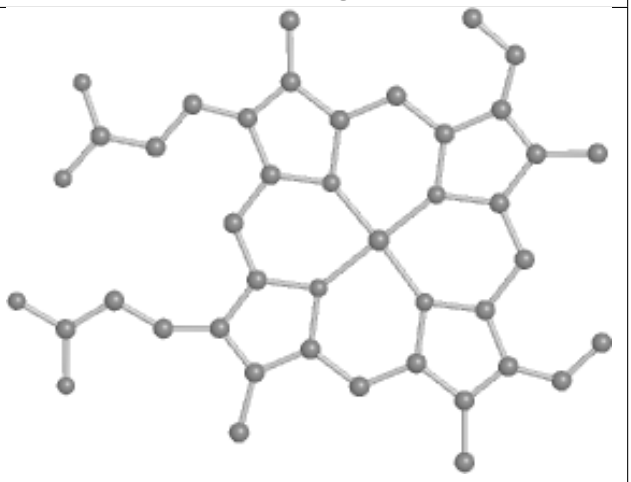
Bond lengths



Bond angles

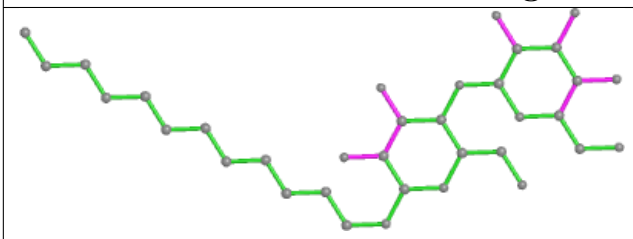


Torsions

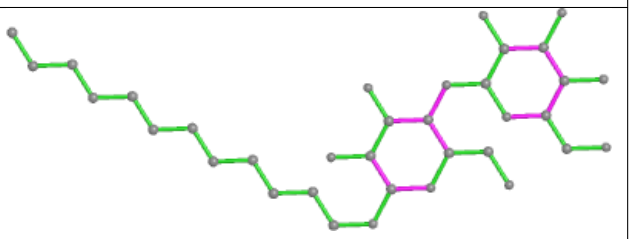


Rings

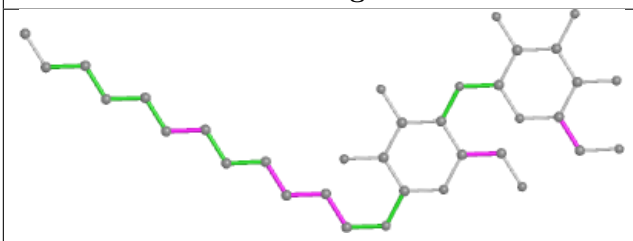
Ligand LMT E 103



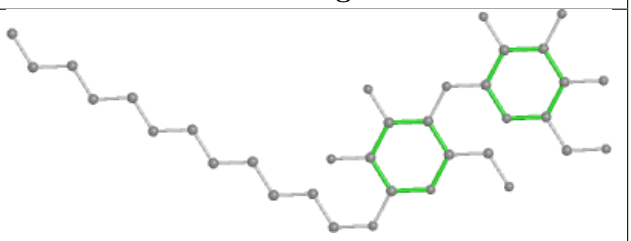
Bond lengths



Bond angles

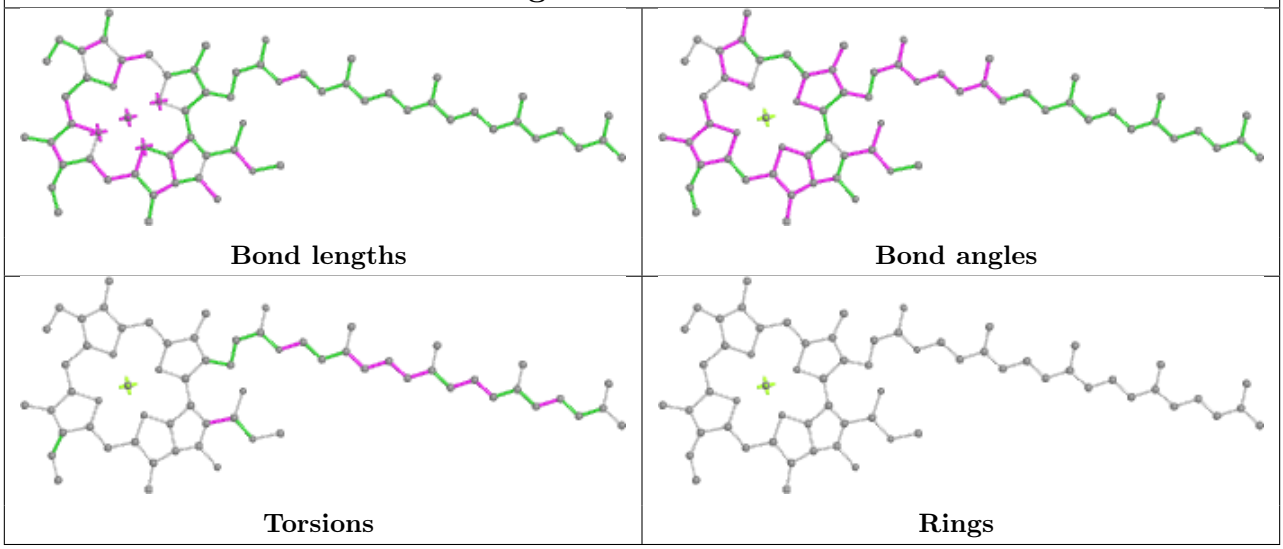


Torsions

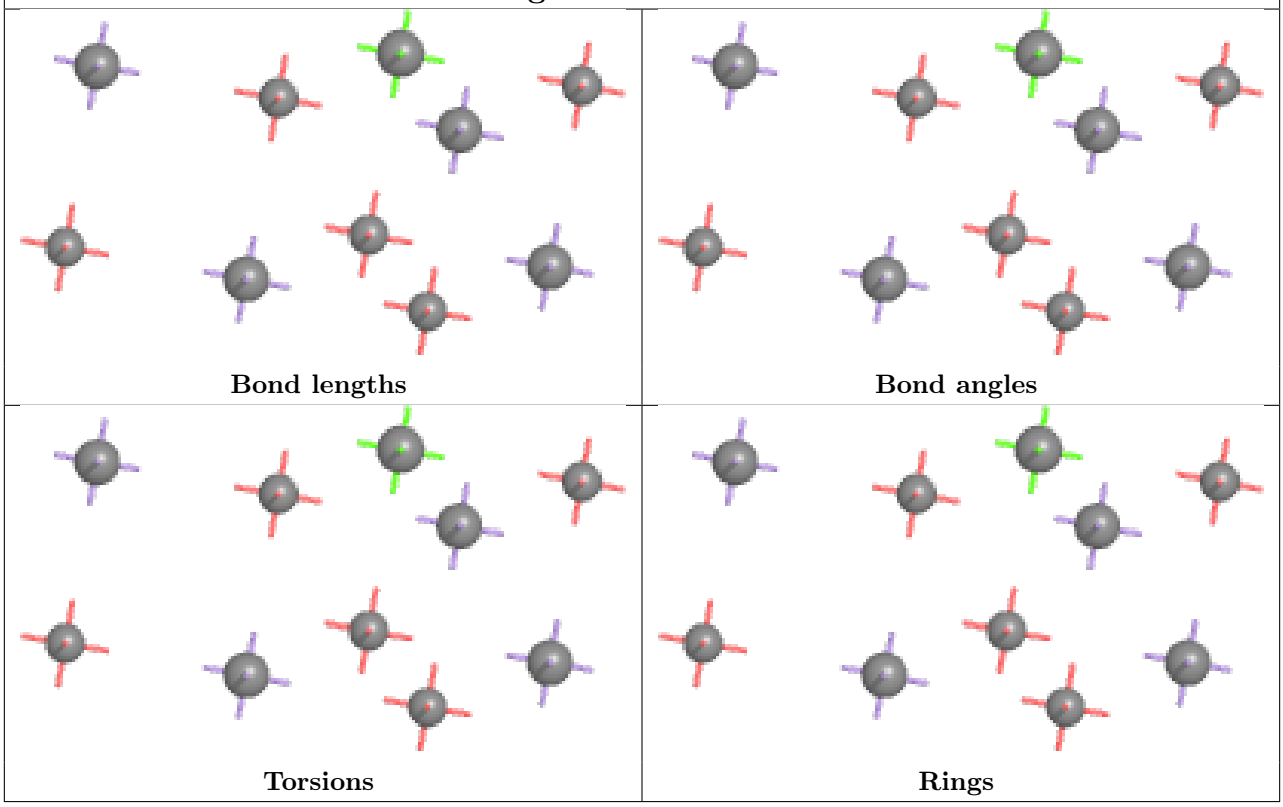


Rings

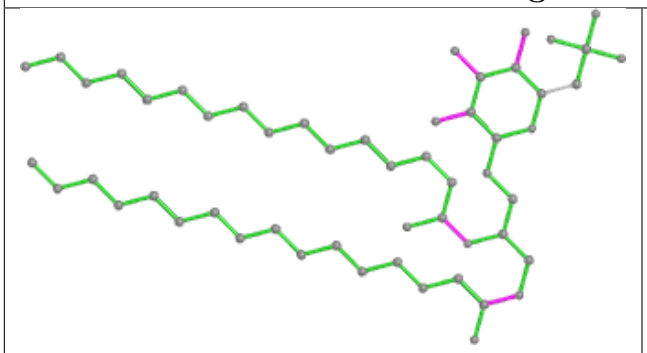
Ligand CLA b 604



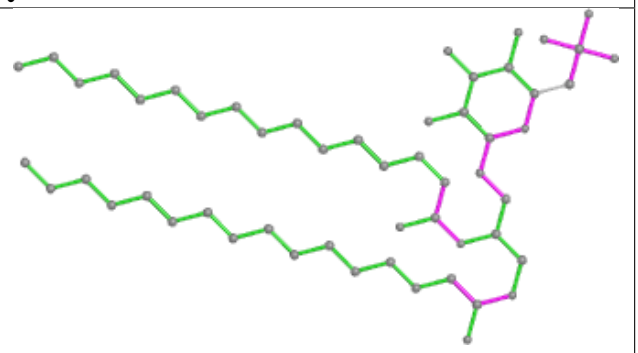
Ligand OEX a 401



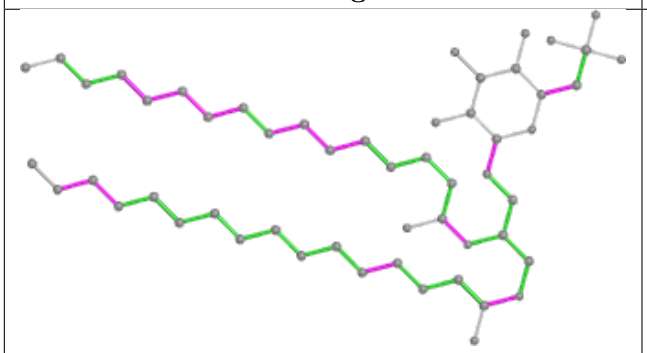
Ligand SQD h 103



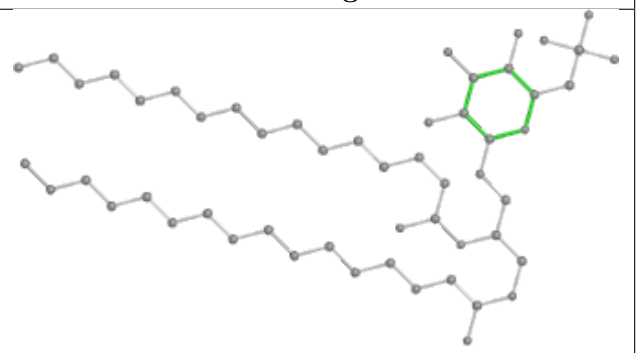
Bond lengths



Bond angles

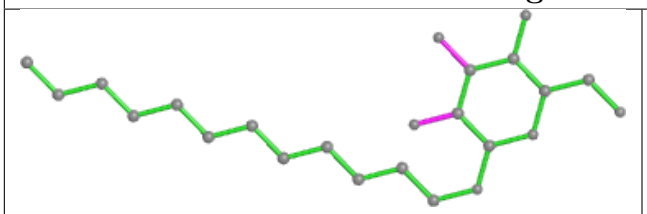


Torsions

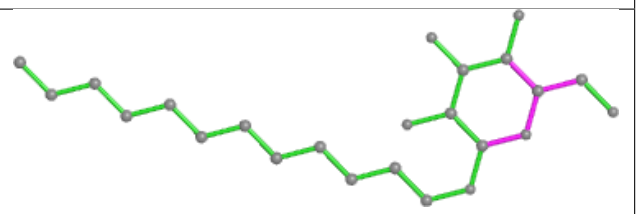


Rings

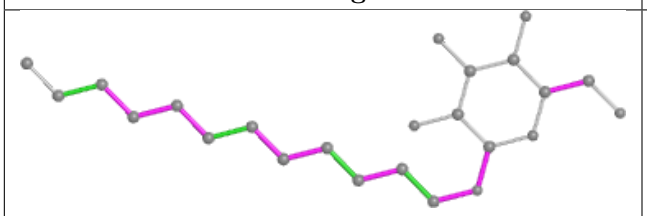
Ligand LMT J 101



