Full wwPDB EM Validation Report

Nov 29, 2022 – 05:53 AM JST

PDB ID	:	7VY2
EMDB ID	:	EMD-32192
Title	:	STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF RHODOBACTER SPHAEROIDES DIMER
Authors	:	Tani, K.; Kanno, R.; Kawamura, S.; Kikuchi, R.; Nagashima, K.V.P.; Hall, M.; Takahashi, A.; Yu, L.-J.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on	:	2021-11-13
Resolution	:	2.75 Å(reported)
Based on initial model	:	7F0L

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:

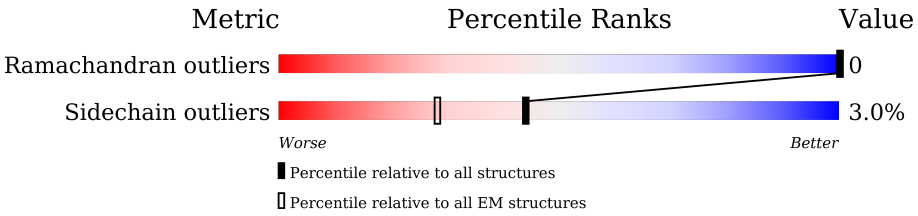
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.75 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	L	281	96% ·
1	l	281	98% ·
2	M	307	96% ·
2	m	307	98% ·
3	H	260	94% · 5%
3	h	260	93% · 5%
4	01	54	98% ·
4	03	54	94% 6%
4	05	54	6% 98% ·

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Mol	Chain	Length	Quality of chain
4	07	54	37% 93% 6%
4	1	54	94% 6%
4	3	54	96%
4	5	54	15% 98%
4	7	54	30% 94% 6%
4	A	54	81% 17%
4	D	54	96%
4	F	54	94% 6%
4	I	54	96%
4	K	54	98%
4	O	54	98%
4	Q	54	94% 6%
4	S	54	93% 7%
4	V	54	98%
4	Y	54	96%
4	a	54	76% 7% 17%
4	d	54	94% 6%
4	f	54	94% 6%
4	i	54	96%
4	k	54	98%
4	o	54	96%
4	q	54	98%
4	s	54	96%
4	v	54	98%
4	y	54	96%

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Mol	Chain	Length	Quality of chain
5	02	48	88% 12%
5	04	48	90% 10%
5	06	48	12% 83% 12%
5	08	48	19% 77% 21%
5	2	48	85% 12%
5	4	48	17% 88% 10%
5	6	48	31% 88% 12%
5	8	48	31% 79% 21%
5	B	48	92% 8%
5	E	48	81% 8% 10%
5	G	48	88% 6% 6%
5	J	48	88% 10%
5	N	48	90% 10%
5	P	48	83% 6% 10%
5	R	48	88% 10%
5	T	48	90% 10%
5	W	48	88% 10%
5	Z	48	88% 10%
5	b	48	88% 10%
5	e	48	85% 10%
5	g	48	92% 6%
5	j	48	88% 10%
5	n	48	85% 10%
5	p	48	88% 10%
5	r	48	85% 10%

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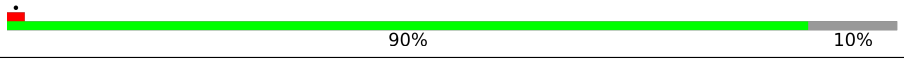
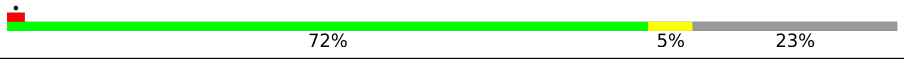
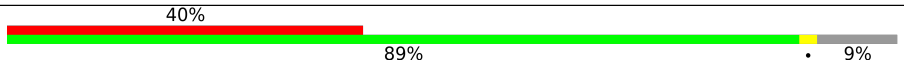
Mol	Chain	Length	Quality of chain
5	t	48	
5	w	48	
5	z	48	
6	X	81	
6	x	81	
7	U	53	
7	u	53	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 46292 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 Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2233	1508	355	362	8		
1	l	281	Total	C	N	O	S	0	0
			2233	1508	355	362	8		

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	306	Total	C	N	O	S	0	0
			2437	1627	398	401	11		
2	m	306	Total	C	N	O	S	0	0
			2437	1627	398	401	11		

- Molecule 3 is a protein called Photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	248	Total	C	N	O	S	0	0
			1884	1209	320	345	10		
3	h	248	Total	C	N	O	S	0	0
			1884	1209	320	345	10		

- Molecule 4 is a protein called Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	45	Total	C	N	O	S	0	0
			386	266	59	58	3		
4	D	54	Total	C	N	O	S	0	0
			455	309	73	70	3		
4	F	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	I	54	Total	C	N	O	S	0	0
			457	311	73	70	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	O	54	Total	C	N	O	S	0	0
			453	308	72	70	3		
4	Q	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	S	54	Total	C	N	O	S	0	0
			448	303	73	70	2		
4	V	54	Total	C	N	O	S	0	0
			451	308	70	70	3		
4	Y	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	1	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	3	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	5	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	7	51	Total	C	N	O	S	0	0
			415	281	68	64	2		
4	a	45	Total	C	N	O	S	0	0
			386	266	59	58	3		
4	d	54	Total	C	N	O	S	0	0
			455	309	73	70	3		
4	f	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	i	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	k	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	o	54	Total	C	N	O	S	0	0
			453	308	72	70	3		
4	q	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	s	54	Total	C	N	O	S	0	0
			454	309	73	70	2		
4	v	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	y	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	01	54	Total	C	N	O	S	0	0
			457	311	73	70	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	03	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	05	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	07	51	Total	C	N	O	S	0	0
			415	281	68	64	2		

- Molecule 5 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	G	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
5	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	N	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	P	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	R	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	T	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	W	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	Z	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	2	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
5	4	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	6	42	Total	C	N	O	S	0	0
			332	222	54	55	1		
5	8	38	Total	C	N	O	S	0	0
			296	202	49	44	1		
5	b	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	e	43	Total	C	N	O	S	0	0
			351	236	55	59	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
5	j	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	n	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	p	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	r	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	t	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	w	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	z	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	02	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
5	04	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	06	42	Total	C	N	O	S	0	0
			332	222	54	55	1		
5	08	38	Total	C	N	O	S	0	0
			296	202	49	44	1		

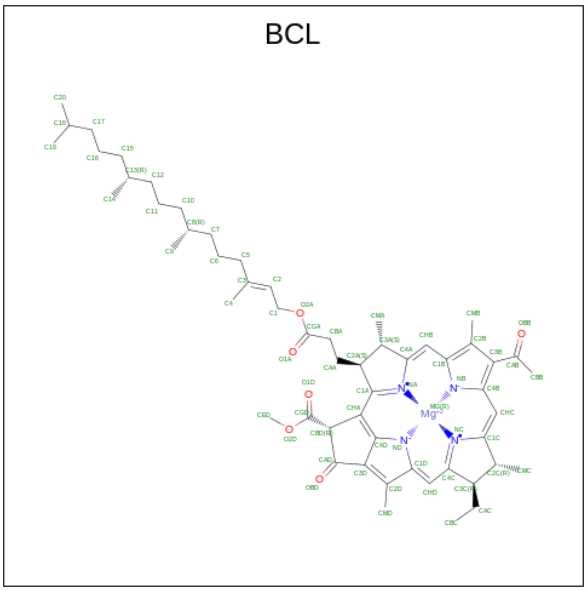
- Molecule 6 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	62	Total	C	N	O	S	0	0
			478	312	84	79	3		
6	x	60	Total	C	N	O	S	0	0
			456	301	78	74	3		

- Molecule 7 is a protein called protein-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	48	Total	C	N	O	S	0	0
			353	242	55	53	3		
7	u	13	Total	C	N	O		0	0
			71	45	13	13			

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
8	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
8	l	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	m	1	Total	C	Mg	N	O	0
			198	165	3	12	18	
8	m	1	Total	C	Mg	N	O	0
			198	165	3	12	18	

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Mol	Chain	Residues	Atoms					AltConf
8	m	1	Total	C	Mg	N	O	0
			198	165	3	12	18	
8	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
8	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	d	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	e	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	f	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	i	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	k	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	s	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	t	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	v	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	w	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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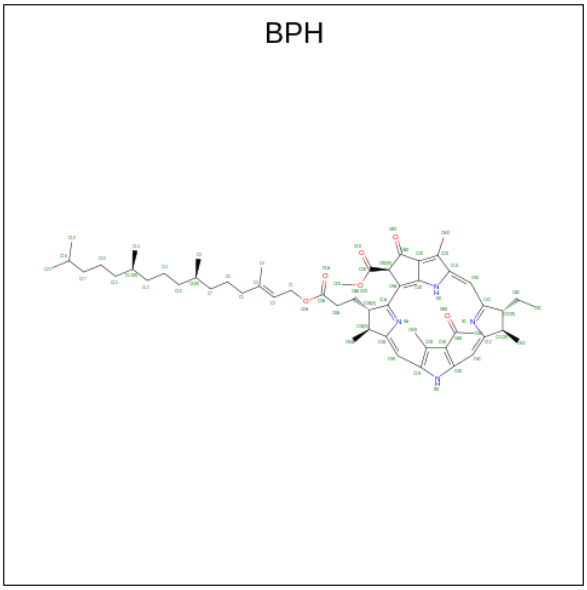
Mol	Chain	Residues	Atoms					AltConf
8	01	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	02	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	03	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	04	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	05	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	06	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	07	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	08	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			65	55	4	6	
9	l	1	Total	C	N	O	0
			65	55	4	6	

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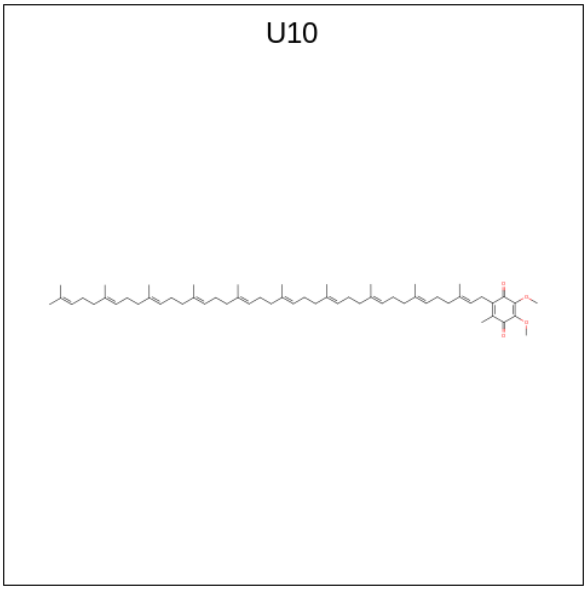
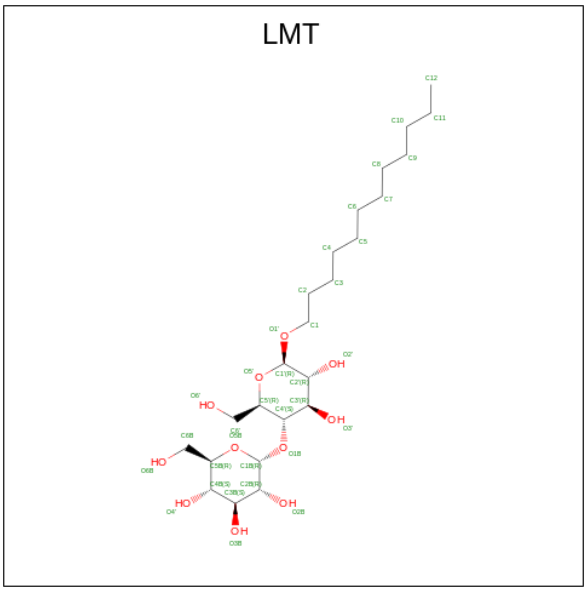
Mol	Chain	Residues	Atoms				AltConf
9	m	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 10 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
10	L	1	Total	C	O	0
			70	62	8	
10	L	1	Total	C	O	0
			70	62	8	
10	M	1	Total	C	O	0
			63	59	4	
10	D	1	Total	C	O	0
			32	28	4	
10	l	1	Total	C	O	0
			70	62	8	
10	l	1	Total	C	O	0
			70	62	8	
10	m	1	Total	C	O	0
			59	55	4	
10	d	1	Total	C	O	0
			30	26	4	

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



Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total	C	O	0
			53	32	21	
11	L	1	Total	C	O	0
			53	32	21	
11	M	1	Total	C	O	0
			115	80	35	
11	M	1	Total	C	O	0
			115	80	35	
11	M	1	Total	C	O	0
			115	80	35	
11	M	1	Total	C	O	0
			115	80	35	
11	H	1	Total	C	O	0
			35	24	11	
11	A	1	Total	C	O	0
			35	24	11	
11	I	1	Total	C	O	0
			35	24	11	
11	Q	1	Total	C	O	0
			24	18	6	
11	3	1	Total	C	O	0
			62	40	22	
11	3	1	Total	C	O	0
			62	40	22	
11	5	1	Total	C	O	0
			33	22	11	
11	U	1	Total	C	O	0
			102	69	33	

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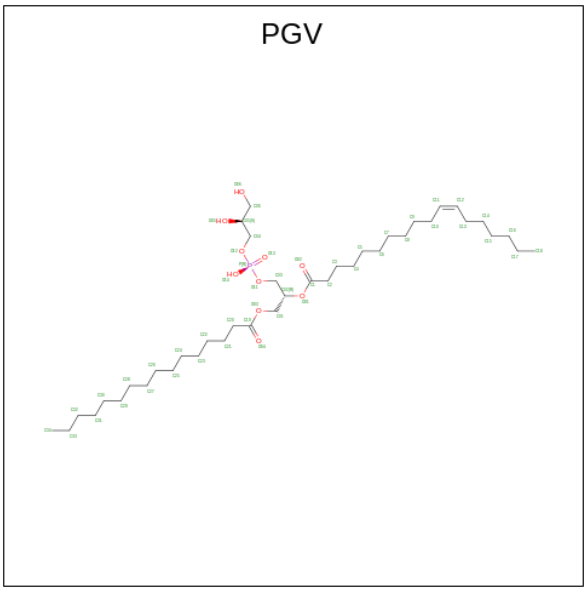
Mol	Chain	Residues	Atoms	AltConf
11	U	1	Total C O 102 69 33	0
11	U	1	Total C O 102 69 33	0
11	m	1	Total C O 68 46 22	0
11	m	1	Total C O 68 46 22	0
11	h	1	Total C O 62 44 18	0
11	h	1	Total C O 62 44 18	0
11	i	1	Total C O 61 40 21	0
11	i	1	Total C O 61 40 21	0
11	q	1	Total C O 24 18 6	0
11	s	1	Total C O 55 38 17	0
11	s	1	Total C O 55 38 17	0
11	03	1	Total C O 62 40 22	0
11	03	1	Total C O 62 40 22	0

- Molecule 12 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total 162	C 118	O 40	P 4	0
12	L	1	Total 162	C 118	O 40	P 4	0
12	L	1	Total 162	C 118	O 40	P 4	0
12	L	1	Total 162	C 118	O 40	P 4	0
12	M	1	Total 38	C 27	O 10	P 1	0
12	H	1	Total 113	C 82	O 28	P 3	0
12	H	1	Total 113	C 82	O 28	P 3	0
12	H	1	Total 113	C 82	O 28	P 3	0
12	F	1	Total 41	C 30	O 10	P 1	0
12	K	1	Total 41	C 34	O 6	P 1	0
12	Q	1	Total 29	C 18	O 10	P 1	0
12	1	1	Total 43	C 32	O 10	P 1	0
12	l	1	Total 144	C 100	O 40	P 4	0
12	l	1	Total 144	C 100	O 40	P 4	0

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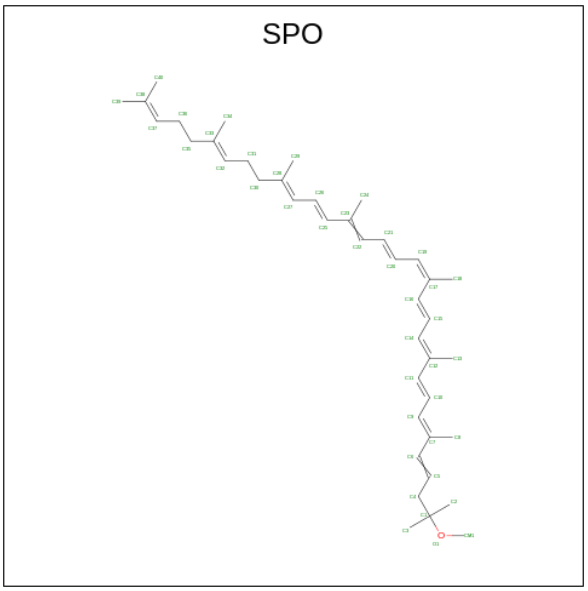
Mol	Chain	Residues	Atoms				AltConf
12	l	1	Total	C	O	P	0
			144	100	40	4	
12	l	1	Total	C	O	P	0
			144	100	40	4	
12	m	1	Total	C	O	P	0
			77	55	20	2	
12	m	1	Total	C	O	P	0
			77	55	20	2	
12	h	1	Total	C	O	P	0
			73	53	18	2	
12	h	1	Total	C	O	P	0
			73	53	18	2	
12	f	1	Total	C	O	P	0
			87	65	20	2	
12	f	1	Total	C	O	P	0
			87	65	20	2	
12	k	1	Total	C	O	P	0
			41	34	6	1	
12	q	1	Total	C	O	P	0
			34	23	10	1	
12	y	1	Total	C	O	P	0
			43	32	10	1	
12	x	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
13	M	1	Total	Fe	0
			1	1	
13	m	1	Total	Fe	0
			1	1	

- Molecule 14 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			42	41	1	
14	A	1	Total	C	O	0
			42	41	1	
14	B	1	Total	C	O	0
			84	82	2	
14	B	1	Total	C	O	0
			84	82	2	
14	E	1	Total	C	O	0
			42	41	1	
14	G	1	Total	C	O	0
			84	82	2	
14	G	1	Total	C	O	0
			84	82	2	
14	I	1	Total	C	O	0
			42	41	1	
14	J	1	Total	C	O	0
			42	41	1	
14	K	1	Total	C	O	0
			42	41	1	
14	N	1	Total	C	O	0
			42	41	1	
14	O	1	Total	C	O	0
			42	41	1	
14	P	1	Total	C	O	0
			42	41	1	
14	Q	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
14	R	1	Total	C	O	0
			42	41	1	
14	S	1	Total	C	O	0
			84	82	2	
14	S	1	Total	C	O	0
			84	82	2	
14	T	1	Total	C	O	0
			42	41	1	
14	V	1	Total	C	O	0
			42	41	1	
14	Y	1	Total	C	O	0
			42	41	1	
14	2	1	Total	C	O	0
			126	123	3	
14	2	1	Total	C	O	0
			126	123	3	
14	2	1	Total	C	O	0
			126	123	3	
14	3	1	Total	C	O	0
			42	41	1	
14	4	1	Total	C	O	0
			42	41	1	
14	5	1	Total	C	O	0
			42	41	1	
14	6	1	Total	C	O	0
			42	41	1	
14	m	1	Total	C	O	0
			42	41	1	
14	a	1	Total	C	O	0
			42	41	1	
14	e	1	Total	C	O	0
			42	41	1	
14	f	1	Total	C	O	0
			84	82	2	
14	f	1	Total	C	O	0
			84	82	2	
14	g	1	Total	C	O	0
			84	82	2	
14	g	1	Total	C	O	0
			84	82	2	
14	j	1	Total	C	O	0
			42	41	1	

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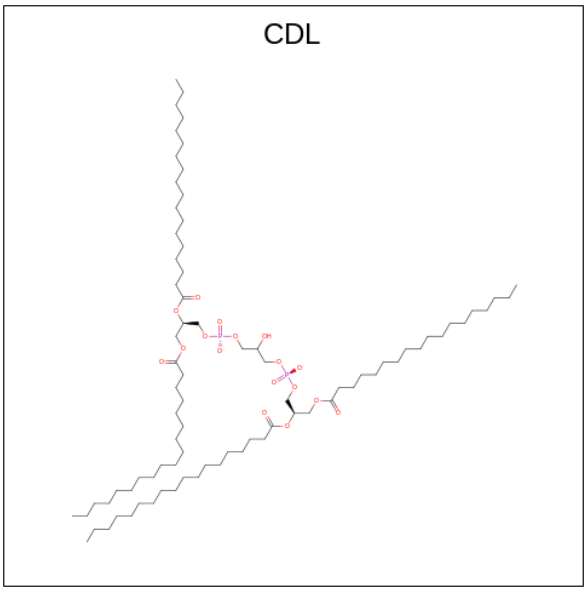
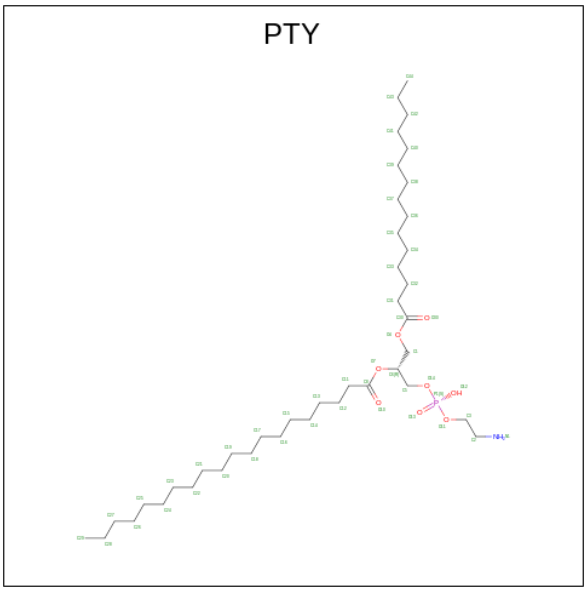
Mol	Chain	Residues	Atoms			AltConf
14	k	1	Total	C	O	0
			42	41	1	
14	n	1	Total	C	O	0
			84	82	2	
14	n	1	Total	C	O	0
			84	82	2	
14	p	1	Total	C	O	0
			42	41	1	
14	q	1	Total	C	O	0
			42	41	1	
14	r	1	Total	C	O	0
			84	82	2	
14	r	1	Total	C	O	0
			84	82	2	
14	s	1	Total	C	O	0
			84	82	2	
14	s	1	Total	C	O	0
			84	82	2	
14	v	1	Total	C	O	0
			42	41	1	
14	w	1	Total	C	O	0
			42	41	1	
14	y	1	Total	C	O	0
			42	41	1	
14	z	1	Total	C	O	0
			42	41	1	
14	01	1	Total	C	O	0
			84	82	2	
14	01	1	Total	C	O	0
			84	82	2	
14	02	1	Total	C	O	0
			42	41	1	
14	05	1	Total	C	O	0
			84	82	2	
14	05	1	Total	C	O	0
			84	82	2	
14	08	1	Total	C	O	0
			42	41	1	