Bond lengths



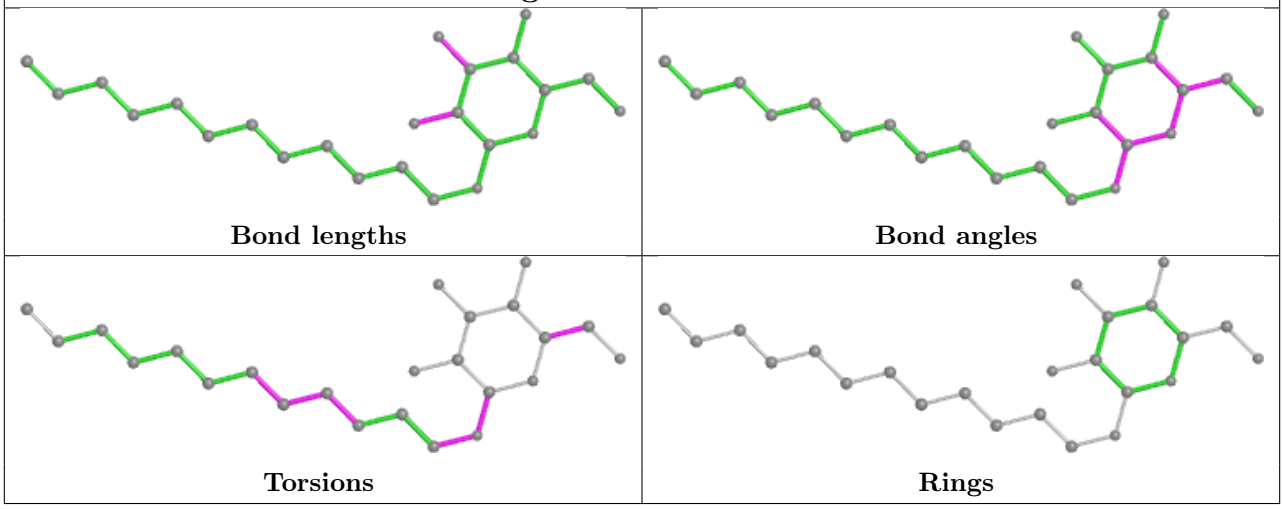
Bond angles



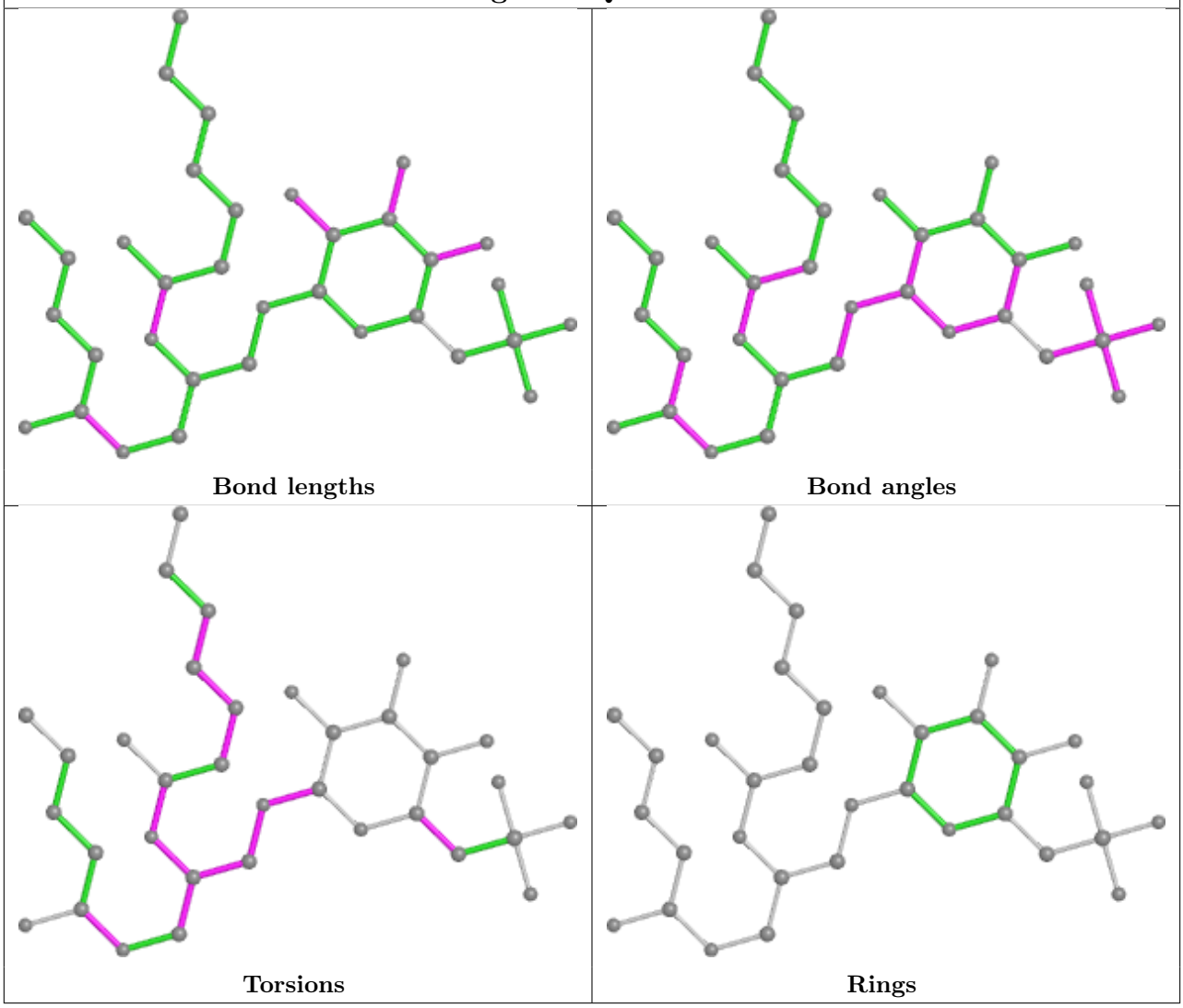
Torsions

Rings

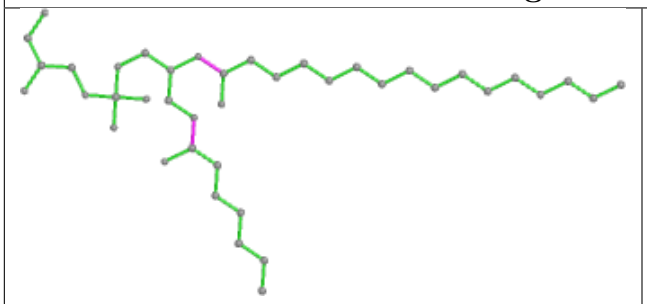
Ligand LMT D 410



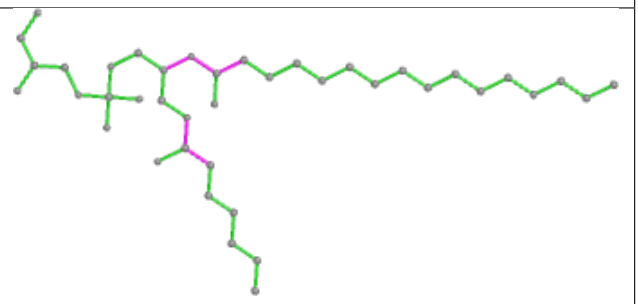
Ligand SQD f 102



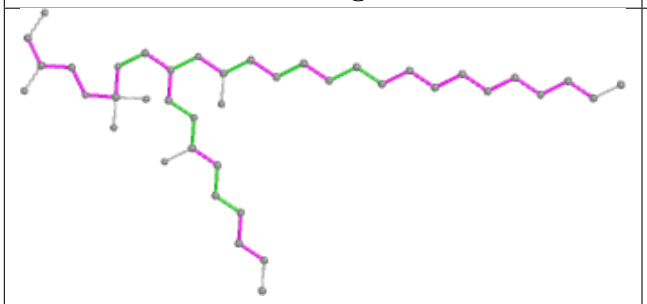
Ligand LHG E 102



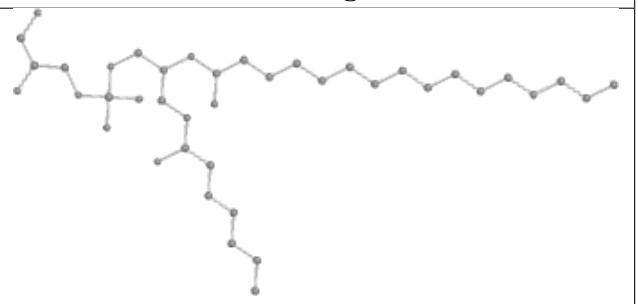
Bond lengths



Bond angles

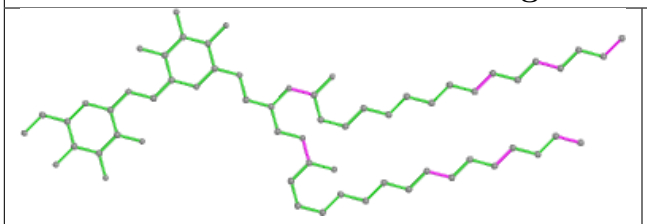


Torsions

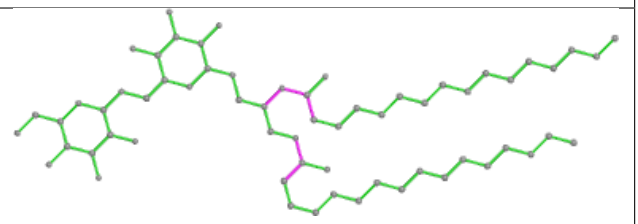


Rings

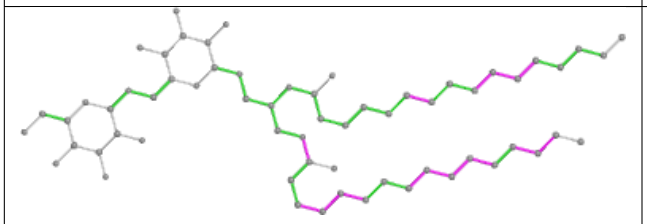
Ligand DGD C 518



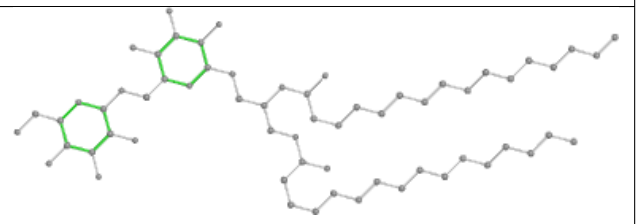
Bond lengths



Bond angles

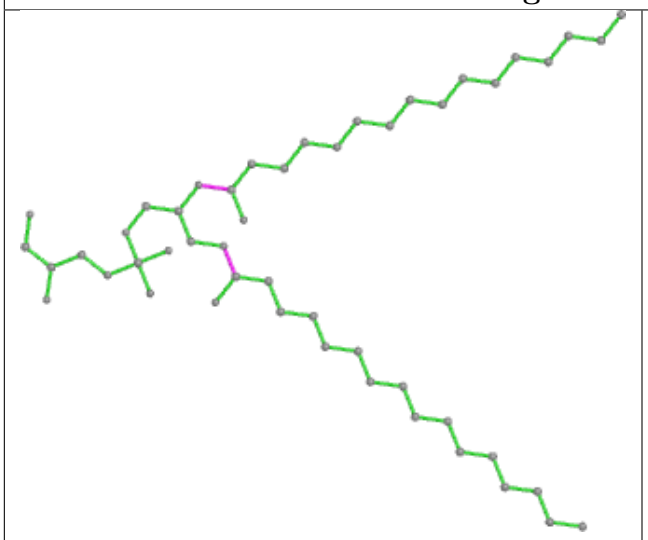


Torsions

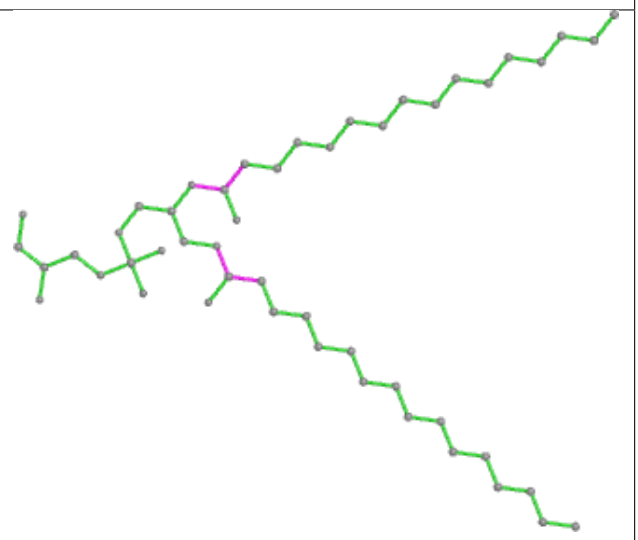


Rings

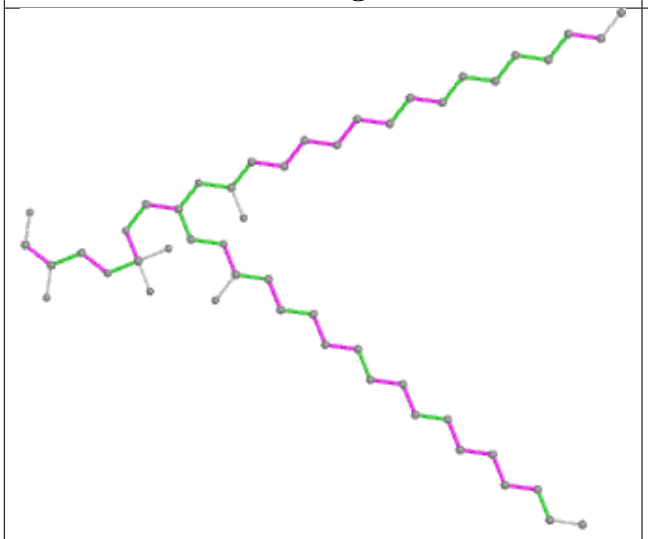
Ligand LHG D 408



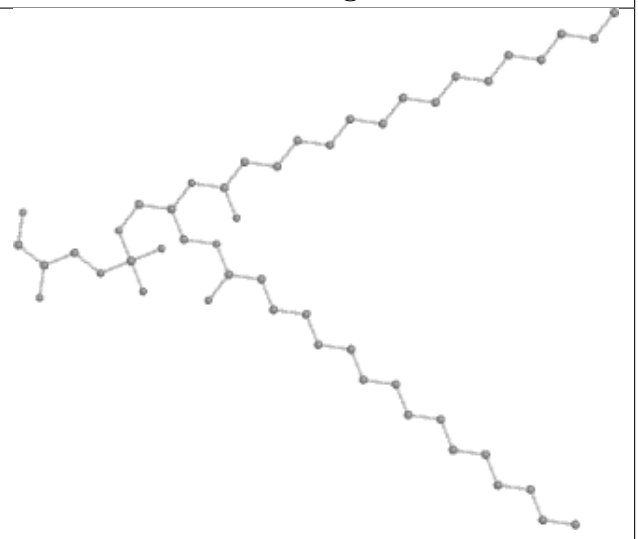