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



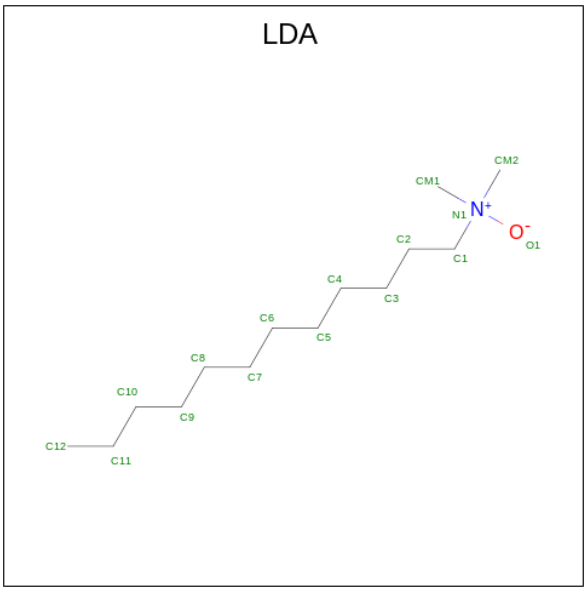
Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			79	60	17	2	
15	K	1	Total	C	O	P	0
			61	42	17	2	
15	Y	1	Total	C	O	P	0
			43	26	15	2	
15	X	1	Total	C	O	P	0
			151	98	47	6	
15	X	1	Total	C	O	P	0
			151	98	47	6	
15	X	1	Total	C	O	P	0
			151	98	47	6	
15	m	1	Total	C	O	P	0
			124	88	32	4	
15	m	1	Total	C	O	P	0
			124	88	32	4	
15	h	1	Total	C	O	P	0
			61	42	17	2	
15	y	1	Total	C	O	P	0
			48	30	16	2	
15	x	1	Total	C	O	P	0
			26	13	11	2	

- Molecule 16 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
16	H	1	Total	C	N	O	P	0
			37	27	1	8	1	
16	F	1	Total	C	N	O	P	0
			41	31	1	8	1	
16	h	1	Total	C	N	O	P	0
			38	28	1	8	1	
16	f	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 17 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



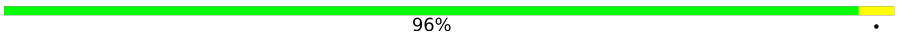
Mol	Chain	Residues	Atoms				AltConf
17	y	1	Total	C	N	O	0
			12	10	1	1	

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.

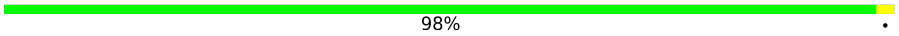
• Molecule 1: Photosynthetic reaction center L subunit

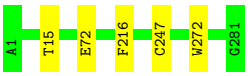
Chain L:



• Molecule 1: Photosynthetic reaction center L subunit

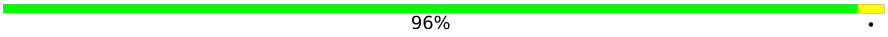
Chain l:

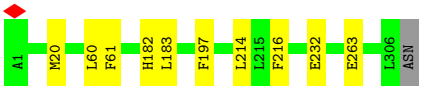




• Molecule 2: Reaction center protein M chain

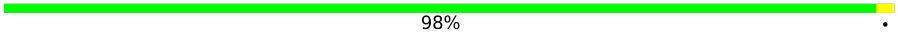
Chain M:

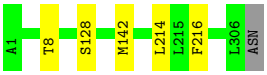




• Molecule 2: Reaction center protein M chain

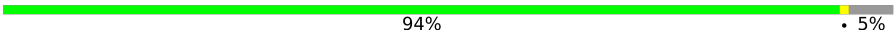
Chain m:

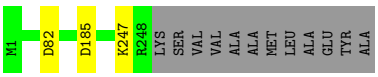




• Molecule 3: Photosynthetic reaction center subunit H

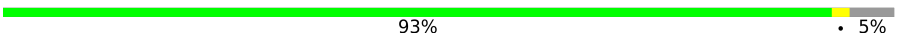
Chain H:

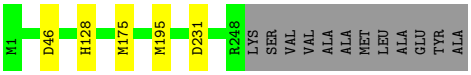




• Molecule 3: Photosynthetic reaction center subunit H

Chain h:



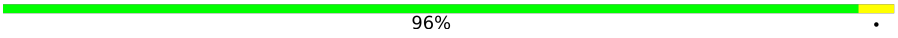


• Molecule 4: Antenna pigment protein alpha chain

Chain A:

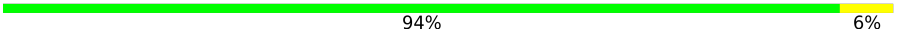
• Molecule 4: Antenna pigment protein alpha chain

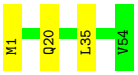
Chain D:



• Molecule 4: Antenna pigment protein alpha chain

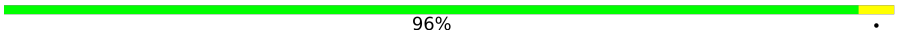
Chain F:





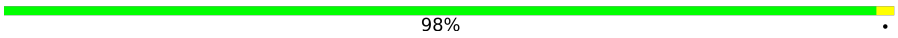
• Molecule 4: Antenna pigment protein alpha chain

Chain I:



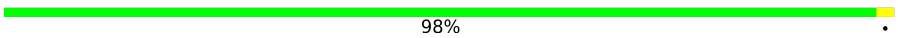
• Molecule 4: Antenna pigment protein alpha chain

Chain K:



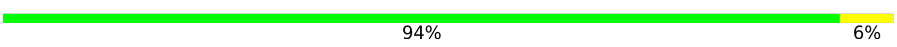
• Molecule 4: Antenna pigment protein alpha chain

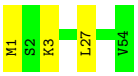
Chain O:



• Molecule 4: Antenna pigment protein alpha chain

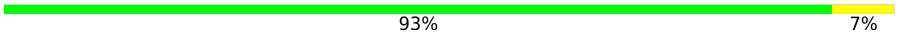
Chain Q:

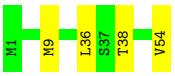




• Molecule 4: Antenna pigment protein alpha chain

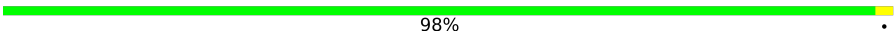
Chain S:





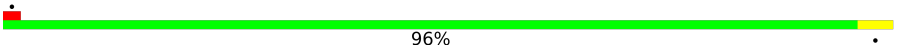
• Molecule 4: Antenna pigment protein alpha chain

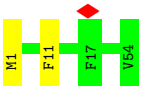
Chain V:



• Molecule 4: Antenna pigment protein alpha chain

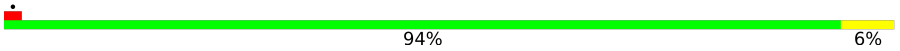
Chain Y:

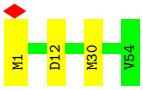




• Molecule 4: Antenna pigment protein alpha chain

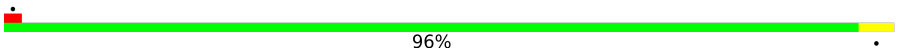
Chain 1:

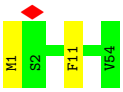




• Molecule 4: Antenna pigment protein alpha chain

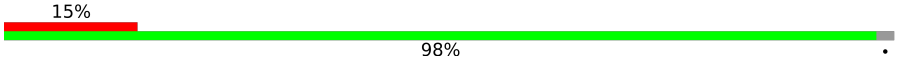
Chain 3:

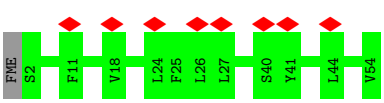




• Molecule 4: Antenna pigment protein alpha chain

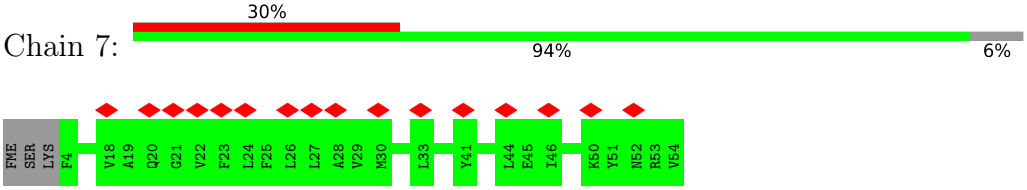
Chain 5:





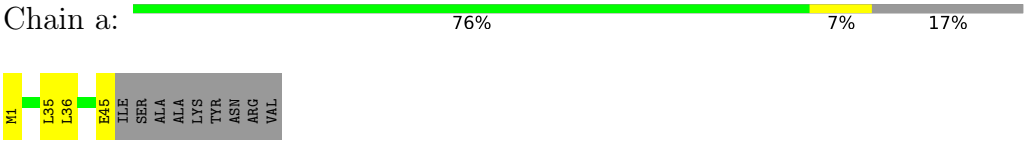
• Molecule 4: Antenna pigment protein alpha chain

Chain 7:



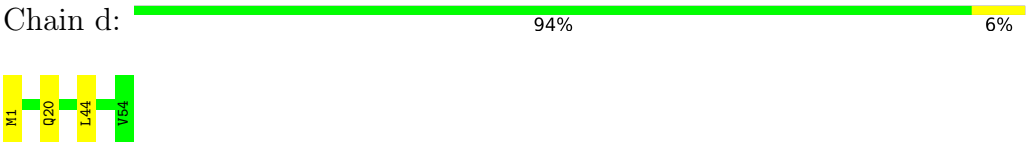
• Molecule 4: Antenna pigment protein alpha chain

Chain a:



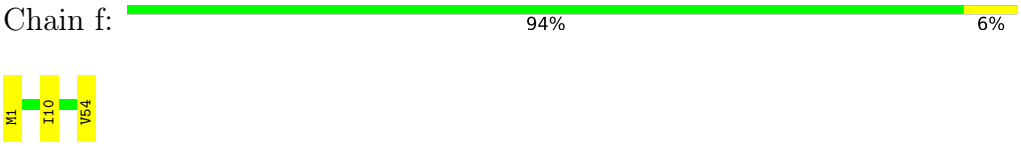
• Molecule 4: Antenna pigment protein alpha chain

Chain d:



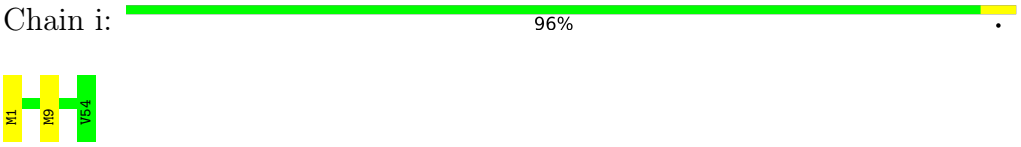
• Molecule 4: Antenna pigment protein alpha chain

Chain f:



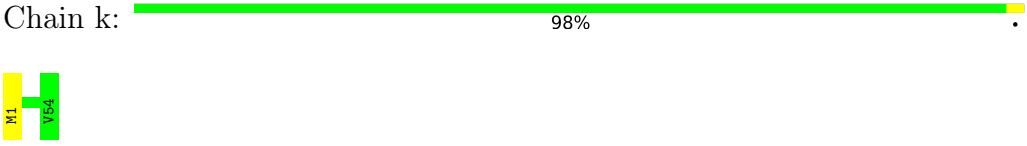
• Molecule 4: Antenna pigment protein alpha chain

Chain i:



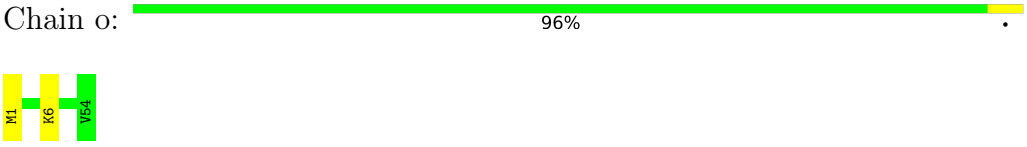
• Molecule 4: Antenna pigment protein alpha chain

Chain k:



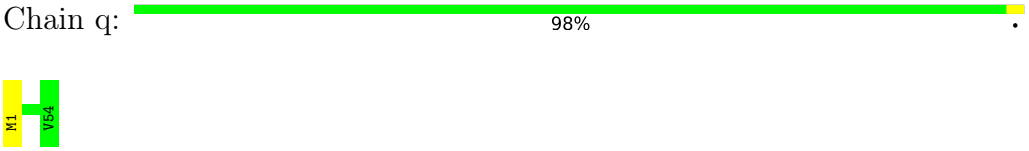
• Molecule 4: Antenna pigment protein alpha chain

Chain o:



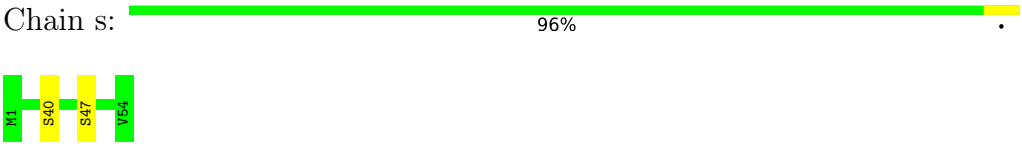
• Molecule 4: Antenna pigment protein alpha chain

Chain q:



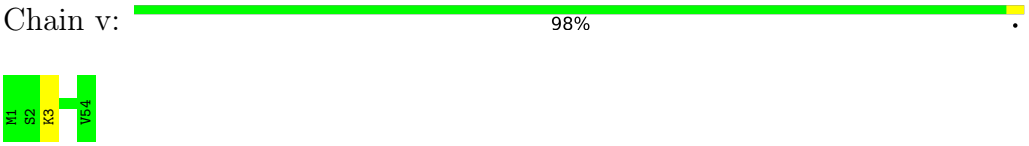
• Molecule 4: Antenna pigment protein alpha chain

Chain s:



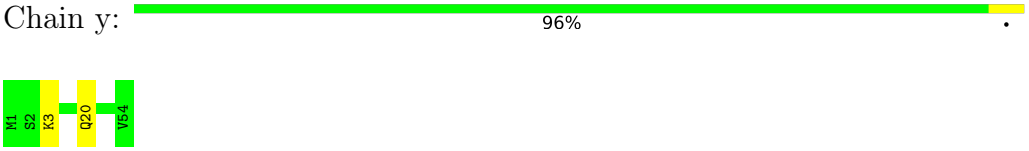
• Molecule 4: Antenna pigment protein alpha chain

Chain v:



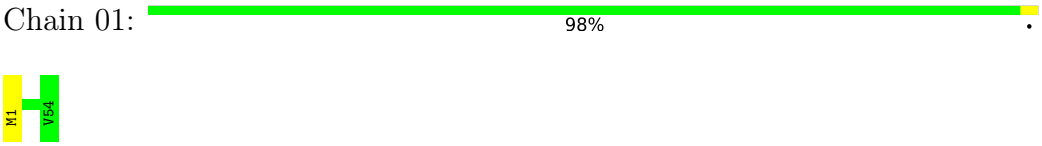
• Molecule 4: Antenna pigment protein alpha chain

Chain y:



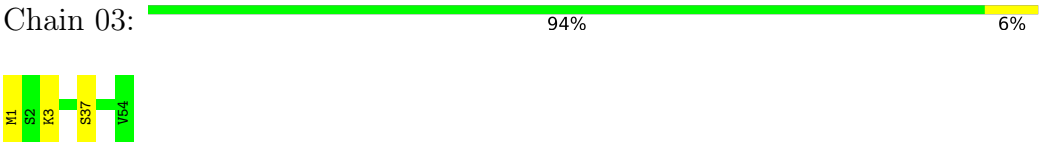
• Molecule 4: Antenna pigment protein alpha chain

Chain 01:



• Molecule 4: Antenna pigment protein alpha chain

Chain 03:



• Molecule 4: Antenna pigment protein alpha chain

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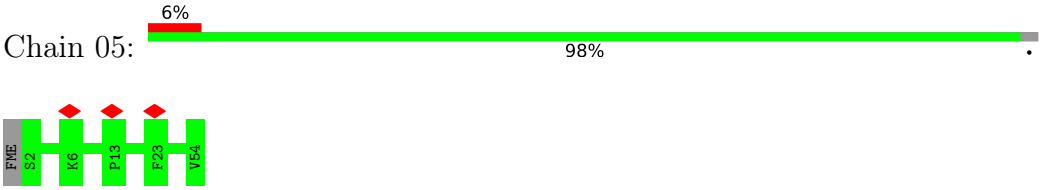
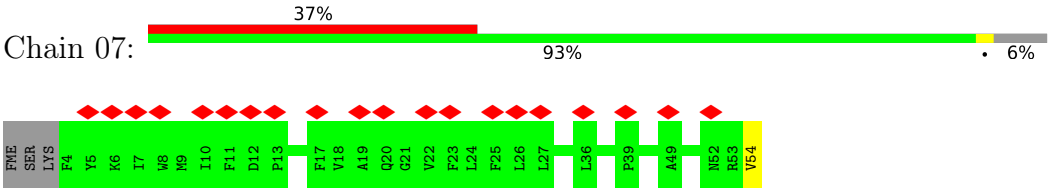


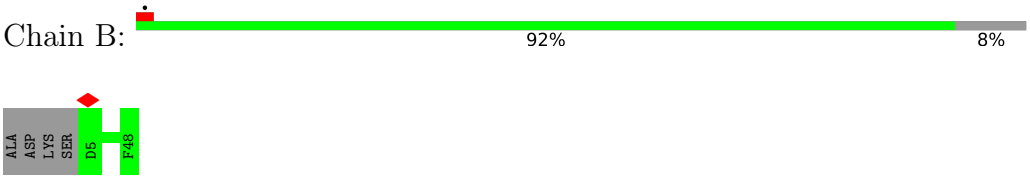
• Molecule 4: Antenna pigment protein alpha chain

Chain 07:



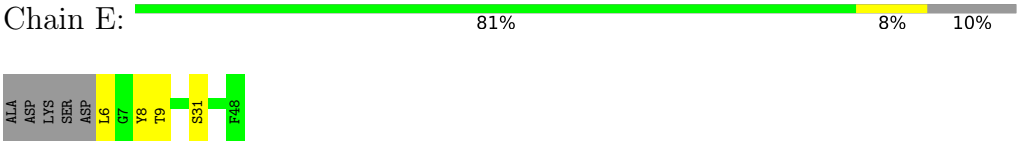
• Molecule 5: Antenna pigment protein beta chain

Chain B:



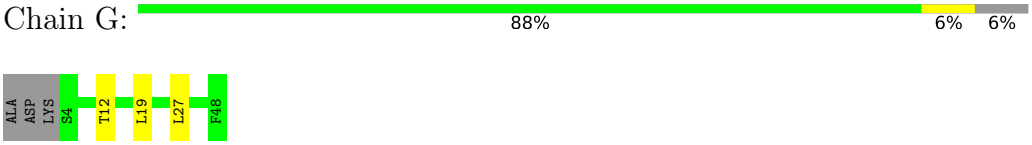
• Molecule 5: Antenna pigment protein beta chain

Chain E:



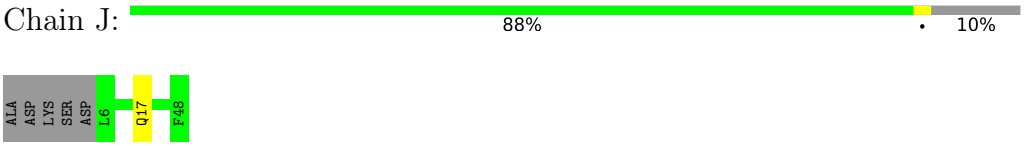
• Molecule 5: Antenna pigment protein beta chain

Chain G:



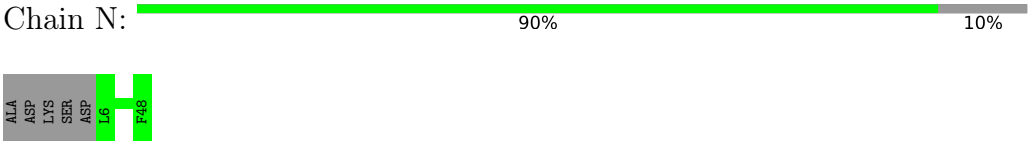
• Molecule 5: Antenna pigment protein beta chain