Bond lengths



Bond angles

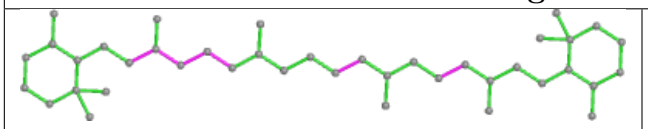


Torsions

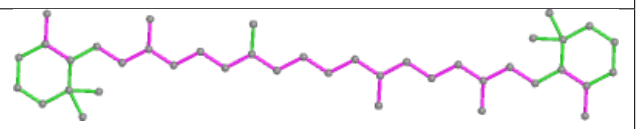


Rings

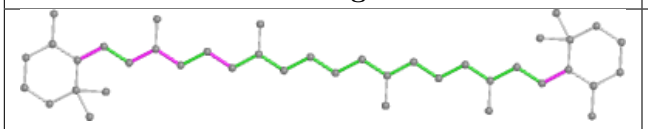
Ligand BCR a 409



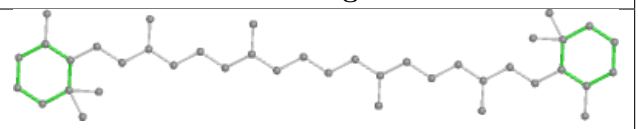
Bond lengths



Bond angles

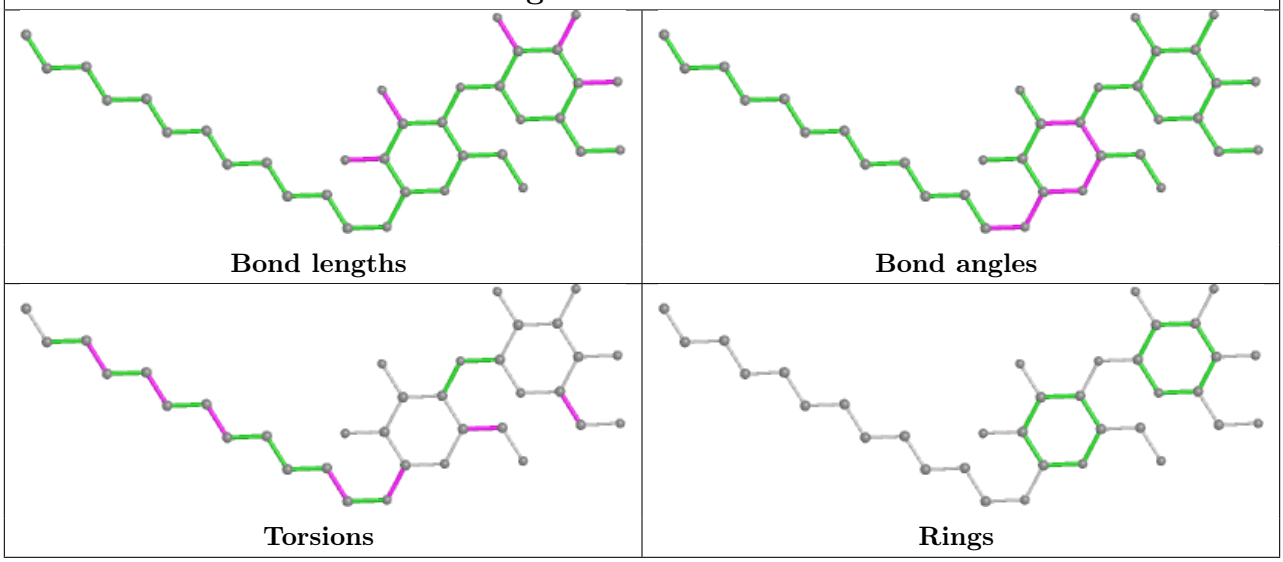


Torsions

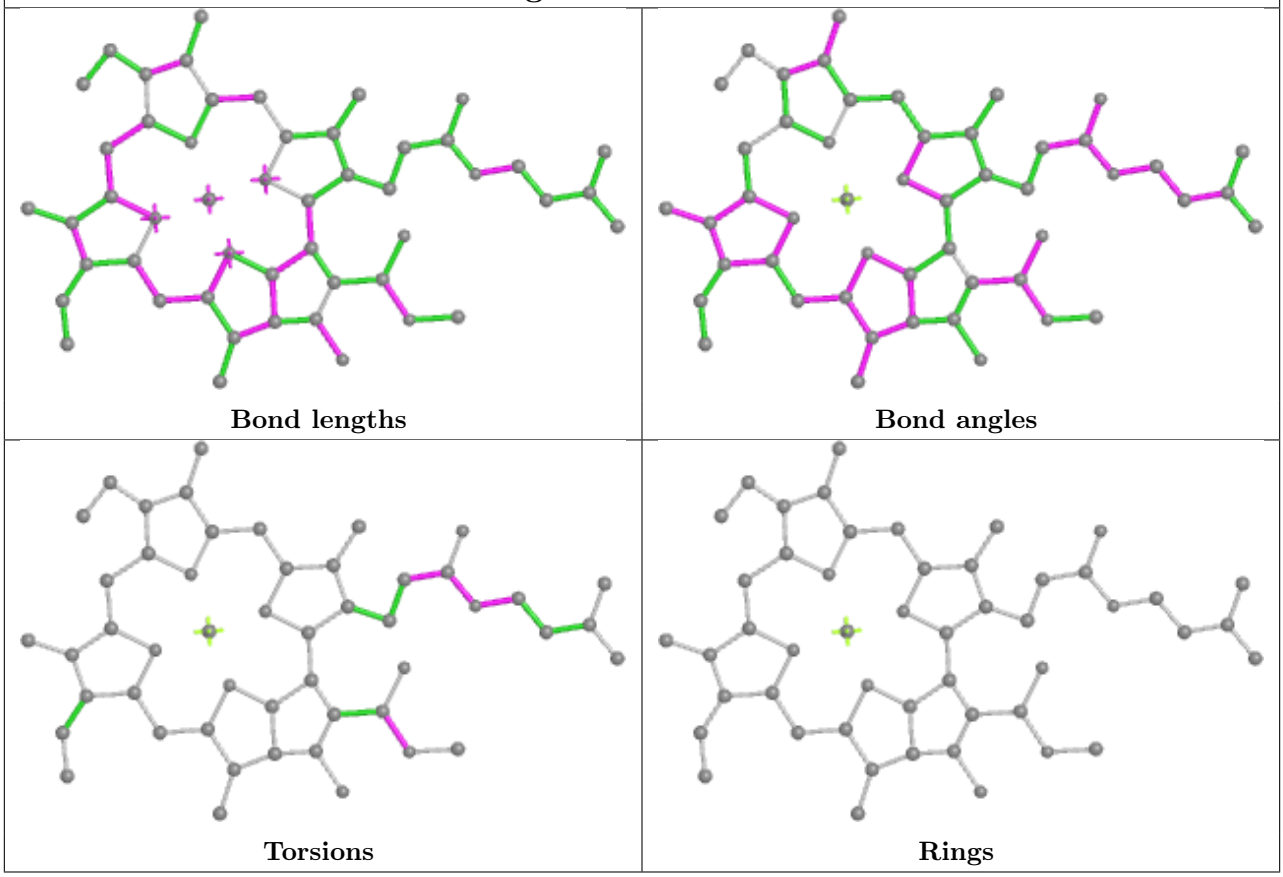


Rings

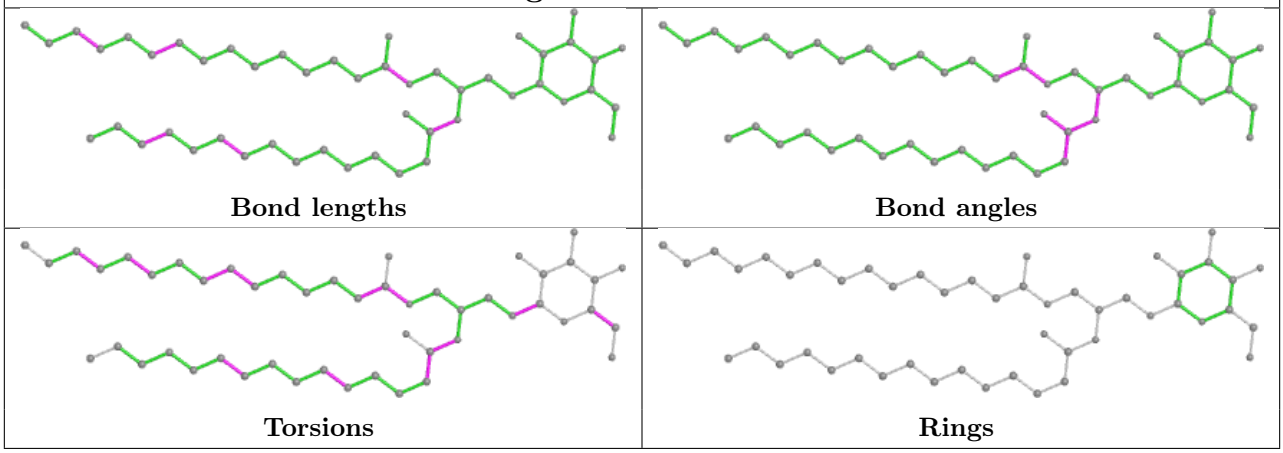
Ligand LMT a 415



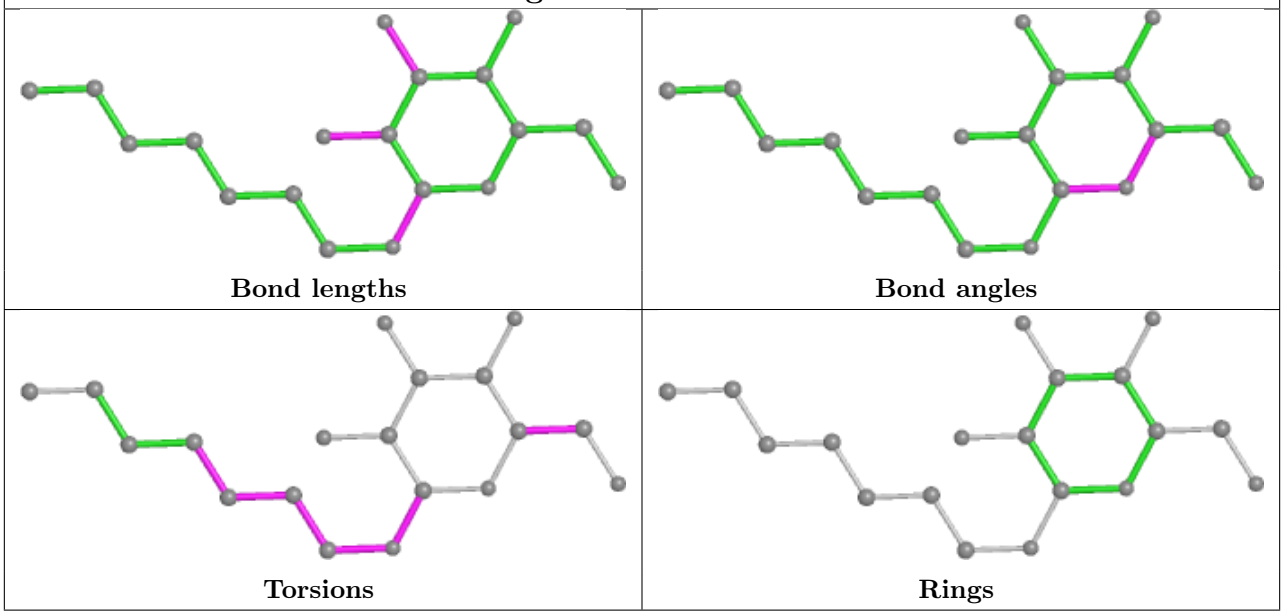
Ligand CLA C 513



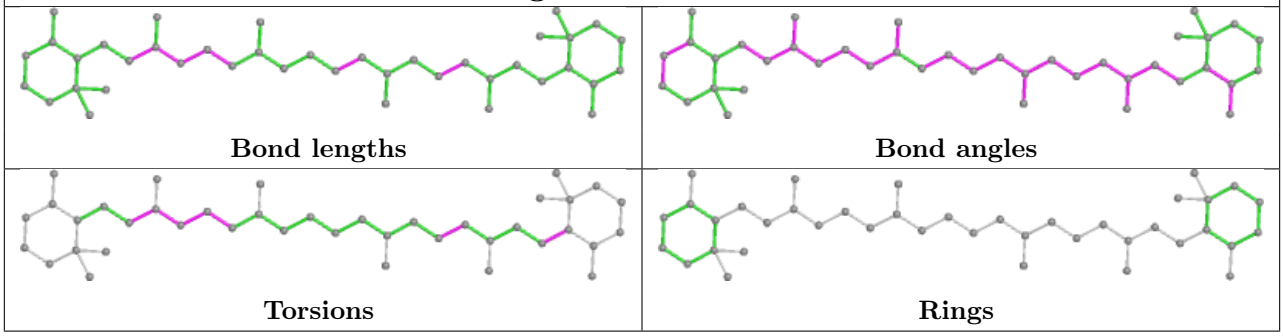
Ligand LMG c 523



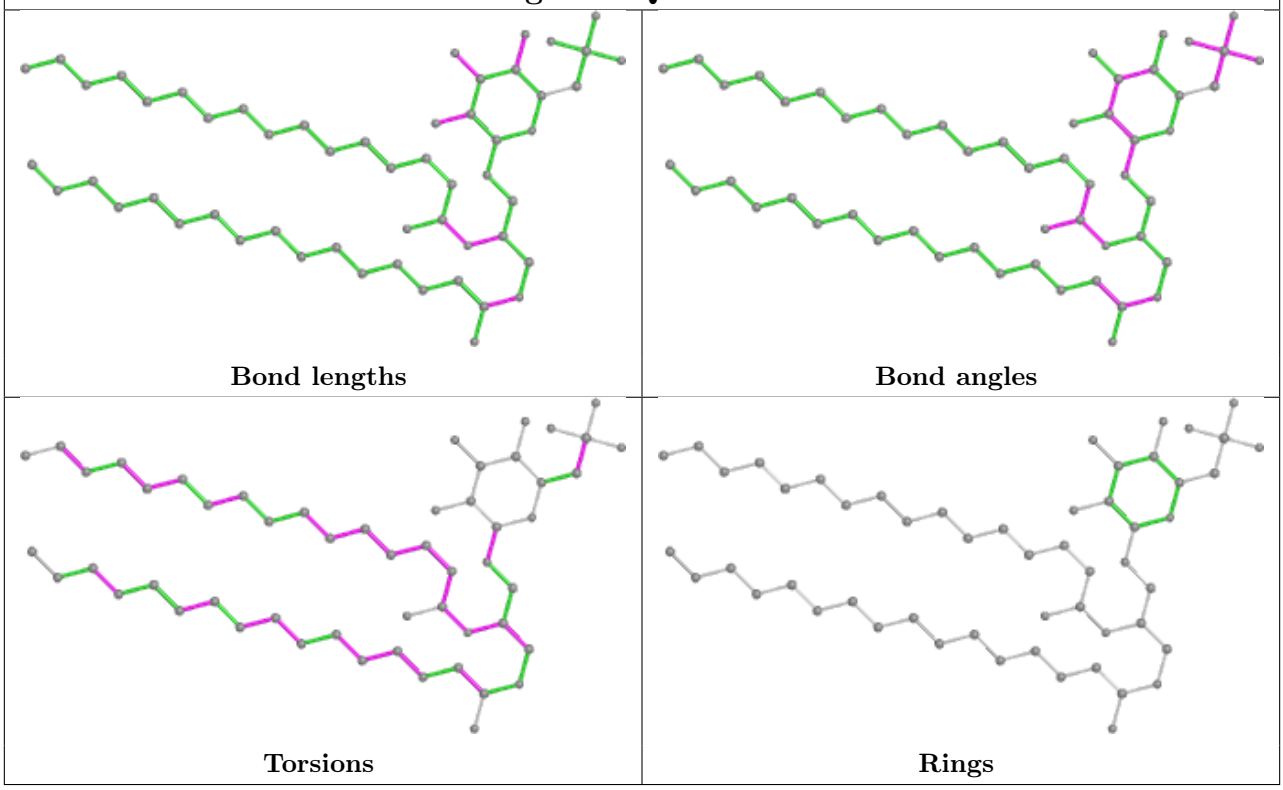
Ligand LMT x 104



Ligand BCR c 515



Ligand SQD C 501



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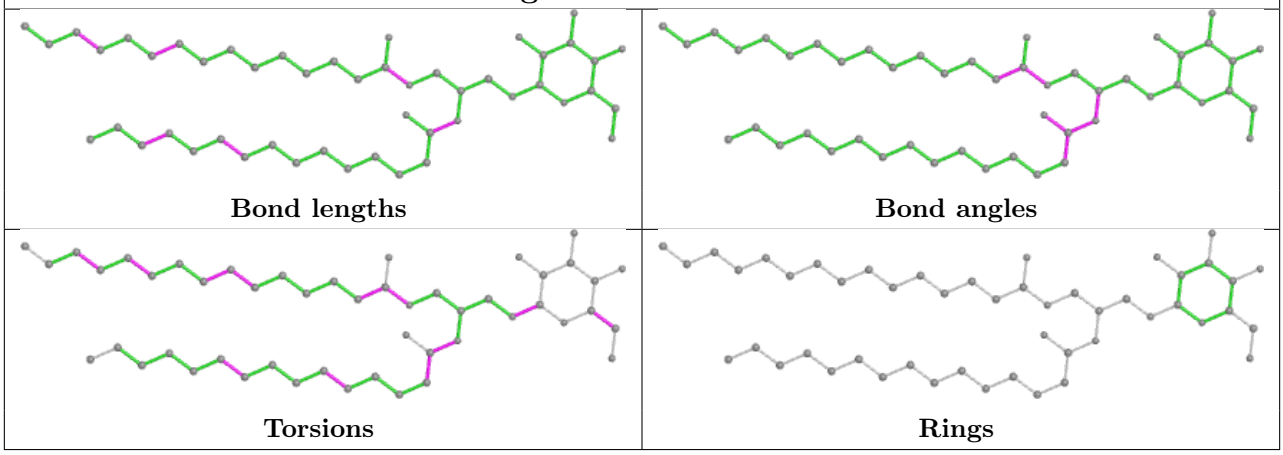
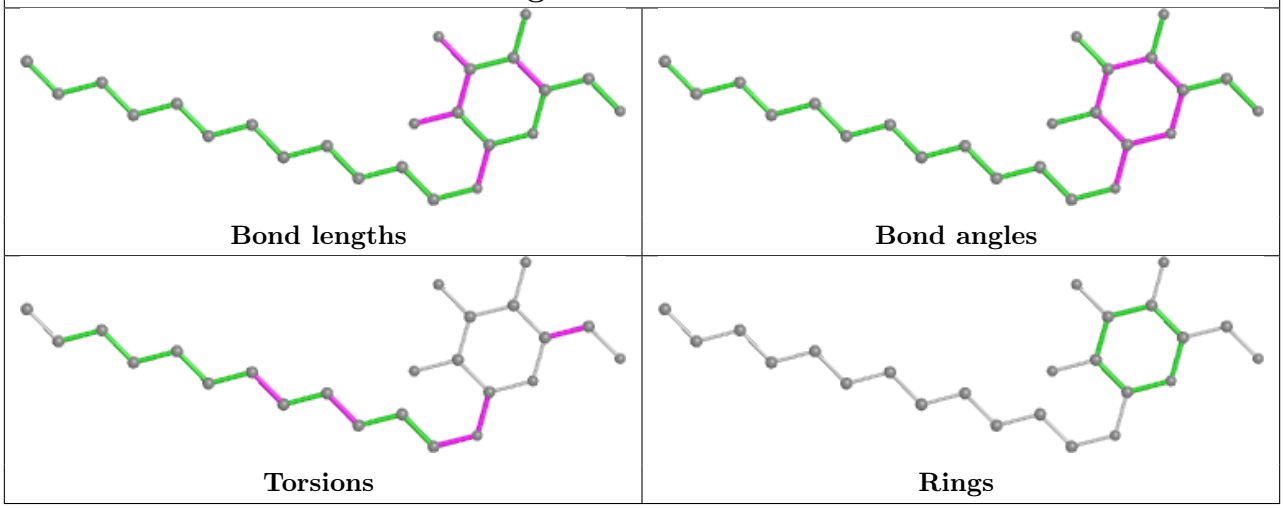
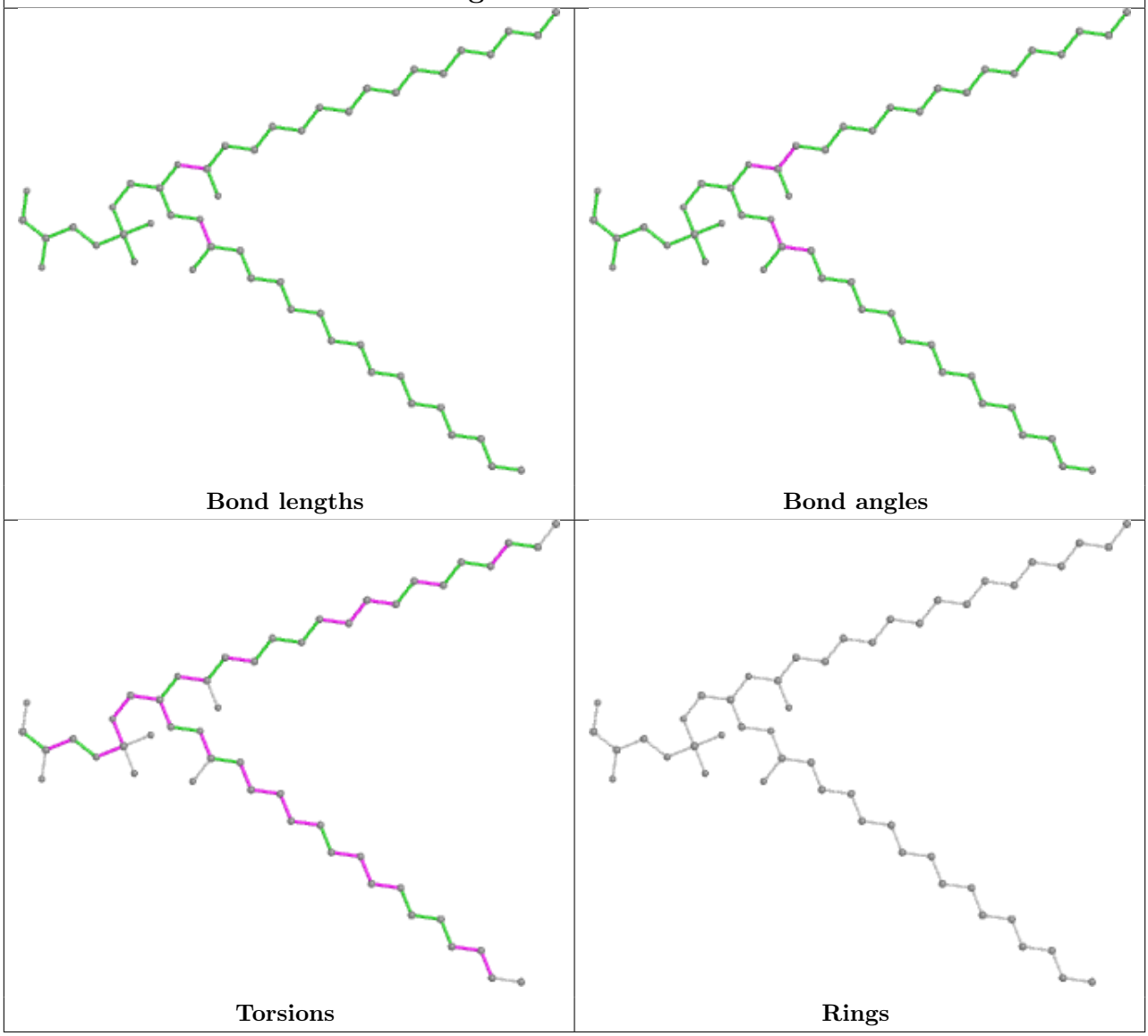