Chain J:



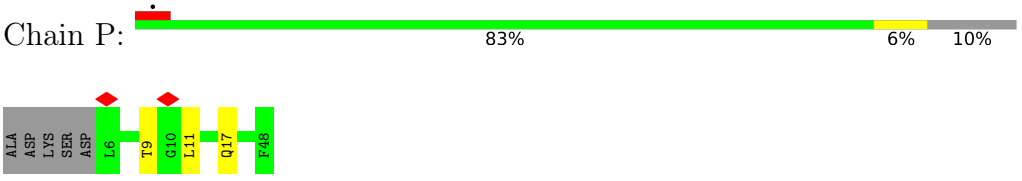
• Molecule 5: Antenna pigment protein beta chain

Chain N:



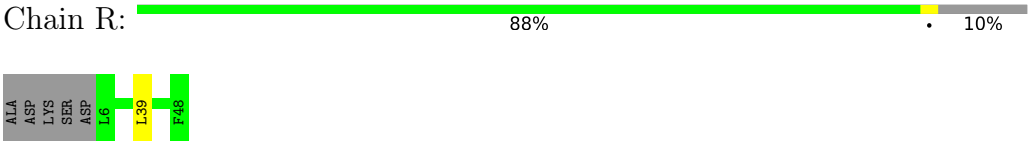
• Molecule 5: Antenna pigment protein beta chain

Chain P:



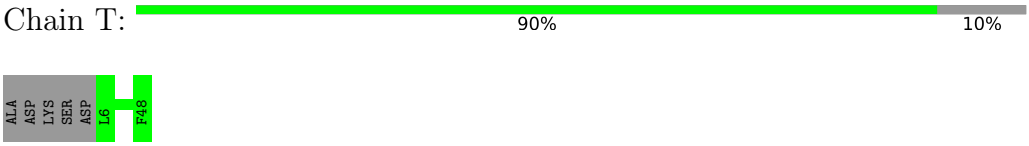
• Molecule 5: Antenna pigment protein beta chain

Chain R:



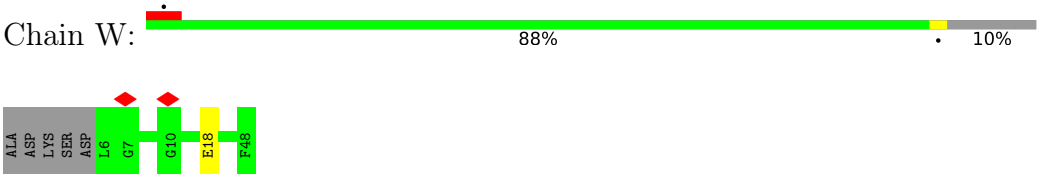
• Molecule 5: Antenna pigment protein beta chain

Chain T:



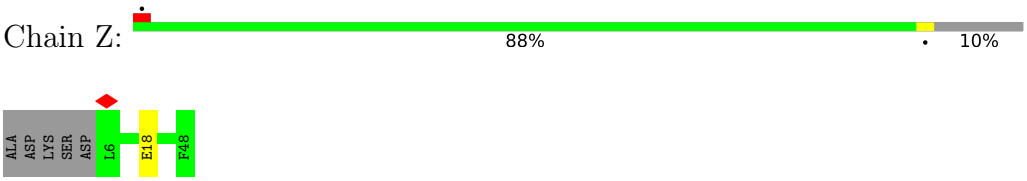
• Molecule 5: Antenna pigment protein beta chain

Chain W:



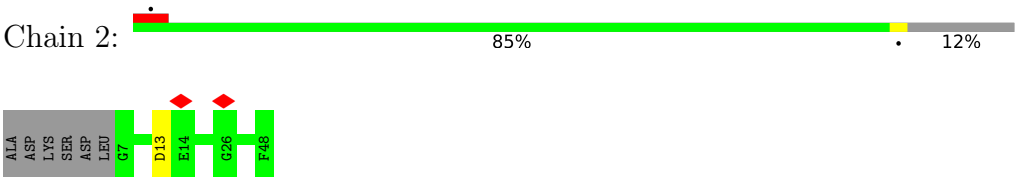
• Molecule 5: Antenna pigment protein beta chain

Chain Z:



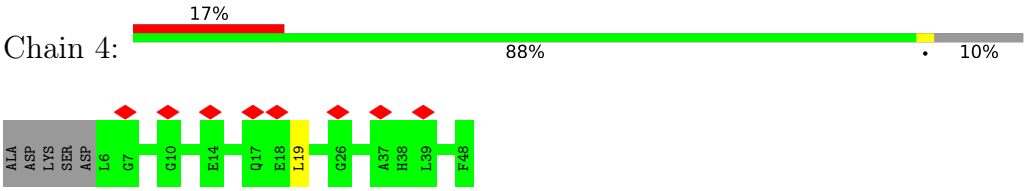
• Molecule 5: Antenna pigment protein beta chain

Chain 2:



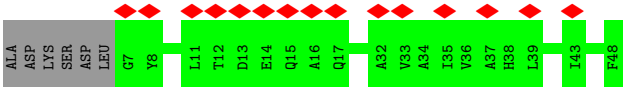
• Molecule 5: Antenna pigment protein beta chain

Chain 4:

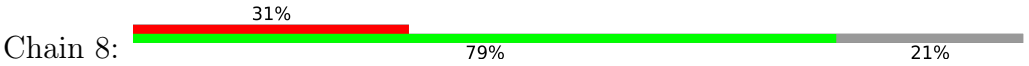


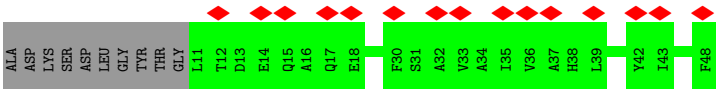
• Molecule 5: Antenna pigment protein beta chain

Chain 6:

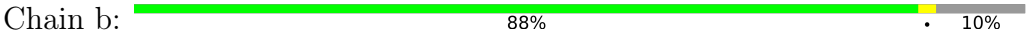


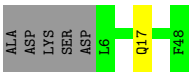
• Molecule 5: Antenna pigment protein beta chain



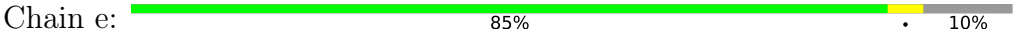


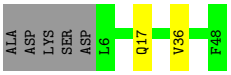
• Molecule 5: Antenna pigment protein beta chain



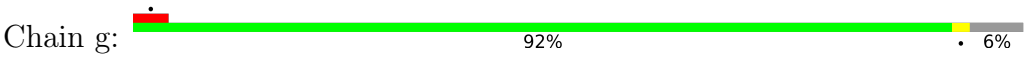


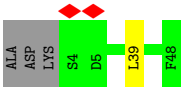
• Molecule 5: Antenna pigment protein beta chain



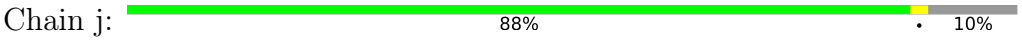


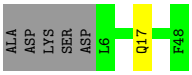
• Molecule 5: Antenna pigment protein beta chain



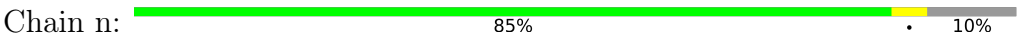


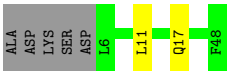
• Molecule 5: Antenna pigment protein beta chain



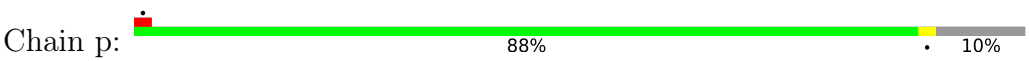


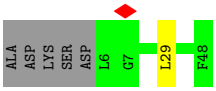
• Molecule 5: Antenna pigment protein beta chain





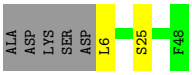
• Molecule 5: Antenna pigment protein beta chain





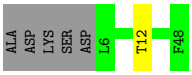
• Molecule 5: Antenna pigment protein beta chain

Chain r:



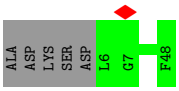
• Molecule 5: Antenna pigment protein beta chain

Chain t:



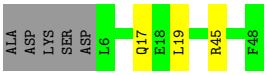
• Molecule 5: Antenna pigment protein beta chain

Chain w:



• Molecule 5: Antenna pigment protein beta chain

Chain z:

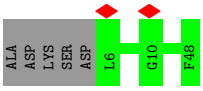


• Molecule 5: Antenna pigment protein beta chain

Chain 02:

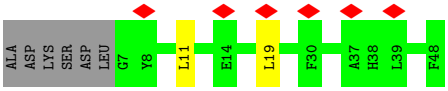
• Molecule 5: Antenna pigment protein beta chain

Chain 04:



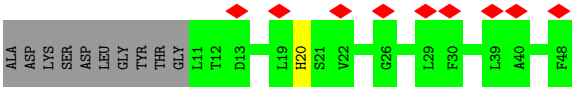
• Molecule 5: Antenna pigment protein beta chain

Chain 06:



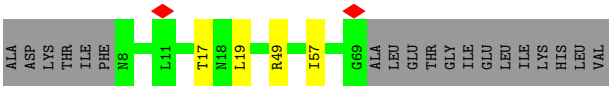
• Molecule 5: Antenna pigment protein beta chain

Chain 08:



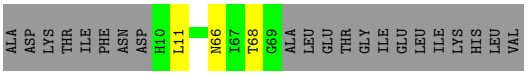
• Molecule 6: PufX

Chain X:



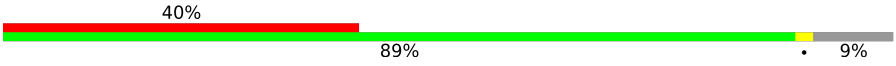
• Molecule 6: PufX

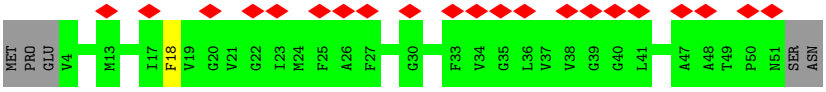
Chain x:



• Molecule 7: protein-U

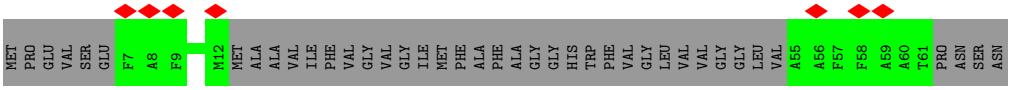
Chain U:





• Molecule 7: protein-U

Chain u:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124916	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	39.517	Depositor
Minimum map value	-18.203	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.2	Depositor
Map size (Å)	369.0, 369.0, 369.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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: PTY, LMT, FME, LDA, BPH, FE, PGV, CDL, U10, BCL, SPO

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	L	0.37	0/2321	0.47	0/3177
1	l	0.38	0/2321	0.46	0/3177
2	M	0.36	0/2530	0.48	0/3455
2	m	0.40	0/2530	0.47	0/3455
3	H	0.32	0/1934	0.49	0/2632
3	h	0.34	0/1934	0.50	0/2632
4	01	0.31	0/461	0.44	0/625
4	03	0.28	0/461	0.45	0/625
4	05	0.27	0/461	0.43	0/625
4	07	0.25	0/427	0.43	0/582
4	1	0.28	0/461	0.44	0/625
4	3	0.27	0/461	0.43	0/625
4	5	0.26	0/461	0.41	0/625
4	7	0.24	0/427	0.41	0/582
4	A	0.33	0/389	0.46	0/528
4	D	0.35	0/459	0.48	0/622
4	F	0.33	0/461	0.46	0/625
4	I	0.32	0/461	0.45	0/625
4	K	0.30	0/461	0.43	0/625
4	O	0.29	0/457	0.44	0/621
4	Q	0.29	0/461	0.44	0/625
4	S	0.29	0/454	0.44	0/616
4	V	0.29	0/455	0.44	0/618
4	Y	0.28	0/461	0.45	0/625
4	a	0.33	0/389	0.48	0/528
4	d	0.35	0/459	0.45	0/622
4	f	0.34	0/461	0.46	0/625
4	i	0.34	0/461	0.45	0/625
4	k	0.32	0/461	0.43	0/625
4	o	0.32	0/457	0.44	0/621
4	q	0.31	0/461	0.46	0/625
4	s	0.32	0/461	0.44	0/625

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
4	v	0.32	0/461	0.44	0/625
4	y	0.32	0/461	0.43	0/625
5	02	0.29	0/356	0.39	0/488
5	04	0.27	0/364	0.42	0/499
5	06	0.24	0/344	0.42	0/472
5	08	0.25	0/308	0.37	0/424
5	2	0.27	0/356	0.41	0/488
5	4	0.28	0/364	0.47	0/499
5	6	0.25	0/344	0.38	0/472
5	8	0.24	0/308	0.36	0/424
5	B	0.30	0/372	0.39	0/510
5	E	0.29	0/364	0.47	0/499
5	G	0.30	0/378	0.40	0/518
5	J	0.31	0/364	0.42	0/499
5	N	0.28	0/364	0.42	0/499
5	P	0.28	0/364	0.44	0/499
5	R	0.28	0/360	0.41	0/494
5	T	0.27	0/364	0.41	0/499
5	W	0.27	0/360	0.42	0/494
5	Z	0.26	0/364	0.40	0/499
5	b	0.30	0/364	0.42	0/499
5	e	0.33	0/364	0.43	0/499
5	g	0.31	0/378	0.41	0/518
5	j	0.33	0/364	0.43	0/499
5	n	0.28	0/364	0.41	0/499
5	p	0.29	0/364	0.41	0/499
5	r	0.29	0/360	0.41	0/494
5	t	0.28	0/364	0.42	0/499
5	w	0.29	0/360	0.44	0/494
5	z	0.31	0/364	0.44	0/499
6	X	0.28	0/492	0.49	0/669
6	x	0.28	0/470	0.48	0/640
7	U	0.28	0/364	0.40	0/493
7	u	0.25	0/70	0.33	0/94
All	All	0.32	0/37681	0.45	0/51389

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	L	279/281 (99%)	270 (97%)	9 (3%)	0	100	100
1	l	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
2	M	304/307 (99%)	289 (95%)	15 (5%)	0	100	100
2	m	304/307 (99%)	292 (96%)	12 (4%)	0	100	100
3	H	246/260 (95%)	232 (94%)	14 (6%)	0	100	100
3	h	246/260 (95%)	236 (96%)	10 (4%)	0	100	100
4	01	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	03	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	05	51/54 (94%)	51 (100%)	0	0	100	100
4	07	49/54 (91%)	48 (98%)	1 (2%)	0	100	100
4	1	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	3	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	5	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
4	7	49/54 (91%)	49 (100%)	0	0	100	100
4	A	43/54 (80%)	41 (95%)	2 (5%)	0	100	100
4	D	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	F	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	I	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	K	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
4	O	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	Q	52/54 (96%)	50 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S	52/54 (96%)	52 (100%)	0	0	100	100
4	V	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	Y	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	a	43/54 (80%)	41 (95%)	2 (5%)	0	100	100
4	d	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	f	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	i	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	k	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	o	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	q	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	s	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	v	52/54 (96%)	52 (100%)	0	0	100	100
4	y	52/54 (96%)	52 (100%)	0	0	100	100
5	02	40/48 (83%)	39 (98%)	1 (2%)	0	100	100
5	04	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
5	06	40/48 (83%)	39 (98%)	1 (2%)	0	100	100
5	08	36/48 (75%)	36 (100%)	0	0	100	100
5	2	40/48 (83%)	40 (100%)	0	0	100	100
5	4	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
5	6	40/48 (83%)	40 (100%)	0	0	100	100
5	8	36/48 (75%)	36 (100%)	0	0	100	100
5	B	42/48 (88%)	42 (100%)	0	0	100	100
5	E	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
5	G	43/48 (90%)	41 (95%)	2 (5%)	0	100	100
5	J	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
5	N	41/48 (85%)	41 (100%)	0	0	100	100
5	P	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
5	R	41/48 (85%)	41 (100%)	0	0	100	100
5	T	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
5	W	41/48 (85%)	41 (100%)	0	0	100	100
5	Z	41/48 (85%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	b	41/48 (85%)	41 (100%)	0	0	100	100
5	e	41/48 (85%)	41 (100%)	0	0	100	100
5	g	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
5	j	41/48 (85%)	41 (100%)	0	0	100	100
5	n	41/48 (85%)	41 (100%)	0	0	100	100
5	p	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
5	r	41/48 (85%)	41 (100%)	0	0	100	100
5	t	41/48 (85%)	41 (100%)	0	0	100	100
5	w	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
5	z	41/48 (85%)	41 (100%)	0	0	100	100
6	X	60/81 (74%)	56 (93%)	4 (7%)	0	100	100
6	x	58/81 (72%)	54 (93%)	4 (7%)	0	100	100
7	U	46/53 (87%)	46 (100%)	0	0	100	100
7	u	9/53 (17%)	9 (100%)	0	0	100	100
All	All	4400/4820 (91%)	4266 (97%)	134 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	L	220/220 (100%)	209 (95%)	11 (5%)	24	42
1	l	220/220 (100%)	215 (98%)	5 (2%)	50	69
2	M	239/240 (100%)	229 (96%)	10 (4%)	30	49
2	m	239/240 (100%)	234 (98%)	5 (2%)	53	71
3	H	199/208 (96%)	196 (98%)	3 (2%)	65	78
3	h	199/208 (96%)	194 (98%)	5 (2%)	47	67
4	01	48/48 (100%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	03	48/48 (100%)	46 (96%)	2 (4%)	30 49
4	05	48/48 (100%)	48 (100%)	0	100 100
4	07	43/48 (90%)	42 (98%)	1 (2%)	50 69
4	1	48/48 (100%)	46 (96%)	2 (4%)	30 49
4	3	48/48 (100%)	47 (98%)	1 (2%)	53 71
4	5	48/48 (100%)	48 (100%)	0	100 100
4	7	43/48 (90%)	43 (100%)	0	100 100
4	A	41/48 (85%)	41 (100%)	0	100 100
4	D	47/48 (98%)	46 (98%)	1 (2%)	53 71
4	F	48/48 (100%)	46 (96%)	2 (4%)	30 49
4	I	48/48 (100%)	47 (98%)	1 (2%)	53 71
4	K	48/48 (100%)	48 (100%)	0	100 100
4	O	47/48 (98%)	47 (100%)	0	100 100
4	Q	48/48 (100%)	46 (96%)	2 (4%)	30 49
4	S	47/48 (98%)	43 (92%)	4 (8%)	10 19
4	V	47/48 (98%)	47 (100%)	0	100 100
4	Y	48/48 (100%)	47 (98%)	1 (2%)	53 71
4	a	41/48 (85%)	38 (93%)	3 (7%)	14 25
4	d	47/48 (98%)	45 (96%)	2 (4%)	29 48
4	f	48/48 (100%)	46 (96%)	2 (4%)	30 49
4	i	48/48 (100%)	47 (98%)	1 (2%)	53 71
4	k	48/48 (100%)	48 (100%)	0	100 100
4	o	47/48 (98%)	46 (98%)	1 (2%)	53 71
4	q	48/48 (100%)	48 (100%)	0	100 100
4	s	48/48 (100%)	46 (96%)	2 (4%)	30 49
4	v	48/48 (100%)	47 (98%)	1 (2%)	53 71
4	y	48/48 (100%)	46 (96%)	2 (4%)	30 49
5	02	34/39 (87%)	34 (100%)	0	100 100
5	04	35/39 (90%)	35 (100%)	0	100 100
5	06	32/39 (82%)	30 (94%)	2 (6%)	18 31
5	08	26/39 (67%)	25 (96%)	1 (4%)	33 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2	34/39 (87%)	33 (97%)	1 (3%)	42	62
5	4	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	6	32/39 (82%)	32 (100%)	0	100	100
5	8	26/39 (67%)	26 (100%)	0	100	100
5	B	36/39 (92%)	36 (100%)	0	100	100
5	E	35/39 (90%)	31 (89%)	4 (11%)	5	9
5	G	37/39 (95%)	34 (92%)	3 (8%)	11	21
5	J	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	N	35/39 (90%)	35 (100%)	0	100	100
5	P	35/39 (90%)	32 (91%)	3 (9%)	10	18
5	R	34/39 (87%)	33 (97%)	1 (3%)	42	62
5	T	35/39 (90%)	35 (100%)	0	100	100
5	W	34/39 (87%)	33 (97%)	1 (3%)	42	62
5	Z	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	b	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	e	35/39 (90%)	33 (94%)	2 (6%)	20	36
5	g	37/39 (95%)	36 (97%)	1 (3%)	44	65
5	j	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	n	35/39 (90%)	33 (94%)	2 (6%)	20	36
5	p	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	r	34/39 (87%)	32 (94%)	2 (6%)	19	34
5	t	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	w	34/39 (87%)	34 (100%)	0	100	100
5	z	35/39 (90%)	32 (91%)	3 (9%)	10	18
6	X	49/65 (75%)	45 (92%)	4 (8%)	11	20
6	x	46/65 (71%)	43 (94%)	3 (6%)	17	30
7	U	32/37 (86%)	31 (97%)	1 (3%)	40	60
7	u	1/37 (3%)	1 (100%)	0	100	100
All	All	3713/3976 (93%)	3602 (97%)	111 (3%)	44	61