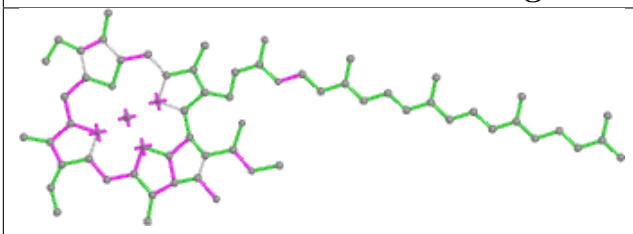
Ligand LMT c 522



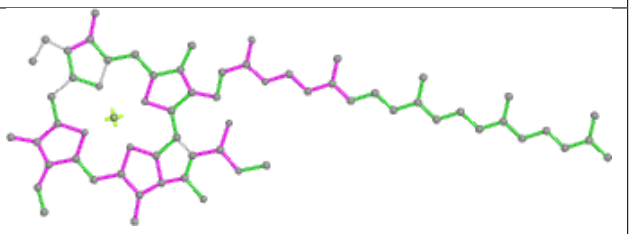
Ligand LHG B 627



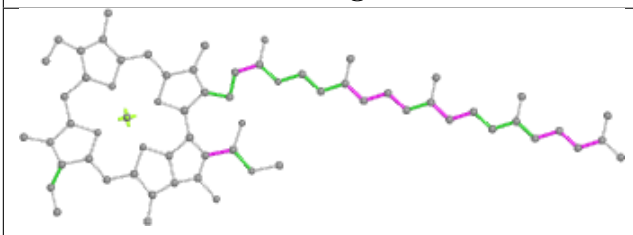
Ligand CLA B 614



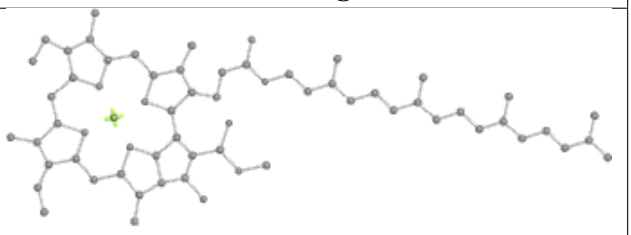
Bond lengths



Bond angles

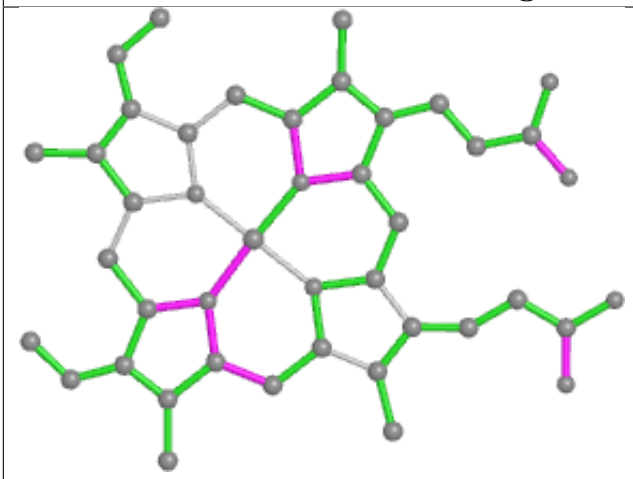


Torsions

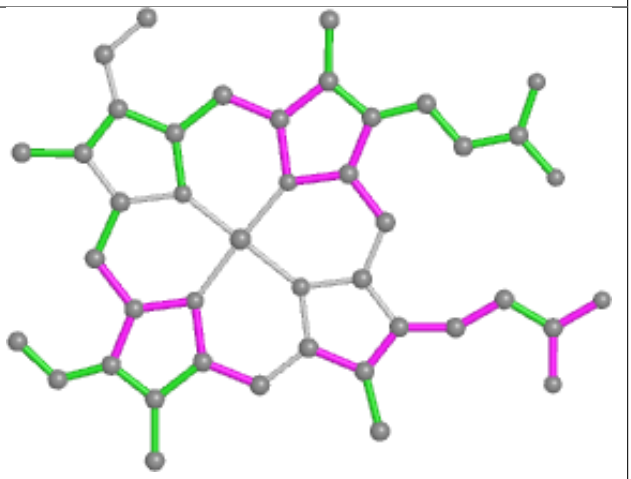


Rings

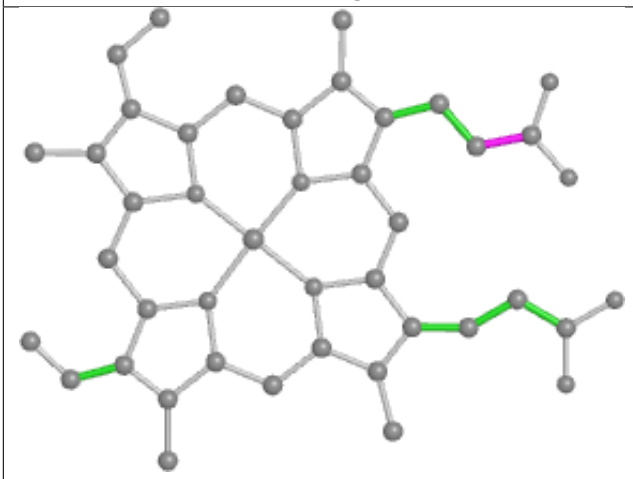
Ligand HEM V 201



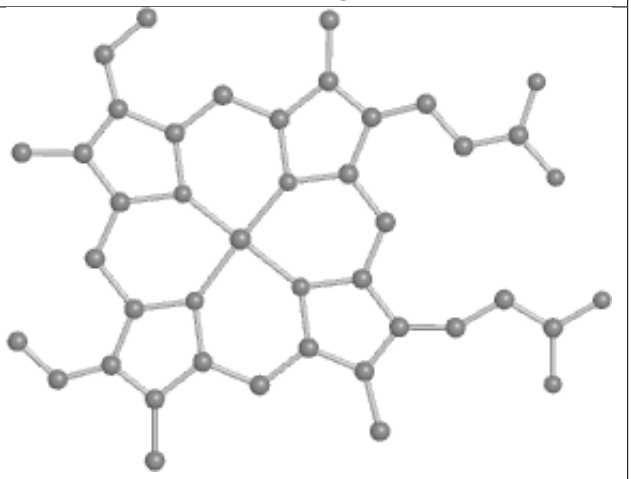
Bond lengths



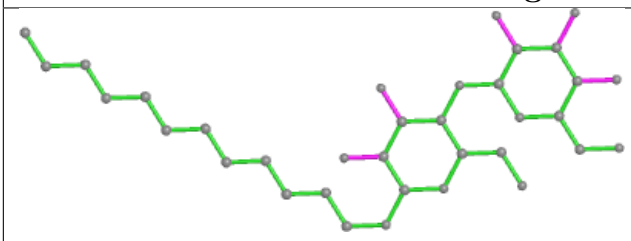
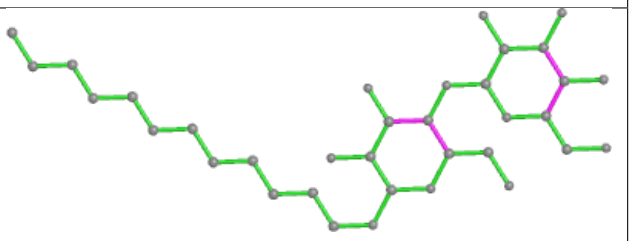
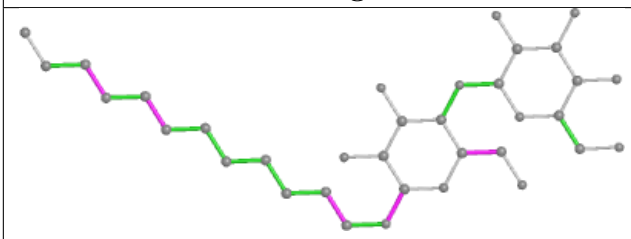
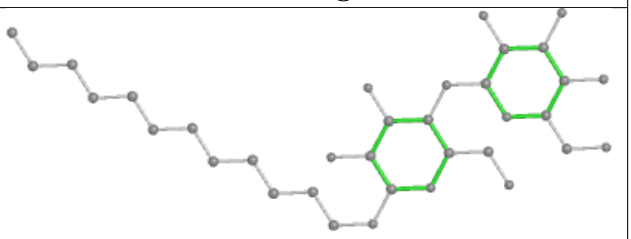
Bond angles

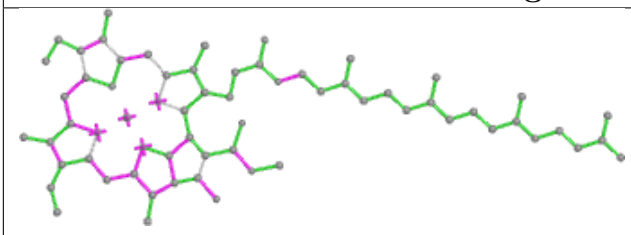
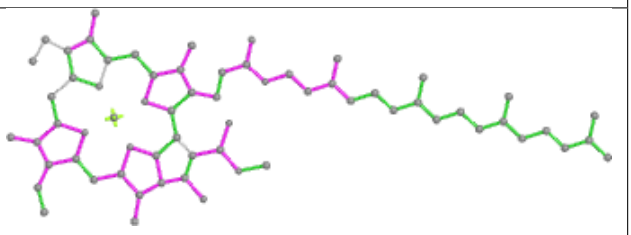
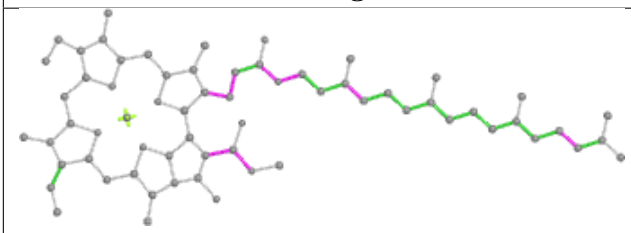
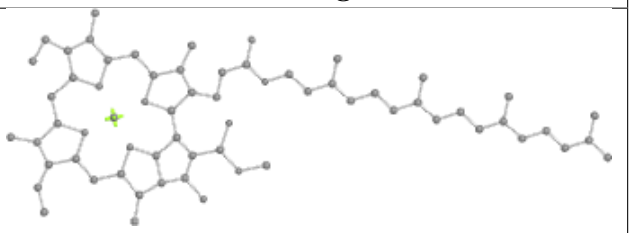


Torsions

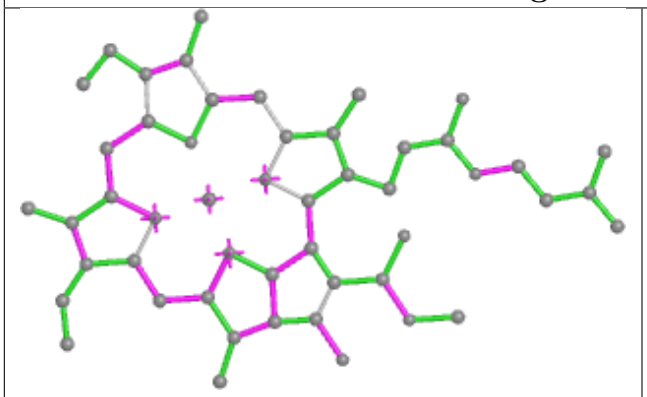


Rings

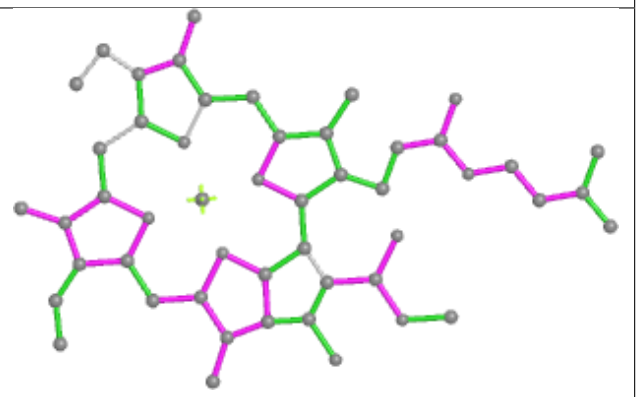
Ligand LMT d 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

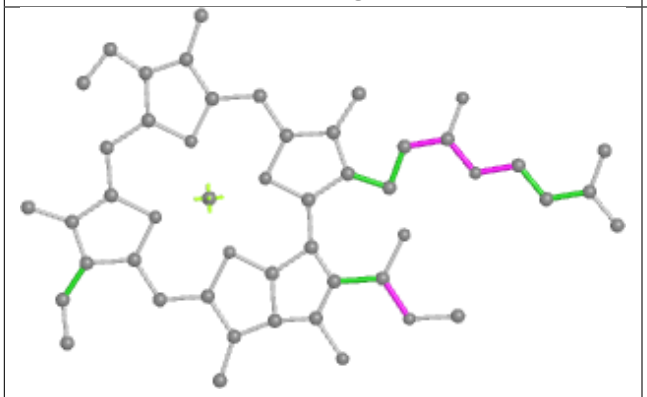
Ligand CLA c 513



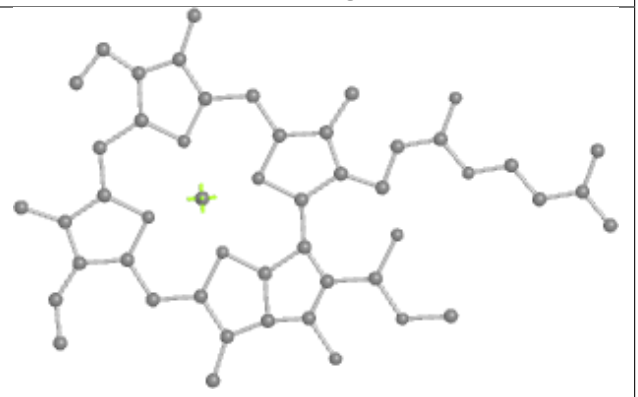
Bond lengths



Bond angles

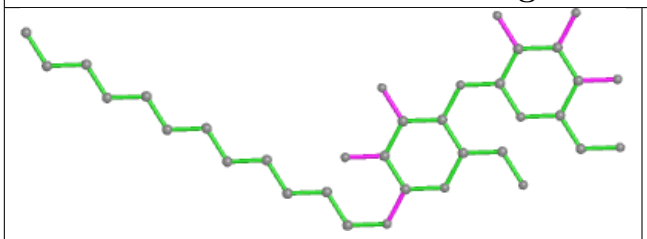


Torsions

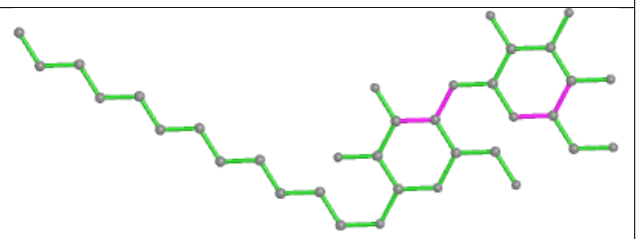


Rings

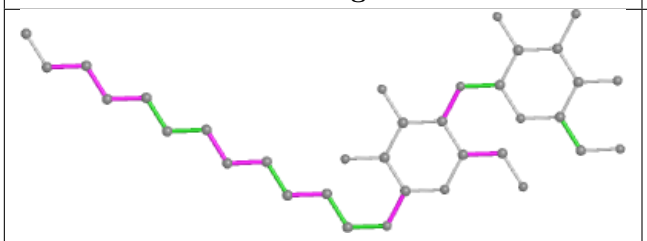
Ligand LMT M 101



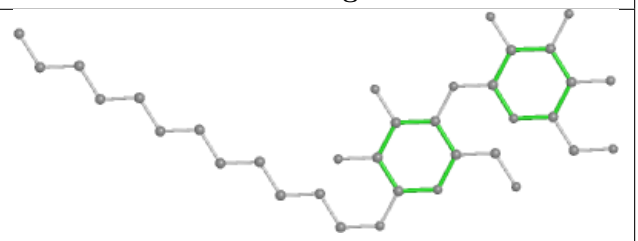
Bond lengths



Bond angles

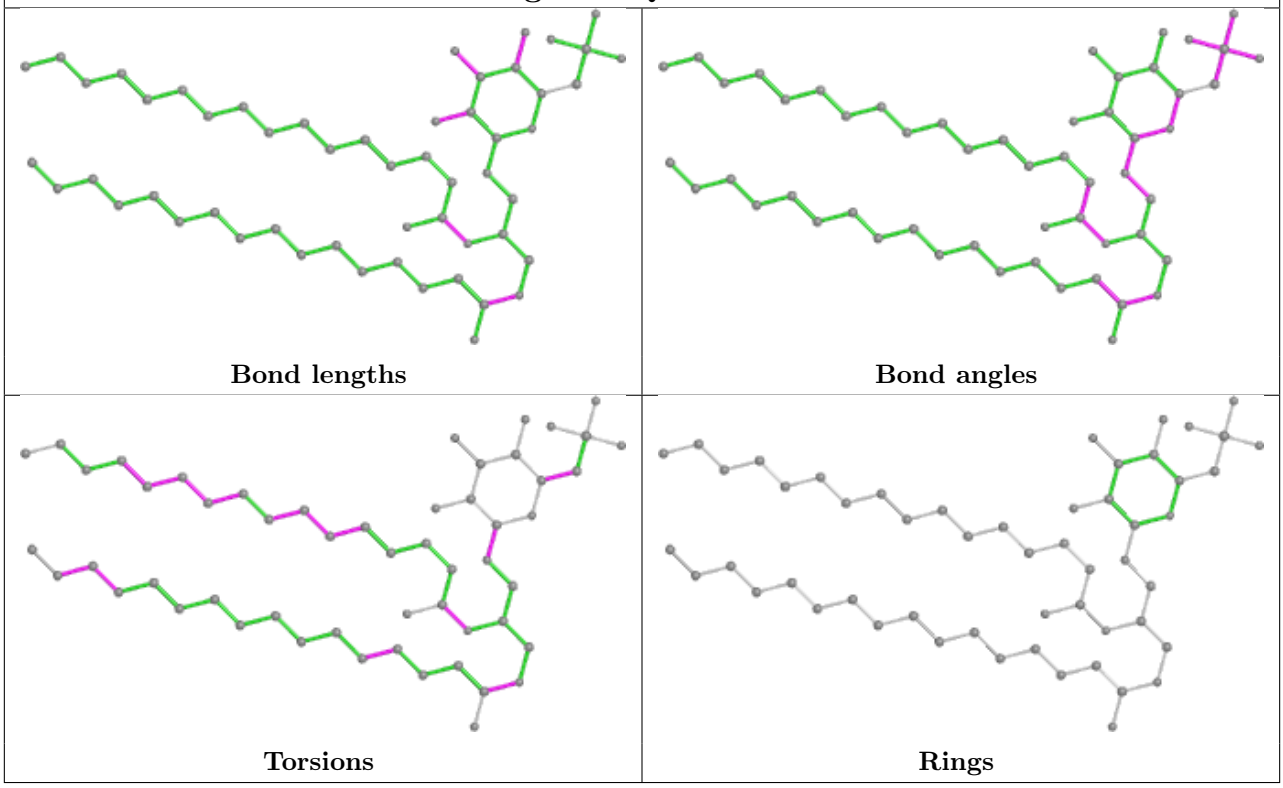


Torsions

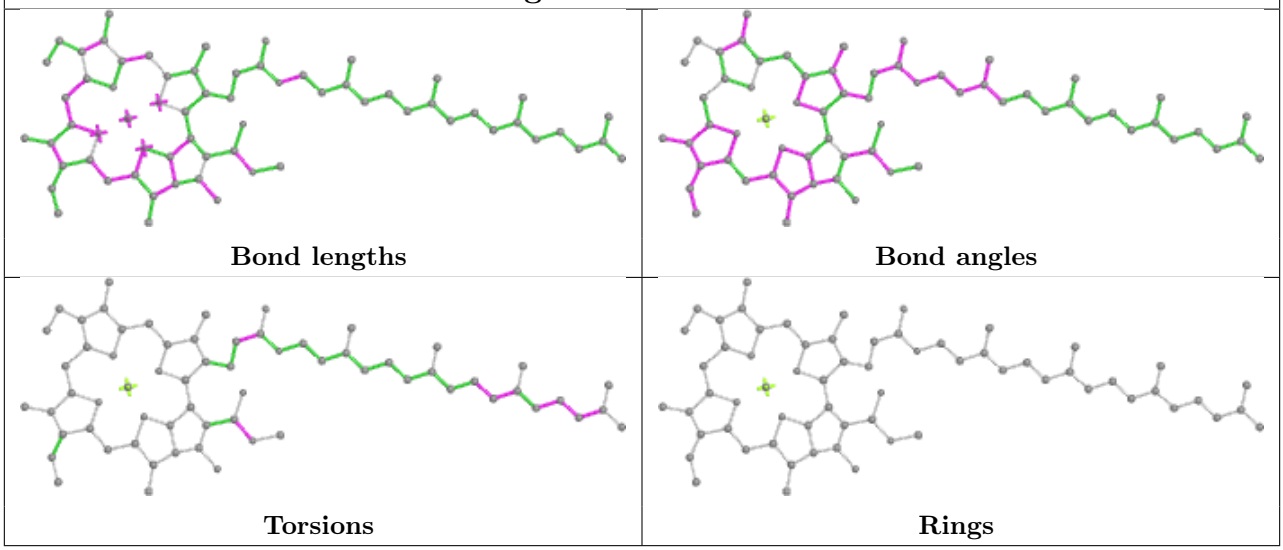


Rings

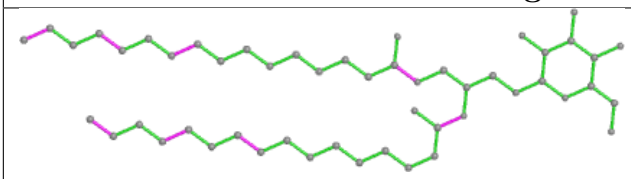
Ligand SQD H 103



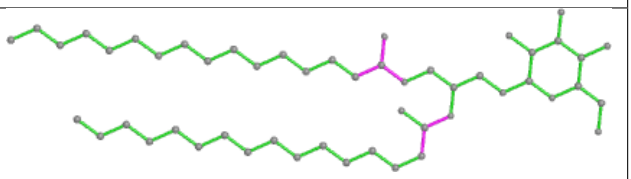
Ligand CLA D 403



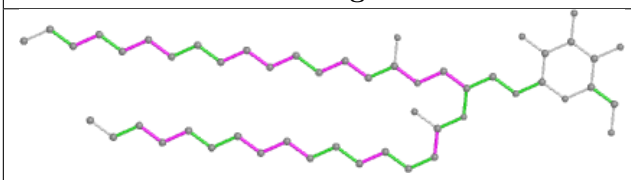
Ligand LMG a 410



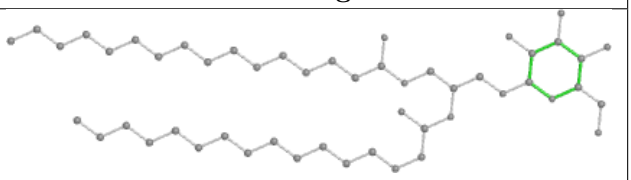
Bond lengths



Bond angles

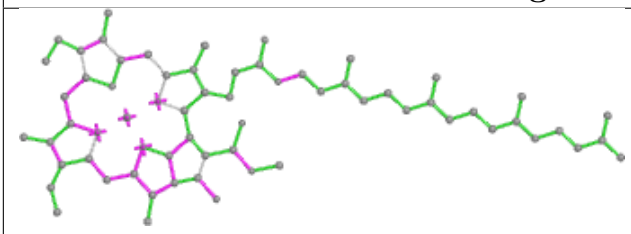


Torsions

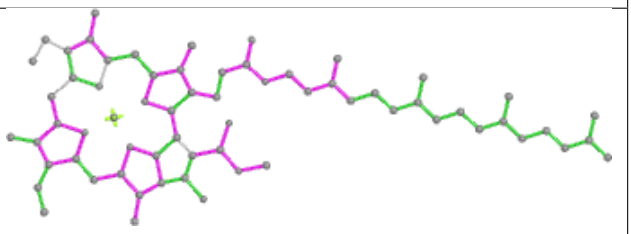


Rings

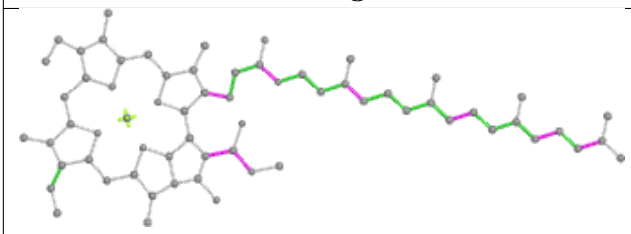
Ligand CLA c 509



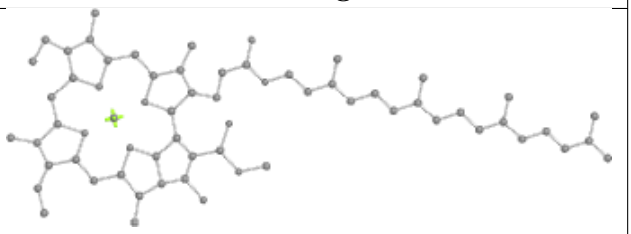
Bond lengths



Bond angles

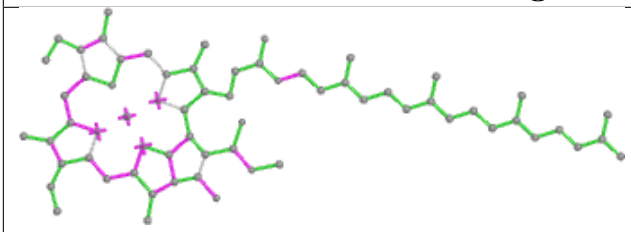


Torsions

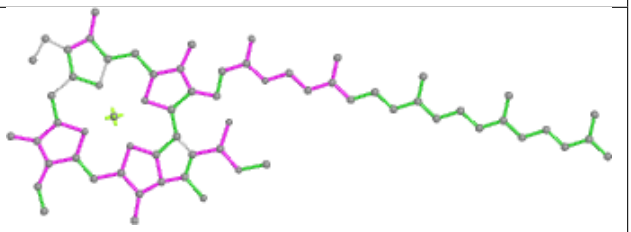


Rings

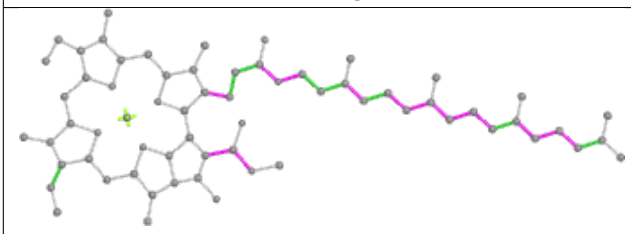
Ligand CLA c 514



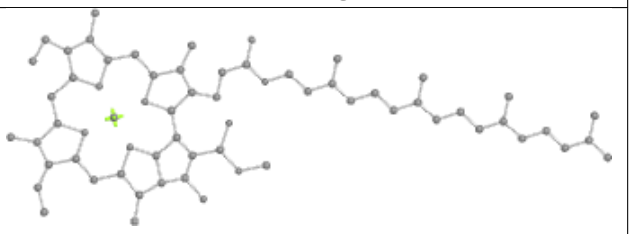
Bond lengths



Bond angles

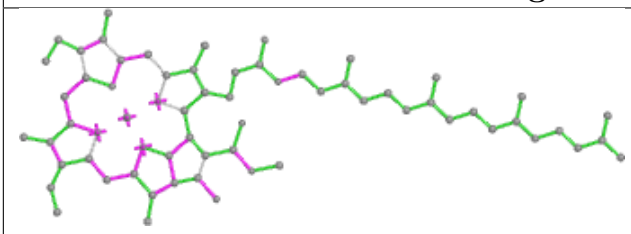


Torsions

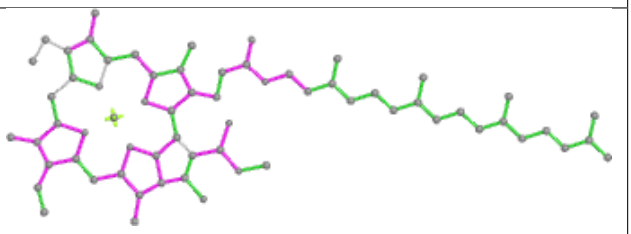


Rings

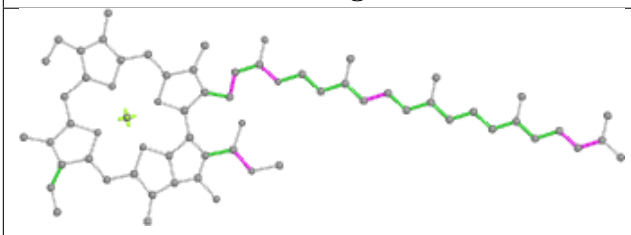
Ligand CLA a 405



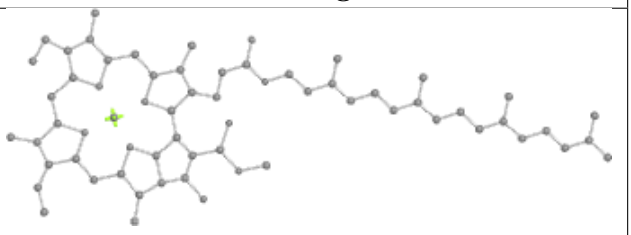
Bond lengths



Bond angles

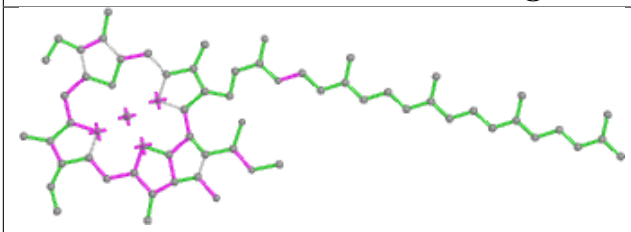


Torsions

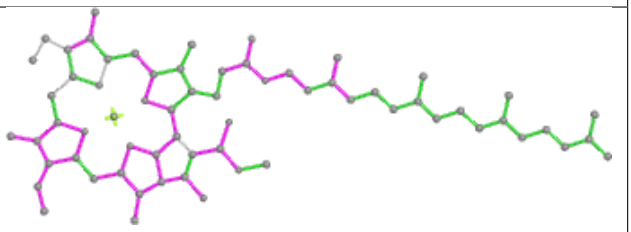


Rings

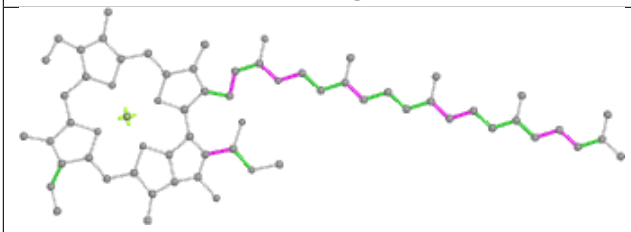
Ligand CLA C 508



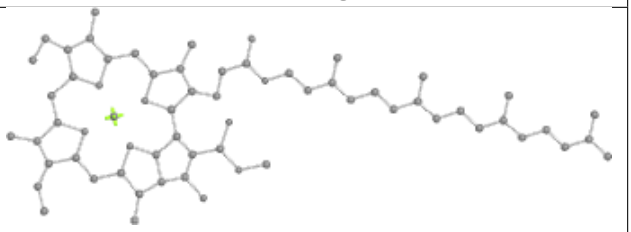
Bond lengths



Bond angles

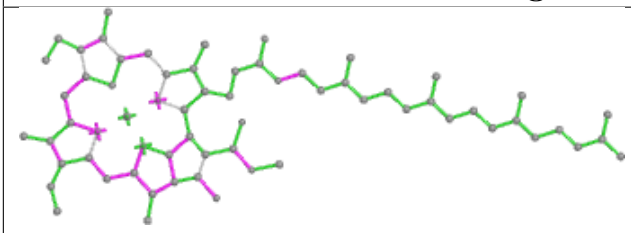


Torsions

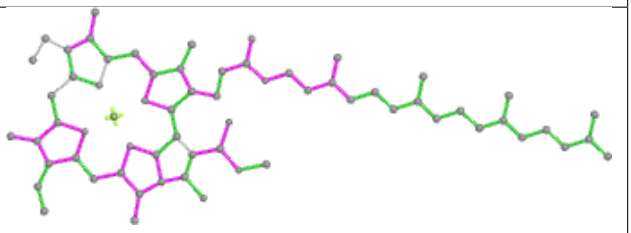


Rings

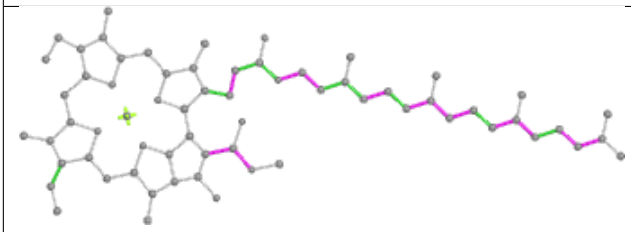