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	54	VAL
1	L	58	THR
1	L	72	GLU
1	L	129	LEU
1	L	208	THR
1	L	216	PHE
1	L	235	LEU
1	L	247	CYS
1	L	257	ASP
1	L	271	TRP
1	L	272	TRP
2	M	20	MET
2	M	60	LEU
2	M	61	PHE
2	M	182	HIS
2	M	183	LEU
2	M	197	PHE
2	M	214	LEU
2	M	216	PHE
2	M	232	GLU
2	M	263	GLU
3	H	82	ASP
3	H	185	ASP
3	H	247	LYS
4	D	44	LEU
5	E	6	LEU
5	E	8	TYR
5	E	9	THR
5	E	31	SER
4	F	20	GLN
4	F	35	LEU
5	G	12	THR
5	G	19	LEU
5	G	27	LEU
4	I	10	ILE
5	J	17	GLN
5	P	9	THR
5	P	11	LEU
5	P	17	GLN
4	Q	3	LYS
4	Q	27	LEU
5	R	39	LEU
4	S	9	MET

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Mol	Chain	Res	Type
4	S	36	LEU
4	S	38	THR
4	S	54	VAL
5	W	18	GLU
4	Y	11	PHE
5	Z	18	GLU
4	1	12	ASP
4	1	30	MET
5	2	13	ASP
4	3	11	PHE
5	4	19	LEU
6	X	17	THR
6	X	19	LEU
6	X	49	ARG
6	X	57	ILE
7	U	18	PHE
1	l	15	THR
1	l	72	GLU
1	l	216	PHE
1	l	247	CYS
1	l	272	TRP
2	m	8	THR
2	m	128	SER
2	m	142	MET
2	m	214	LEU
2	m	216	PHE
3	h	46	ASP
3	h	128	HIS
3	h	175	MET
3	h	195	MET
3	h	231	ASP
4	a	35	LEU
4	a	36	LEU
4	a	45	GLU
5	b	17	GLN
4	d	20	GLN
4	d	44	LEU
5	e	17	GLN
5	e	36	VAL
4	f	10	ILE
4	f	54	VAL
5	g	39	LEU

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Mol	Chain	Res	Type
4	i	9	MET
5	j	17	GLN
5	n	11	LEU
5	n	17	GLN
4	o	6	LYS
5	p	29	LEU
5	r	6	LEU
5	r	25	SER
4	s	40	SER
4	s	47	SER
5	t	12	THR
4	v	3	LYS
4	y	3	LYS
4	y	20	GLN
5	z	17	GLN
5	z	19	LEU
5	z	45	ARG
4	03	3	LYS
4	03	37	SER
5	06	11	LEU
5	06	19	LEU
4	07	54	VAL
5	08	20	HIS
6	x	11	LEU
6	x	66	ASN
6	x	68	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	183	ASN
2	M	301	HIS
3	H	52	ASN
4	A	42	ASN
5	E	38	HIS
5	G	15	GLN
5	J	17	GLN
5	J	38	HIS
5	N	15	GLN
5	P	17	GLN
4	Q	20	GLN
5	R	17	GLN

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Mol	Chain	Res	Type
5	T	17	GLN
4	V	20	GLN
5	W	17	GLN
5	2	15	GLN
5	2	20	HIS
5	6	15	GLN
4	7	20	GLN
6	X	66	ASN
1	l	199	ASN
2	m	81	ASN
2	m	259	ASN
2	m	301	HIS
3	h	44	ASN
3	h	199	GLN
3	h	206	ASN
5	b	17	GLN
4	d	20	GLN
5	e	17	GLN
5	e	20	HIS
5	e	38	HIS
4	f	20	GLN
5	j	17	GLN
5	n	15	GLN
5	n	17	GLN
4	q	20	GLN
5	r	15	GLN
5	w	15	GLN
4	y	20	GLN
4	y	52	ASN
5	z	17	GLN
4	01	20	GLN
5	02	17	GLN
4	03	20	GLN
5	04	17	GLN
4	07	20	GLN
6	x	60	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

24 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	$\#\|Z\|>2$
4	FME	K	1	4	8,9,10	0.51	0	7,9,11	0.92	1 (14%)
4	FME	A	1	4	8,9,10	0.50	0	7,9,11	0.99	1 (14%)
4	FME	S	1	4	5,6,10	0.77	0	3,6,11	0.76	0
4	FME	o	1	4	8,9,10	0.52	0	7,9,11	1.09	1 (14%)
4	FME	O	1	4	8,9,10	0.52	0	7,9,11	1.01	1 (14%)
4	FME	V	1	4	8,9,10	0.53	0	7,9,11	0.87	1 (14%)
4	FME	d	1	4	8,9,10	0.51	0	7,9,11	0.92	1 (14%)
4	FME	k	1	4	8,9,10	0.49	0	7,9,11	1.01	1 (14%)
4	FME	q	1	4	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
4	FME	i	1	4	8,9,10	0.51	0	7,9,11	0.97	1 (14%)
4	FME	Q	1	4	8,9,10	0.52	0	7,9,11	0.99	1 (14%)
4	FME	03	1	4	8,9,10	0.52	0	7,9,11	0.96	1 (14%)
4	FME	Y	1	4	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
4	FME	f	1	4	8,9,10	0.49	0	7,9,11	0.95	1 (14%)
4	FME	v	1	4	3,4,10	0.94	0	2,4,11	1.35	0
4	FME	s	1	4	5,6,10	0.78	0	3,6,11	0.64	0
4	FME	a	1	4	8,9,10	0.50	0	7,9,11	1.12	1 (14%)
4	FME	01	1	4	8,9,10	0.52	0	7,9,11	1.01	1 (14%)
4	FME	F	1	4	8,9,10	0.50	0	7,9,11	0.97	1 (14%)
4	FME	I	1	4	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
4	FME	D	1	4	8,9,10	0.51	0	7,9,11	1.08	1 (14%)
4	FME	3	1	4	8,9,10	0.50	0	7,9,11	0.96	1 (14%)
4	FME	y	1	4	3,4,10	0.94	0	2,4,11	1.38	0
4	FME	1	1	4	8,9,10	0.51	0	7,9,11	1.01	1 (14%)

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
4	FME	K	1	4	-	1/7/9/11	-
4	FME	A	1	4	-	1/7/9/11	-
4	FME	S	1	4	-	1/2/5/11	-
4	FME	o	1	4	-	1/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	V	1	4	-	1/7/9/11	-
4	FME	d	1	4	-	1/7/9/11	-
4	FME	k	1	4	-	1/7/9/11	-
4	FME	q	1	4	-	0/7/9/11	-
4	FME	i	1	4	-	2/7/9/11	-
4	FME	Q	1	4	-	0/7/9/11	-
4	FME	03	1	4	-	0/7/9/11	-
4	FME	Y	1	4	-	1/7/9/11	-
4	FME	f	1	4	-	1/7/9/11	-
4	FME	v	1	4	-	0/0/2/11	-
4	FME	s	1	4	-	1/2/5/11	-
4	FME	a	1	4	-	0/7/9/11	-
4	FME	01	1	4	-	0/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	I	1	4	-	1/7/9/11	-
4	FME	D	1	4	-	0/7/9/11	-
4	FME	3	1	4	-	0/7/9/11	-
4	FME	y	1	4	-	0/0/2/11	-
4	FME	1	1	4	-	0/7/9/11	-

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	o	1	FME	O-C-CA	-2.63	117.89	124.78
4	D	1	FME	O-C-CA	-2.61	117.95	124.78
4	O	1	FME	O-C-CA	-2.53	118.14	124.78
4	a	1	FME	O-C-CA	-2.52	118.17	124.78
4	A	1	FME	O-C-CA	-2.52	118.17	124.78
4	01	1	FME	O-C-CA	-2.52	118.19	124.78
4	1	1	FME	O-C-CA	-2.51	118.20	124.78
4	I	1	FME	O-C-CA	-2.50	118.23	124.78
4	Y	1	FME	O-C-CA	-2.48	118.27	124.78
4	k	1	FME	O-C-CA	-2.48	118.29	124.78
4	03	1	FME	O-C-CA	-2.45	118.37	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	i	1	FME	O-C-CA	-2.44	118.40	124.78
4	q	1	FME	O-C-CA	-2.43	118.40	124.78
4	3	1	FME	O-C-CA	-2.42	118.42	124.78
4	f	1	FME	O-C-CA	-2.42	118.44	124.78
4	F	1	FME	O-C-CA	-2.41	118.46	124.78
4	K	1	FME	O-C-CA	-2.37	118.57	124.78
4	d	1	FME	O-C-CA	-2.37	118.58	124.78
4	Q	1	FME	O-C-CA	-2.33	118.67	124.78
4	V	1	FME	O-C-CA	-2.27	118.82	124.78

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	F	1	FME	O1-CN-N-CA
4	K	1	FME	O1-CN-N-CA
4	O	1	FME	O1-CN-N-CA
4	S	1	FME	O1-CN-N-CA
4	Y	1	FME	O1-CN-N-CA
4	d	1	FME	O1-CN-N-CA
4	f	1	FME	O1-CN-N-CA
4	i	1	FME	O1-CN-N-CA
4	k	1	FME	O1-CN-N-CA
4	o	1	FME	O1-CN-N-CA
4	s	1	FME	O1-CN-N-CA
4	i	1	FME	N-CA-CB-CG
4	V	1	FME	N-CA-CB-CG
4	I	1	FME	N-CA-CB-CG