Ligand CLA b 602



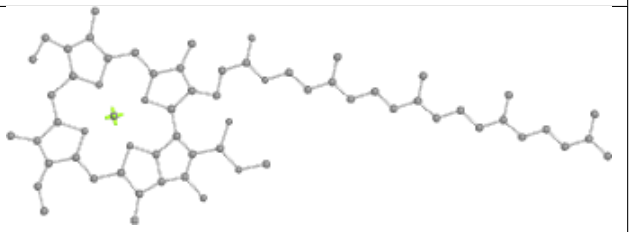
Bond lengths



Bond angles

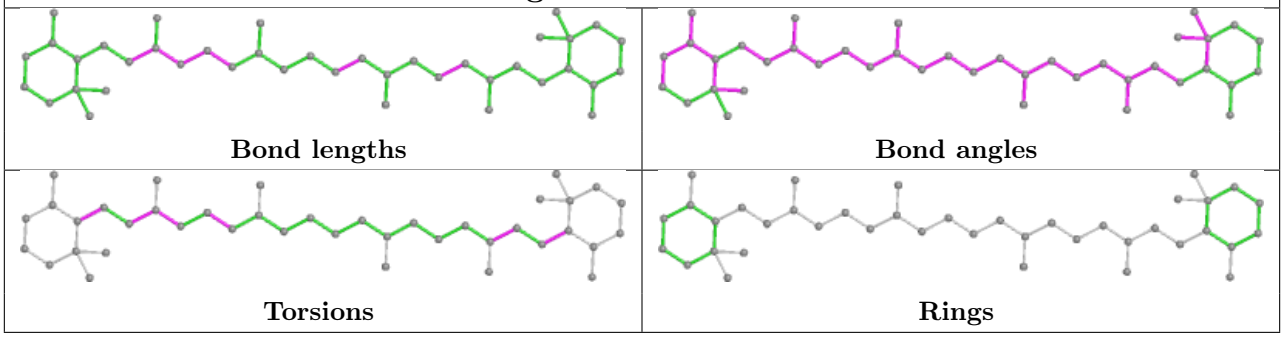


Torsions

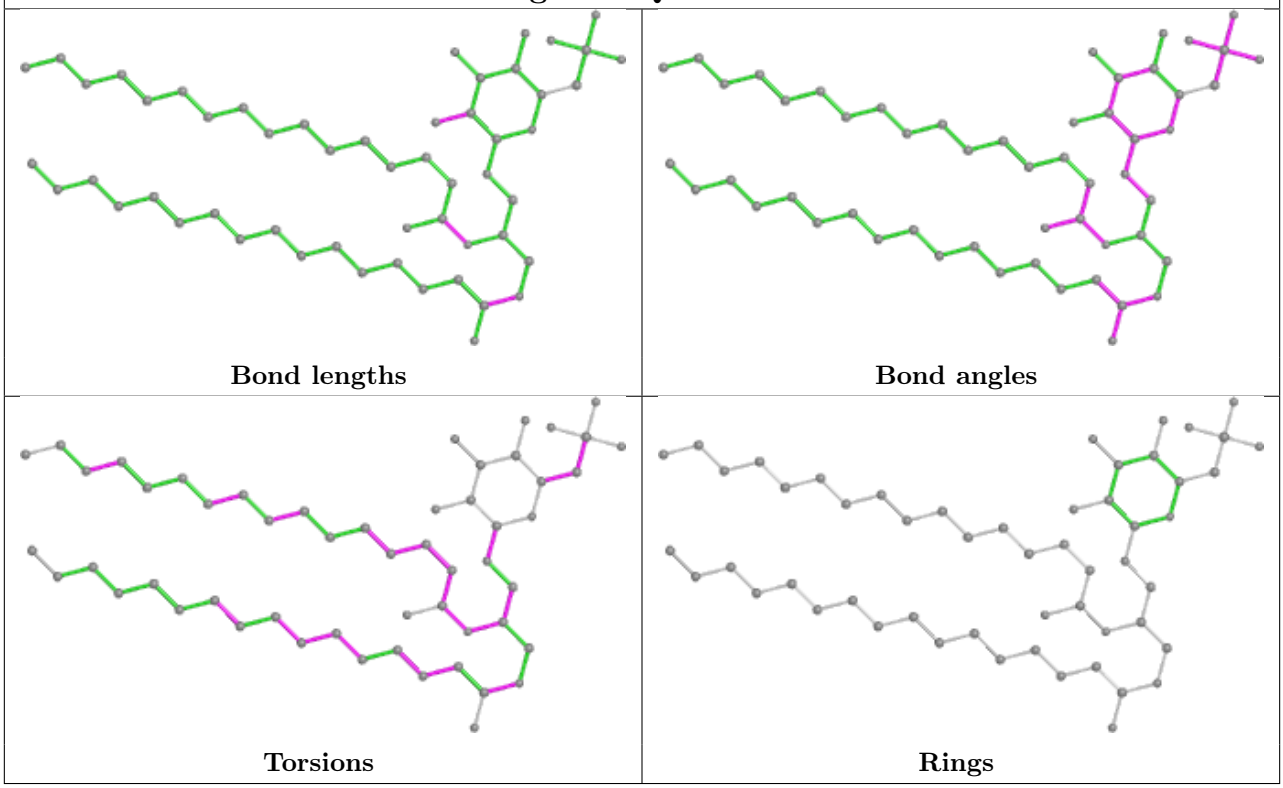


Rings

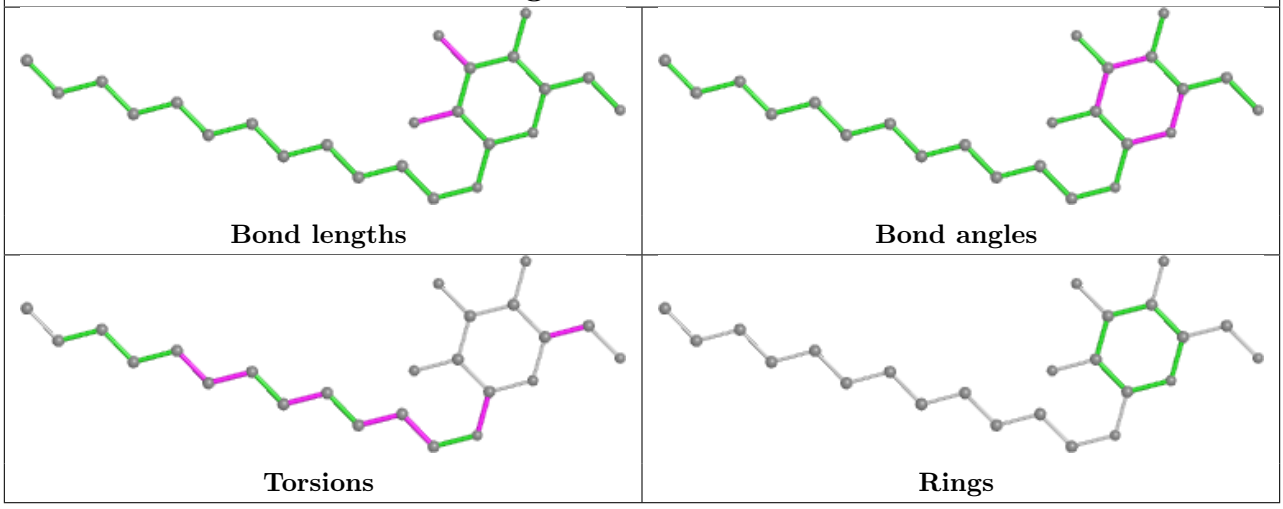
Ligand BCR b 619



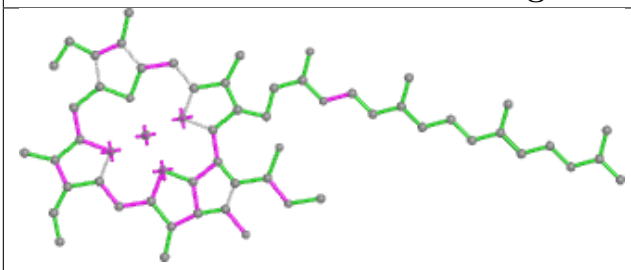
Ligand SQD a 412



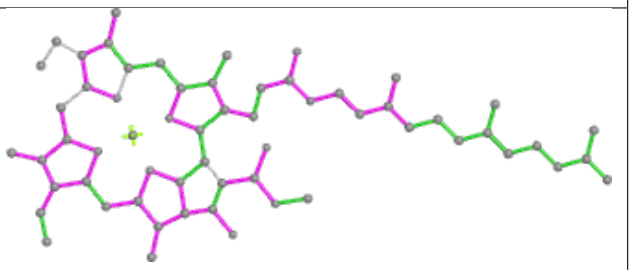
Ligand LMT h 102



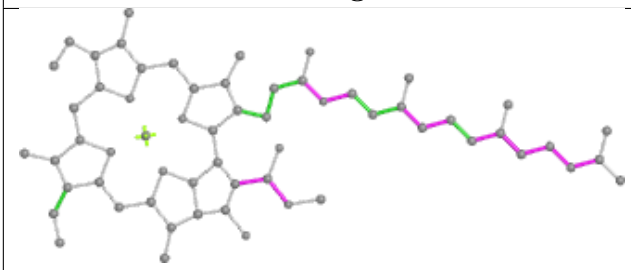
Ligand CLA b 616



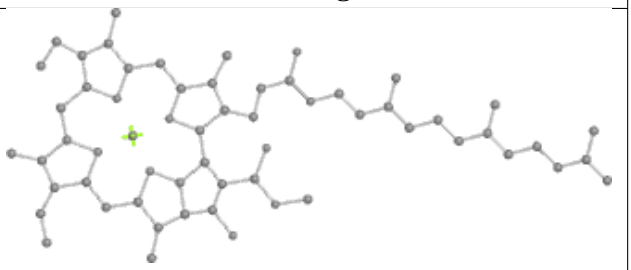
Bond lengths



Bond angles

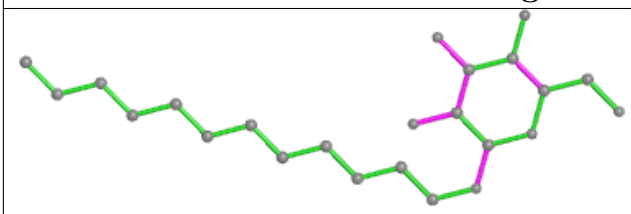


Torsions

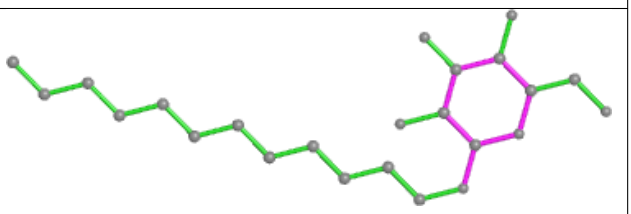


Rings

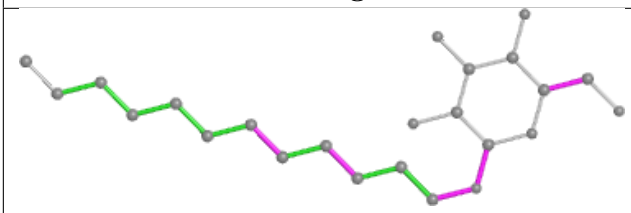
Ligand LMT C 522



Bond lengths



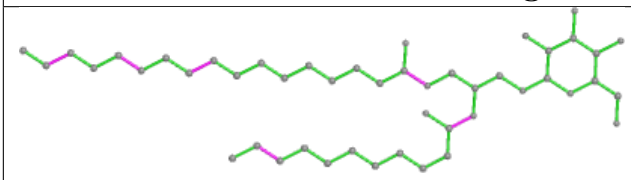
Bond angles



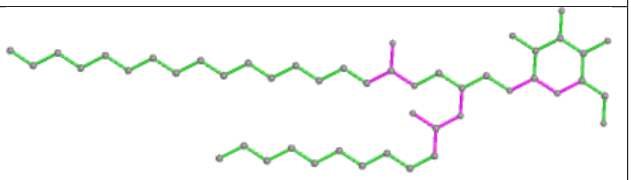
Torsions

Rings

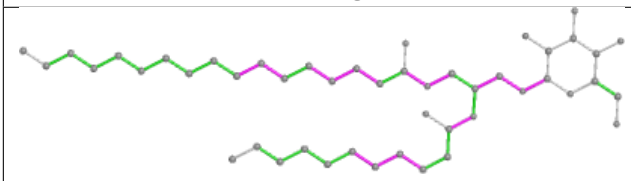
Ligand LMG h 105



Bond lengths



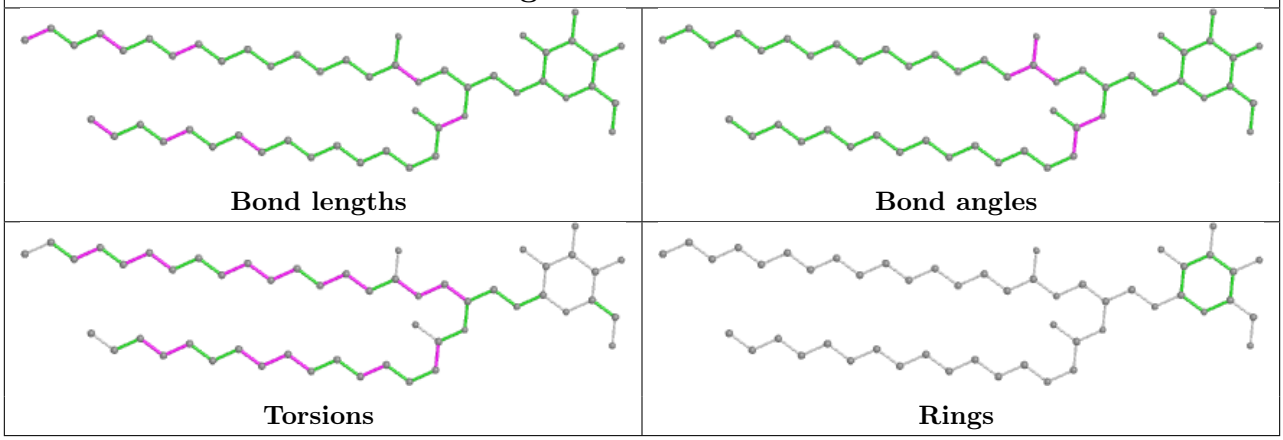
Bond angles



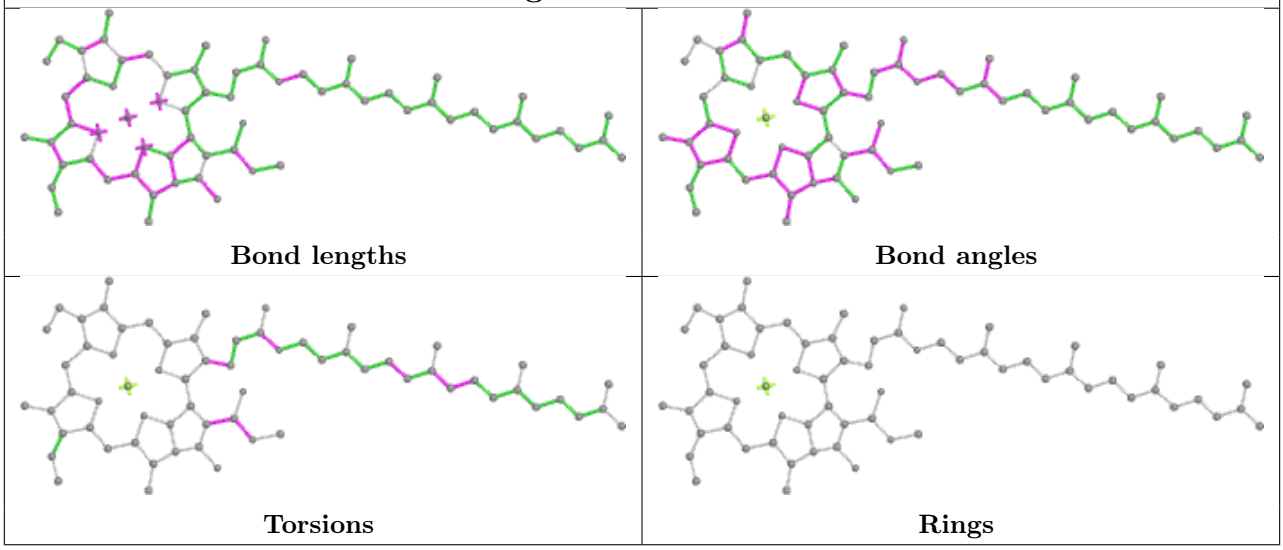
Torsions

Rings

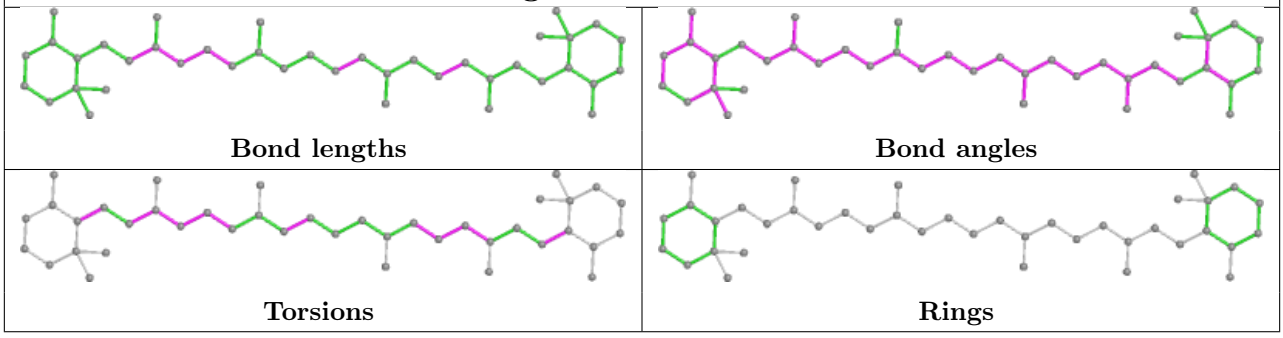
Ligand LMG A 410



Ligand CLA B 605



Ligand BCR K 102



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.

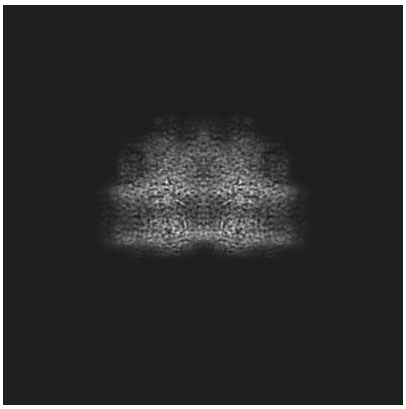
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-41460. These allow visual inspection of the internal detail of the map and identification of artifacts.

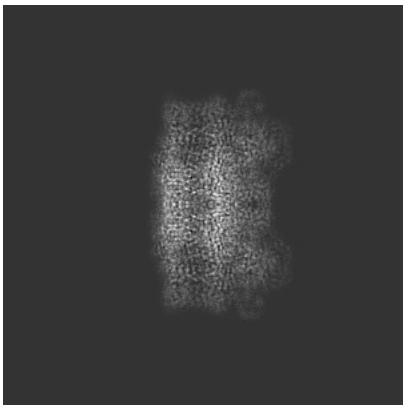
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

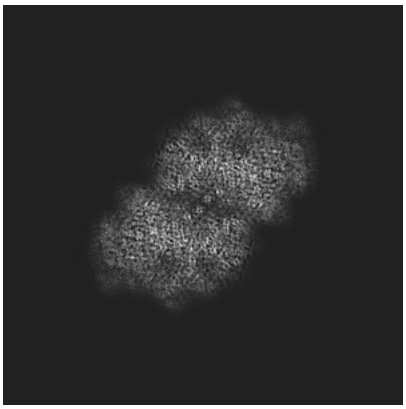
6.1.1 Primary map



X

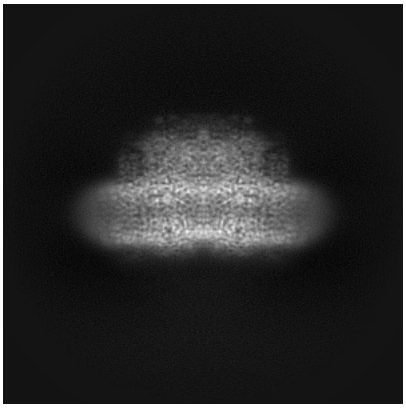


Y

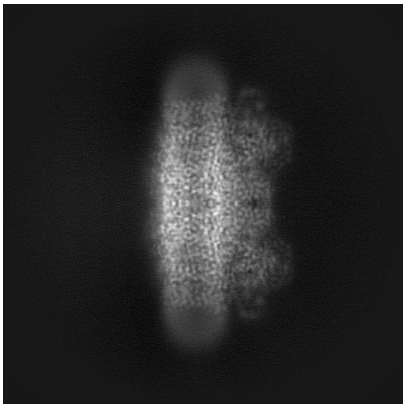


Z

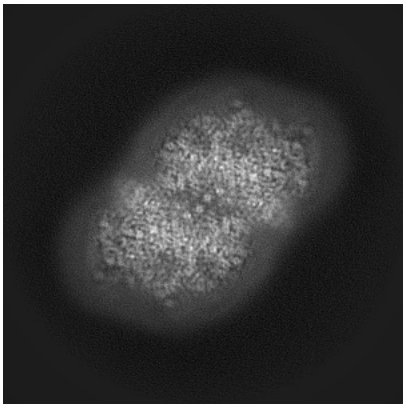
6.1.2 Raw map



X



Y



Z

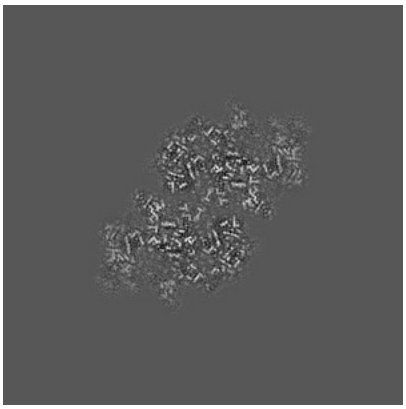
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

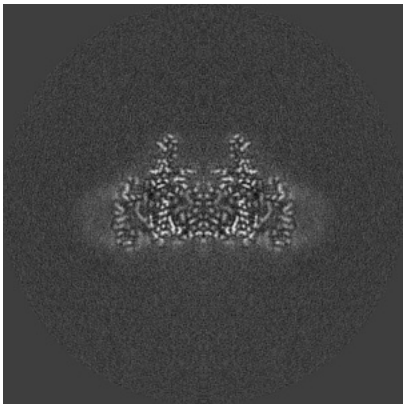
X Index: 180

Y Index: 180

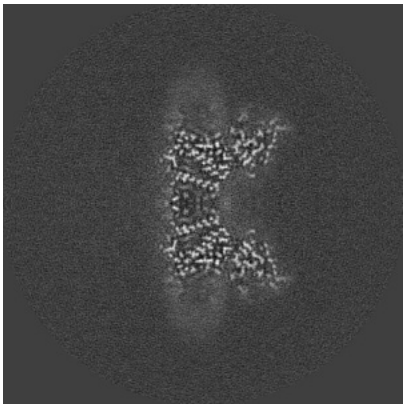


Z Index: 180

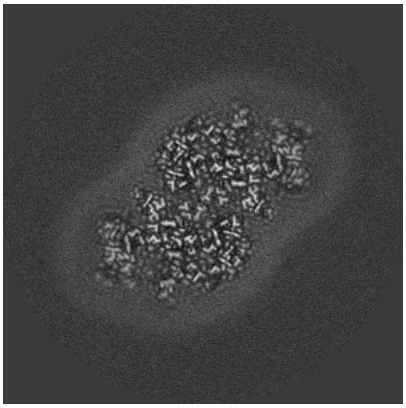
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

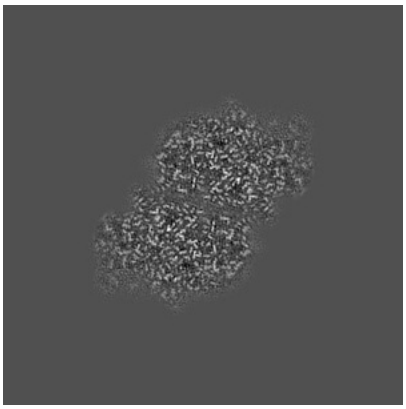
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

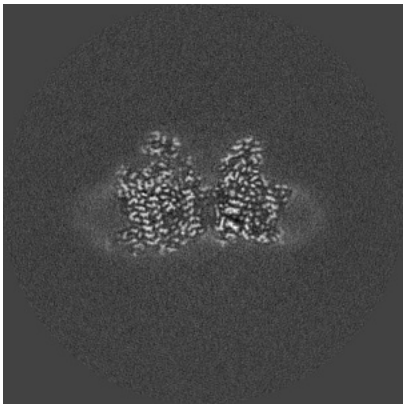
X Index: 192

Y Index: 146

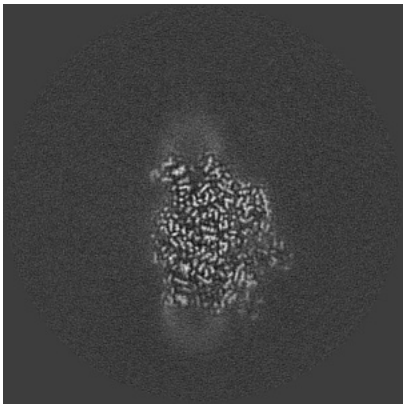


Z Index: 191

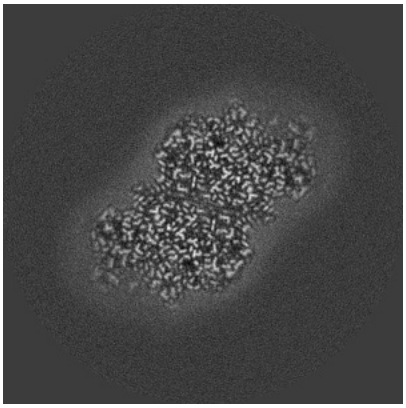
6.3.2 Raw map



X Index: 168



Y Index: 146

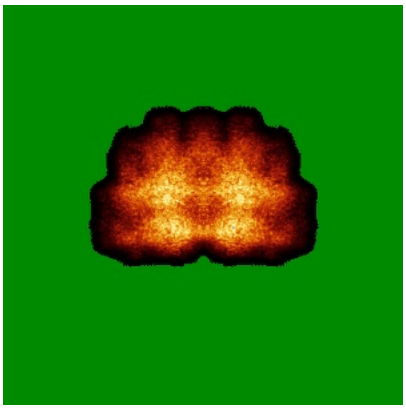


Z Index: 191

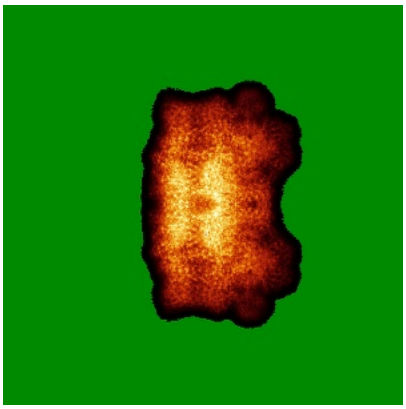
The images above show the largest variance slices of the map in three orthogonal directions.

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

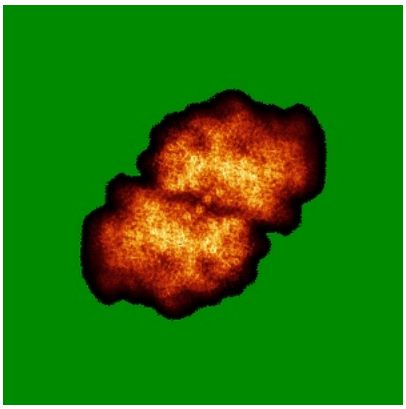
6.4.1 Primary map



X

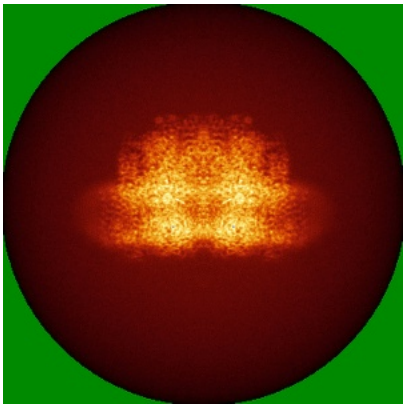


Y

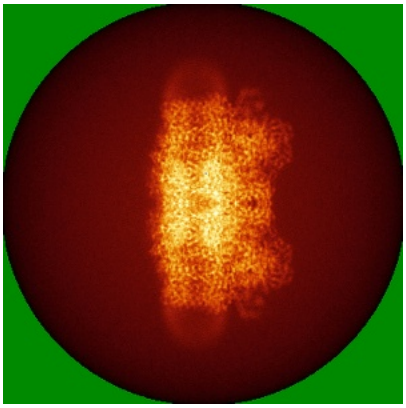


Z

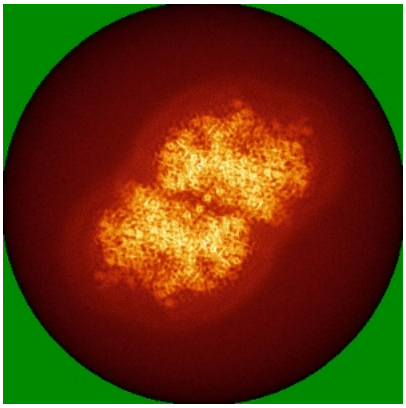
6.4.2 Raw map



X



Y

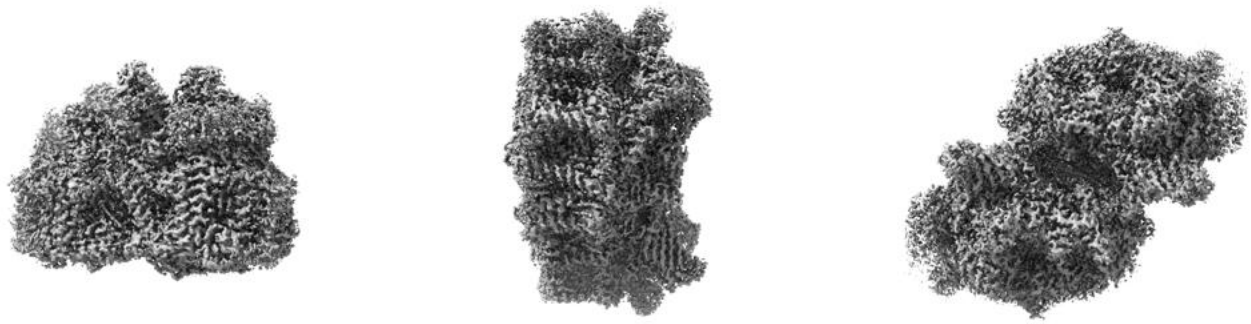


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

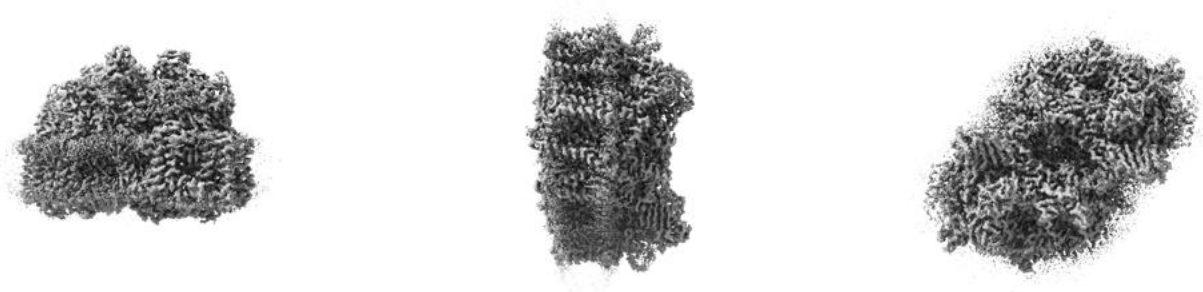
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00432. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

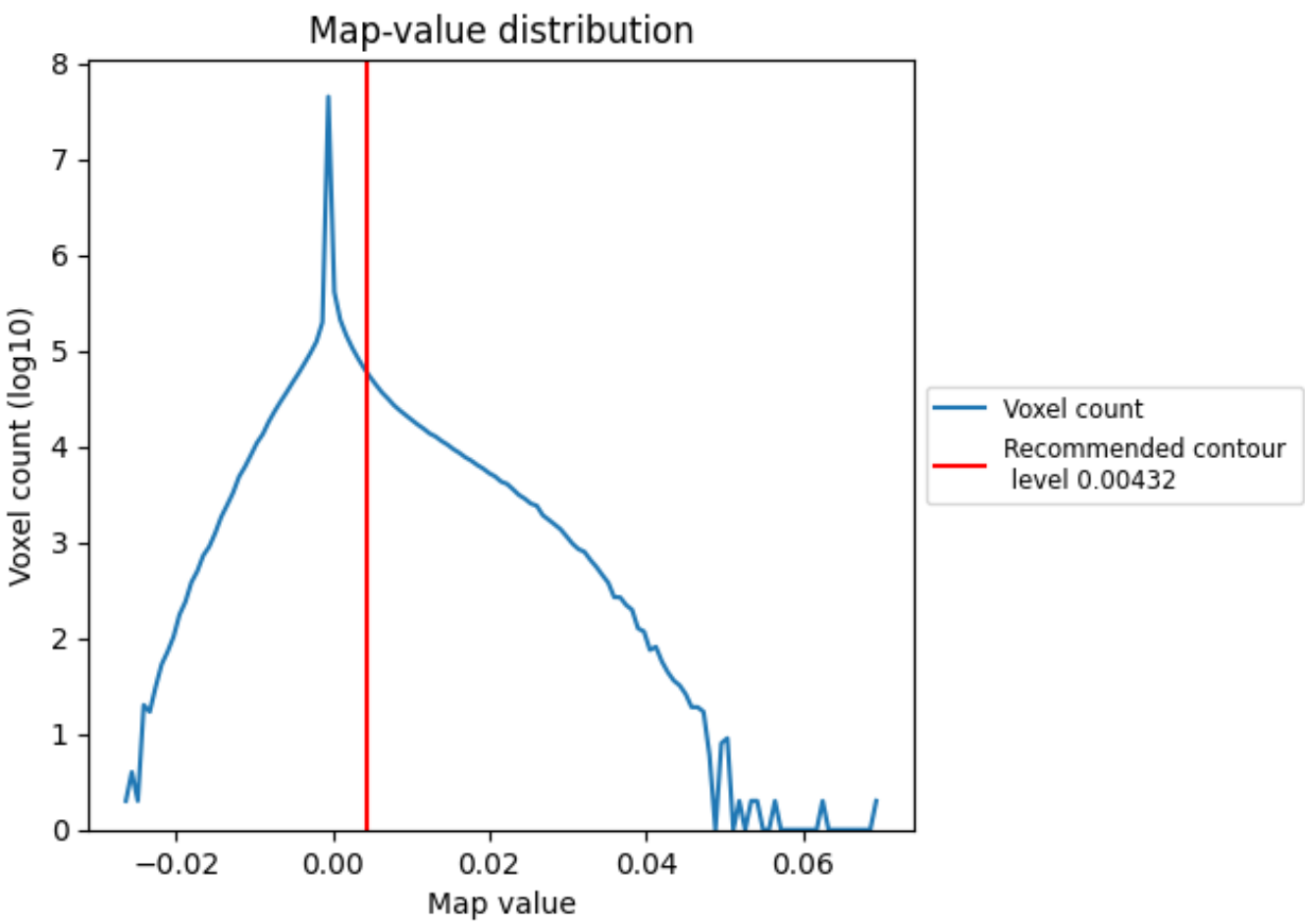
6.6 Mask visualisation (i)

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

7 Map analysis (i)

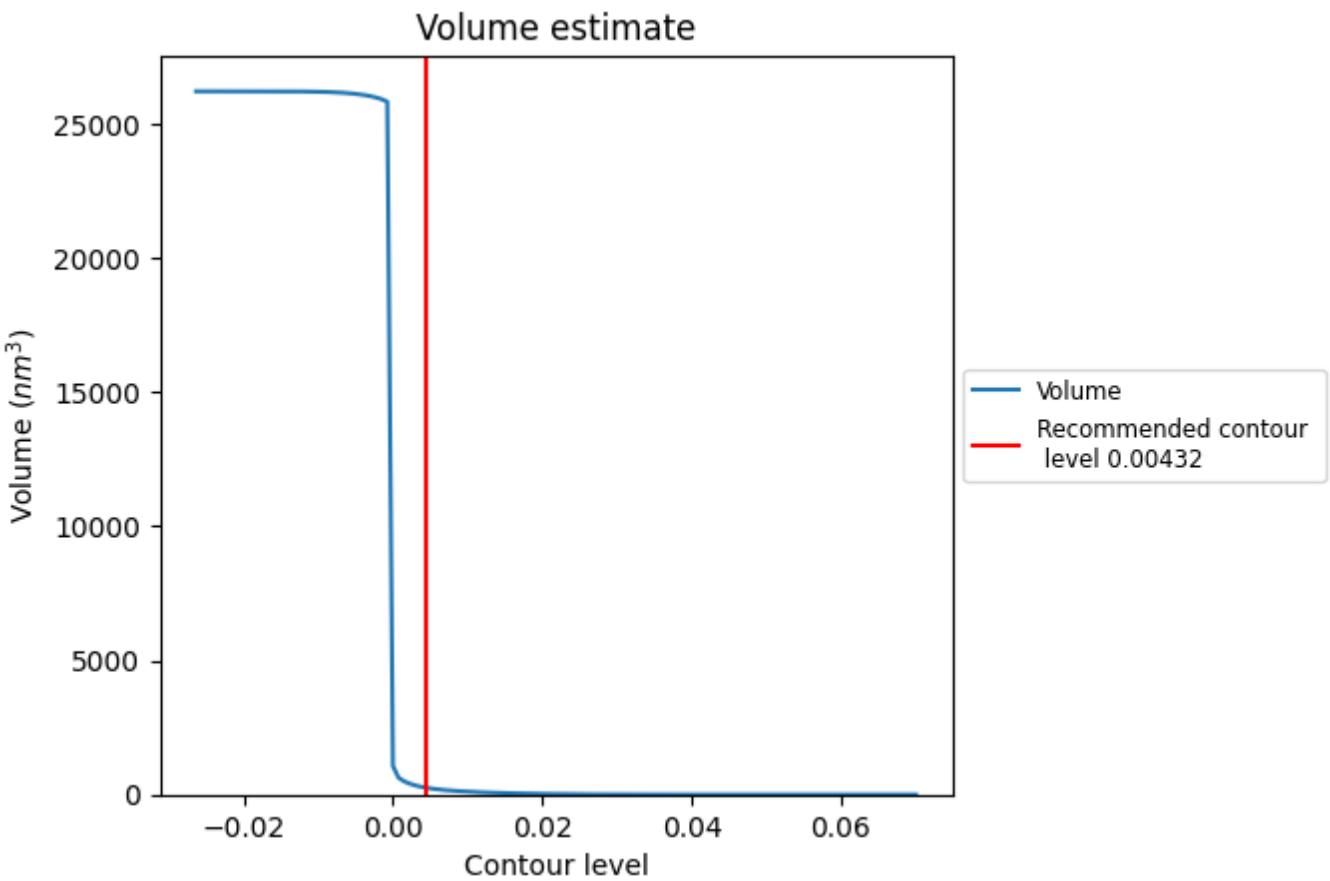
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

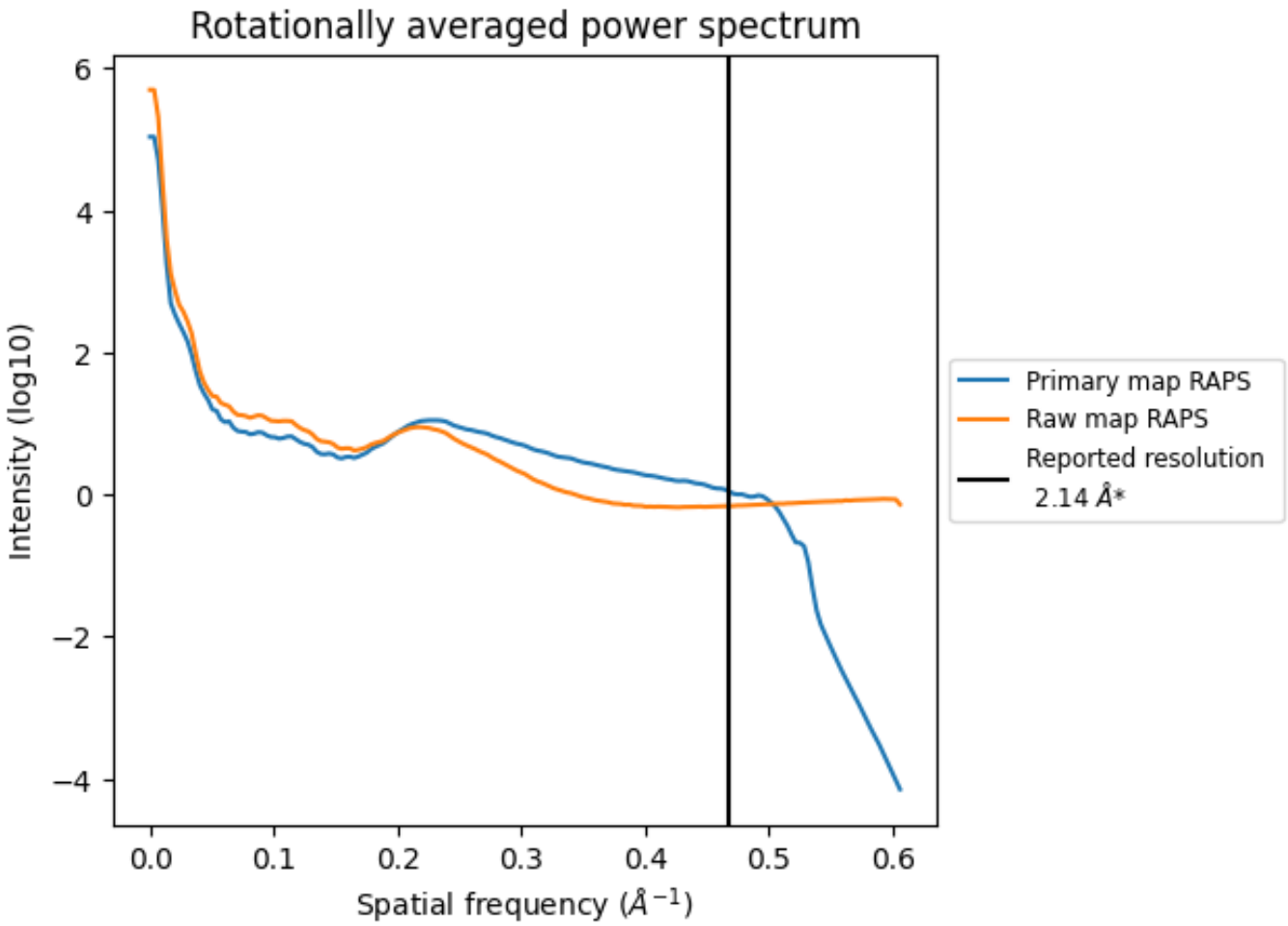
7.2 Volume estimate (i)



The volume at the recommended contour level is 262 nm^3; this corresponds to an approximate mass of 237 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)

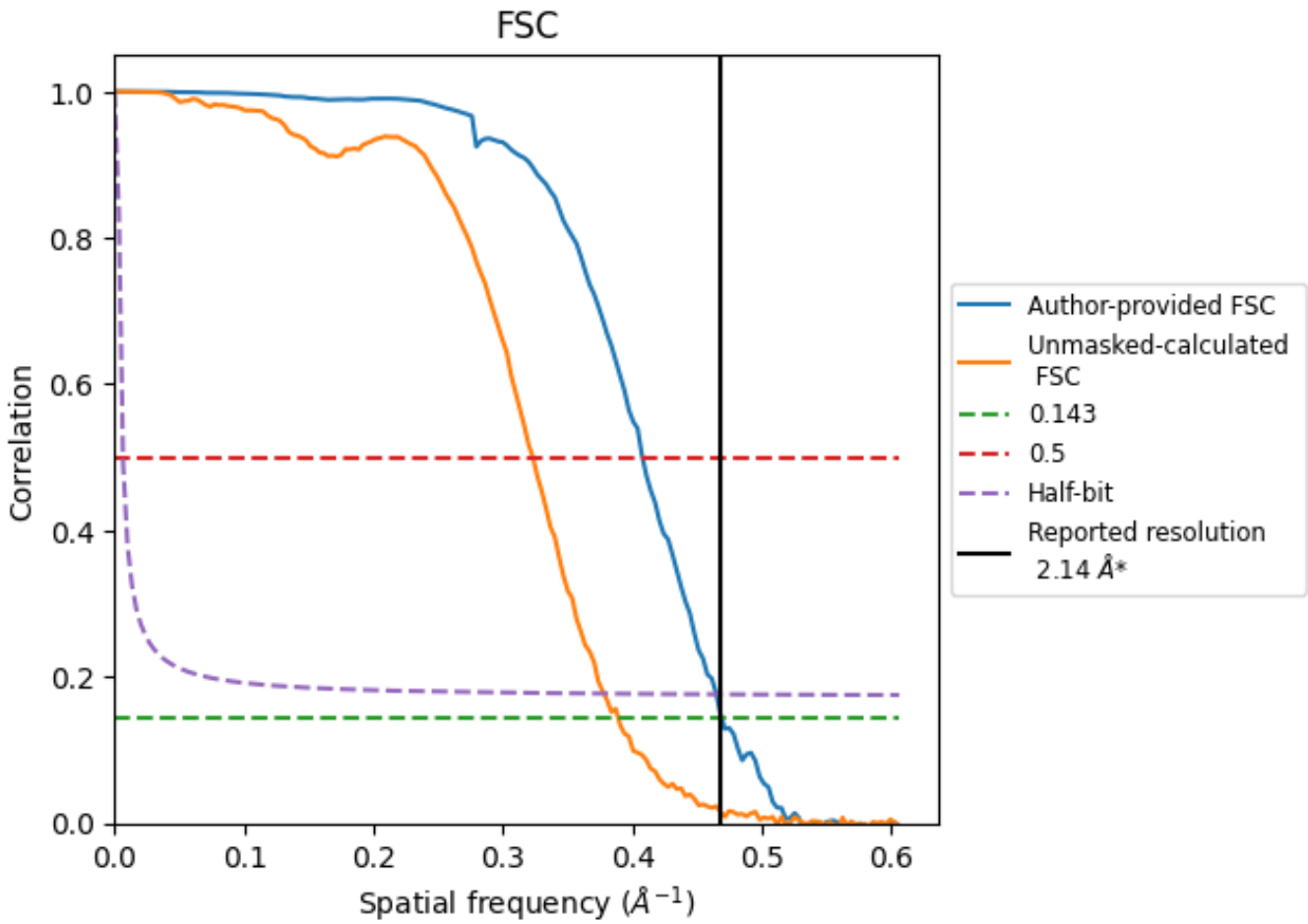


*Reported resolution corresponds to spatial frequency of 0.467 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.467 Å^{-1}

8.2 Resolution estimates (i)

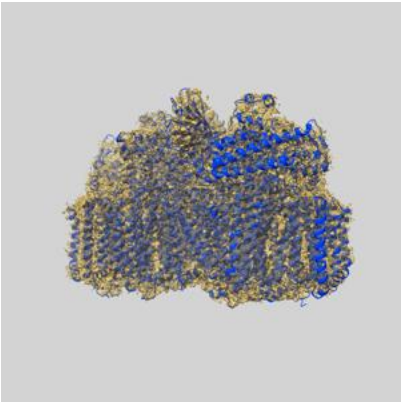
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.13	2.45	2.15
Unmasked-calculated*	2.57	3.09	2.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.57 differs from the reported value 2.14 by more than 10 %

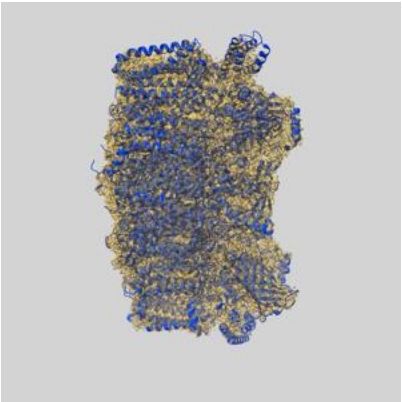
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-41460 and PDB model 8TOW. Per-residue inclusion information can be found in section 3 on page 32.

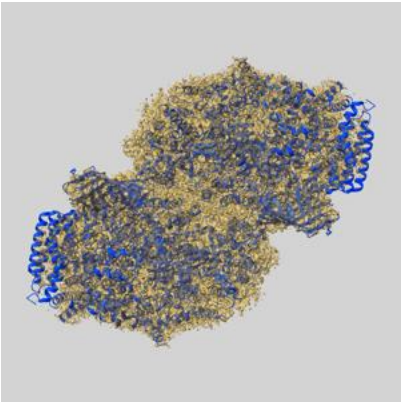
9.1 Map-model overlay (i)



X



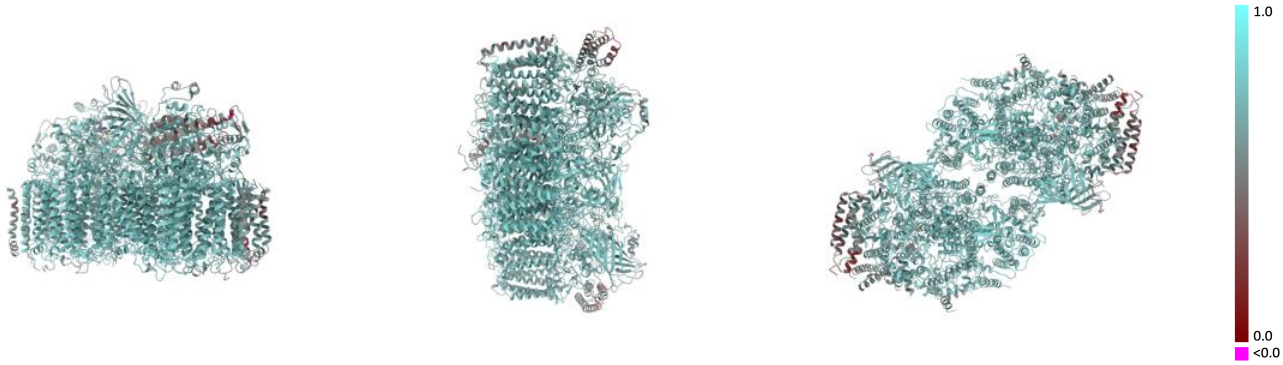
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00432 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.

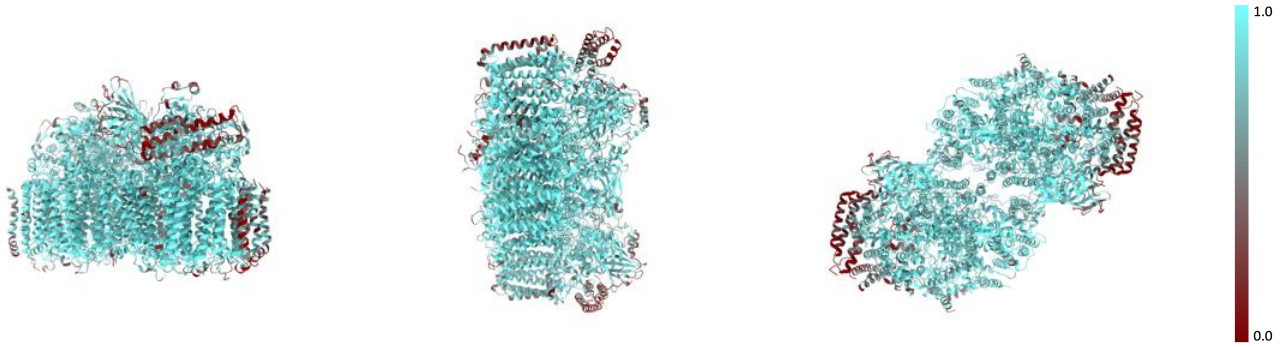
9.2 Q-score mapped to coordinate model (i)



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.

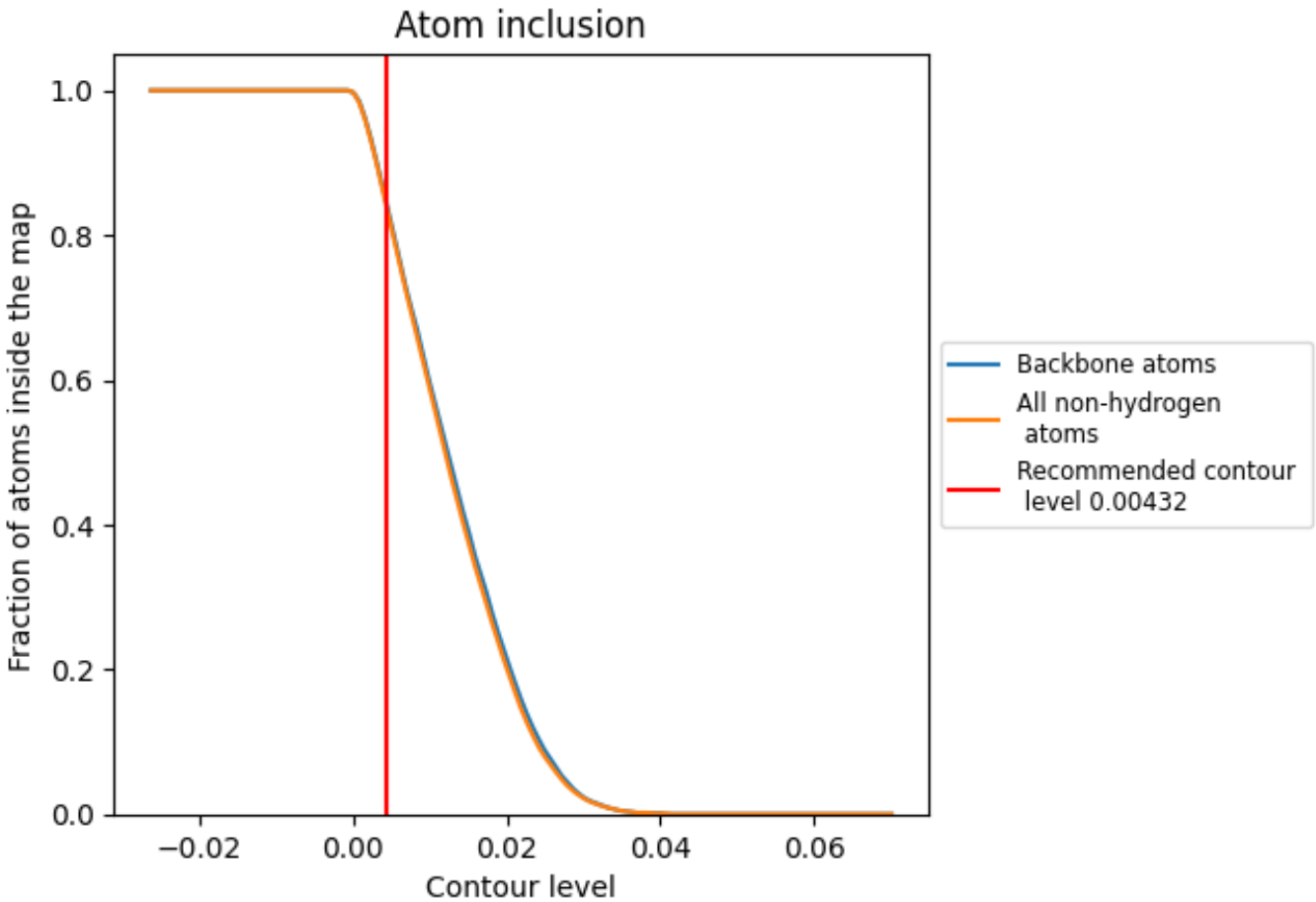
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00432).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00432) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8390	0.6860
A	0.9280	0.7330
B	0.9220	0.7210
C	0.8760	0.6950
D	0.9540	0.7430
E	0.8100	0.6680
F	0.7770	0.6340
H	0.8390	0.6850
I	0.6350	0.6560
J	0.7250	0.6350
K	0.7770	0.6040
L	0.9680	0.7420
M	0.8880	0.6880
O	0.7630	0.6520
Q	0.3080	0.4660
R	0.5280	0.5230
T	0.9040	0.7030
U	0.7290	0.6390
V	0.8060	0.6640
X	0.6730	0.6300
Y	0.6020	0.5660
Z	0.4320	0.5510
a	0.9270	0.7340
b	0.9220	0.7210
c	0.8770	0.6960
d	0.9540	0.7430
e	0.8090	0.6670
f	0.7800	0.6360
h	0.8360	0.6850
i	0.6370	0.6550
j	0.7280	0.6340
k	0.7800	0.6020
l	0.9640	0.7440
m	0.8850	0.6900
o	0.7610	0.6540

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Chain	Atom inclusion	Q-score
q	0.3070	0.4660
r	0.5280	0.5180
t	0.9040	0.7080
u	0.7290	0.6370
v	0.8080	0.6650
x	0.6780	0.6360
y	0.5900	0.5640
z	0.4320	0.5470