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 201 ligands modelled in this entry, 2 are monoatomic - leaving 199 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	$\#\|Z\| > 2$
15	CDL	K	401	-	60,60,99	1.20	4 (6%)	66,72,111	1.09	4 (6%)
11	LMT	L	305	-	28,28,36	0.53	0	39,39,47	1.35	6 (15%)
8	BCL	m	402	-	58,74,74	1.61	11 (18%)	69,115,115	1.67	13 (18%)
11	LMT	H	802	-	36,36,36	0.39	0	47,47,47	1.16	3 (6%)
11	LMT	h	802	-	27,27,36	0.48	0	32,33,47	0.69	0
12	PGV	L	307	-	38,38,50	1.03	2 (5%)	41,44,56	1.06	2 (4%)
14	SPO	01	103	-	40,41,41	0.64	0	47,50,50	1.83	15 (31%)
8	BCL	02	101	-	58,74,74	1.69	10 (17%)	69,115,115	1.63	12 (17%)
14	SPO	m	407	-	40,41,41	0.65	0	47,50,50	1.70	8 (17%)
12	PGV	L	310	-	38,38,50	1.00	2 (5%)	41,44,56	1.18	4 (9%)
14	SPO	R	101	-	40,41,41	0.66	0	47,50,50	2.09	13 (27%)
14	SPO	3	103	-	40,41,41	0.64	0	47,50,50	1.80	14 (29%)
9	BPH	l	302	-	51,70,70	0.66	2 (3%)	52,101,101	0.71	0
8	BCL	05	101	-	58,74,74	1.65	11 (18%)	69,115,115	1.66	16 (23%)
14	SPO	Q	104	-	40,41,41	0.63	0	47,50,50	1.70	11 (23%)
11	LMT	Q	101	-	24,24,36	0.43	0	29,29,47	0.56	0
8	BCL	2	103	-	58,74,74	1.68	9 (15%)	69,115,115	1.64	12 (17%)
12	PGV	f	103	-	39,39,50	1.03	2 (5%)	42,45,56	1.26	6 (14%)
14	SPO	I	103	-	40,41,41	0.62	0	47,50,50	1.78	14 (29%)
12	PGV	x	101	-	38,38,50	1.06	2 (5%)	41,44,56	1.03	2 (4%)
8	BCL	Z	101	-	58,74,74	1.62	9 (15%)	69,115,115	1.60	12 (17%)
8	BCL	O	101	-	58,74,74	1.66	9 (15%)	69,115,115	1.72	15 (21%)
11	LMT	s	104	-	31,31,36	0.40	0	42,42,47	0.63	0
16	PTY	f	105	-	36,36,49	0.34	0	39,41,54	0.40	0
8	BCL	f	102	-	58,74,74	1.59	8 (13%)	69,115,115	1.81	16 (23%)
14	SPO	05	103	-	40,41,41	0.63	0	47,50,50	2.04	13 (27%)
14	SPO	s	105	-	40,41,41	0.66	0	47,50,50	1.98	15 (31%)
15	CDL	y	102	-	47,47,99	1.18	3 (6%)	52,58,111	1.04	3 (5%)
14	SPO	E	102	-	40,41,41	0.65	0	47,50,50	1.78	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	PGV	L	309	-	32,32,50	1.13	2 (6%)	35,38,56	1.22	3 (8%)
14	SPO	O	102	-	40,41,41	0.63	0	47,50,50	1.82	12 (25%)
15	CDL	X	101	-	58,58,99	1.21	4 (6%)	64,70,111	1.19	5 (7%)
14	SPO	A	703	-	40,41,41	0.65	0	47,50,50	2.05	19 (40%)
14	SPO	n	101	-	40,41,41	0.63	0	47,50,50	1.92	14 (29%)
8	BCL	b	101	-	58,74,74	1.61	8 (13%)	69,115,115	1.73	15 (21%)
11	LMT	M	407	-	27,27,36	0.46	0	32,33,47	0.70	0
14	SPO	G	101	-	40,41,41	0.63	0	47,50,50	1.64	10 (21%)
12	PGV	k	103	-	38,40,50	1.03	2 (5%)	40,42,56	1.08	3 (7%)
8	BCL	w	102	-	58,74,74	1.64	9 (15%)	69,115,115	1.62	13 (18%)
12	PGV	l	308	-	23,23,50	1.32	2 (8%)	26,29,56	1.38	4 (15%)
12	PGV	l	306	-	50,50,50	0.90	2 (4%)	53,56,56	1.14	3 (5%)
8	BCL	F	502	-	58,74,74	1.62	8 (13%)	69,115,115	1.75	13 (18%)
14	SPO	n	103	-	40,41,41	0.66	0	47,50,50	1.70	13 (27%)
14	SPO	08	101	-	40,41,41	0.65	0	47,50,50	2.05	15 (31%)
14	SPO	2	104	-	40,41,41	0.62	0	47,50,50	2.00	15 (31%)
8	BCL	1	202	-	58,74,74	1.65	9 (15%)	69,115,115	1.73	16 (23%)
8	BCL	W	101	-	58,74,74	1.65	9 (15%)	69,115,115	1.60	13 (18%)
11	LMT	U	101	-	33,33,36	0.41	0	44,44,47	0.68	1 (2%)
14	SPO	z	101	-	40,41,41	0.68	0	47,50,50	1.77	13 (27%)
8	BCL	S	101	-	58,74,74	1.65	9 (15%)	69,115,115	1.72	17 (24%)
10	U10	L	303	-	35,35,63	0.83	2 (5%)	42,45,79	0.63	0
8	BCL	L	301	-	58,74,74	1.63	9 (15%)	69,115,115	1.70	15 (21%)
10	U10	M	405	-	63,63,63	0.66	2 (3%)	76,79,79	0.60	0
8	BCL	Q	103	-	58,74,74	1.65	9 (15%)	69,115,115	1.75	17 (24%)
14	SPO	f	106	-	40,41,41	0.61	0	47,50,50	1.69	10 (21%)
14	SPO	r	103	-	40,41,41	0.63	0	47,50,50	1.66	13 (27%)
8	BCL	m	403	-	58,74,74	1.66	10 (17%)	69,115,115	1.78	14 (20%)
15	CDL	Y	101	-	42,42,99	1.02	2 (4%)	46,52,111	0.92	2 (4%)
12	PGV	h	801	-	46,46,50	0.91	2 (4%)	49,52,56	1.10	4 (8%)
16	PTY	F	501	-	40,40,49	0.31	0	43,45,54	0.41	0
8	BCL	B	102	-	58,74,74	1.63	8 (13%)	69,115,115	1.75	13 (18%)
12	PGV	m	412	-	38,38,50	1.05	2 (5%)	41,44,56	1.09	3 (7%)
9	BPH	m	404	-	51,70,70	0.63	1 (1%)	52,101,101	0.83	4 (7%)
8	BCL	q	103	-	58,74,74	1.64	10 (17%)	69,115,115	1.76	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	LMT	U	102	-	36,36,36	0.38	0	47,47,47	0.83	2 (4%)
11	LMT	U	103	-	36,36,36	0.37	0	47,47,47	0.79	1 (2%)
8	BCL	P	102	-	58,74,74	1.65	9 (15%)	69,115,115	1.63	13 (18%)
14	SPO	01	102	-	40,41,41	0.63	0	47,50,50	1.74	11 (23%)
14	SPO	G	103	-	40,41,41	0.65	0	47,50,50	2.16	14 (29%)
8	BCL	M	402	-	58,74,74	1.65	10 (17%)	69,115,115	1.82	15 (21%)
8	BCL	7	101	-	58,74,74	1.71	11 (18%)	69,115,115	1.68	12 (17%)
14	SPO	K	404	-	40,41,41	0.63	0	47,50,50	1.73	10 (21%)
17	LDA	y	101	-	8,11,15	2.60	1 (12%)	10,13,17	0.43	0
8	BCL	03	102	-	58,74,74	1.65	9 (15%)	69,115,115	1.66	12 (17%)
8	BCL	Y	102	-	58,74,74	1.67	9 (15%)	69,115,115	1.80	18 (26%)
8	BCL	01	101	-	58,74,74	1.64	8 (13%)	69,115,115	1.74	17 (24%)
11	LMT	M	408	-	25,25,36	0.38	0	30,30,47	0.63	0
8	BCL	p	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.73	15 (21%)
14	SPO	p	101	-	40,41,41	0.67	0	47,50,50	2.28	19 (40%)
11	LMT	q	101	-	24,24,36	0.39	0	29,29,47	0.65	0
10	U10	D	102	-	32,32,63	0.88	2 (6%)	38,41,79	0.67	0
11	LMT	L	306	-	27,27,36	0.49	0	38,38,47	0.92	1 (2%)
8	BCL	j	102	-	58,74,74	1.67	9 (15%)	69,115,115	1.65	13 (18%)
10	U10	d	102	-	30,30,63	0.88	2 (6%)	36,39,79	0.68	0
11	LMT	m	408	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
14	SPO	S	102	-	40,41,41	0.67	0	47,50,50	1.85	16 (34%)
8	BCL	6	101	-	58,74,74	1.74	11 (18%)	69,115,115	1.63	13 (18%)
8	BCL	d	101	-	58,74,74	1.61	9 (15%)	69,115,115	1.85	15 (21%)
8	BCL	t	101	-	58,74,74	1.64	9 (15%)	69,115,115	1.68	13 (18%)
8	BCL	8	101	-	52,68,74	1.83	11 (21%)	61,107,115	1.71	10 (16%)
14	SPO	4	102	-	40,41,41	0.65	0	47,50,50	2.03	13 (27%)
8	BCL	A	702	-	53,69,74	1.73	10 (18%)	63,109,115	1.77	14 (22%)
8	BCL	R	102	-	58,74,74	1.69	11 (18%)	69,115,115	1.61	14 (20%)
14	SPO	B	103	-	40,41,41	0.63	0	47,50,50	1.64	11 (23%)
8	BCL	L	311	-	58,74,74	1.59	8 (13%)	69,115,115	1.76	14 (20%)
11	LMT	I	101	-	36,36,36	0.42	0	47,47,47	0.73	1 (2%)
14	SPO	N	101	-	40,41,41	0.64	0	47,50,50	1.70	10 (21%)
14	SPO	r	101	-	40,41,41	0.64	0	47,50,50	1.79	12 (25%)
8	BCL	r	102	-	58,74,74	1.64	9 (15%)	69,115,115	1.70	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	LMT	M	412	-	31,31,36	0.43	0	42,42,47	0.71	1 (2%)
8	BCL	J	102	-	58,74,74	1.64	8 (13%)	69,115,115	1.60	13 (18%)
14	SPO	5	103	-	40,41,41	0.65	0	47,50,50	1.88	14 (29%)
12	PGV	q	102	-	33,33,50	1.10	2 (6%)	36,39,56	1.15	3 (8%)
14	SPO	a	102	-	40,41,41	0.64	0	47,50,50	1.84	15 (31%)
12	PGV	L	308	-	50,50,50	0.91	2 (4%)	53,56,56	1.04	3 (5%)
16	PTY	H	803	-	36,36,49	0.32	0	39,41,54	0.41	0
8	BCL	N	102	-	58,74,74	1.66	8 (13%)	69,115,115	1.65	13 (18%)
11	LMT	3	104	-	28,28,36	0.45	0	39,39,47	0.71	0
11	LMT	03	101	-	36,36,36	0.38	0	47,47,47	0.71	1 (2%)
11	LMT	s	101	-	25,25,36	0.37	0	30,30,47	0.64	0
10	U10	L	304	-	35,35,63	0.77	2 (5%)	42,45,79	0.68	0
10	U10	l	303	-	35,35,63	0.87	2 (5%)	42,45,79	0.67	0
8	BCL	m	401	-	58,74,74	1.61	9 (15%)	69,115,115	1.78	14 (20%)
12	PGV	H	804	-	25,25,50	1.28	2 (8%)	28,30,56	1.33	3 (10%)
8	BCL	K	402	-	58,74,74	1.64	9 (15%)	69,115,115	1.72	17 (24%)
16	PTY	h	804	-	37,37,49	0.33	0	40,42,54	0.49	0
8	BCL	M	401	-	58,74,74	1.64	9 (15%)	69,115,115	1.67	15 (21%)
12	PGV	Q	102	-	28,28,50	1.22	2 (7%)	31,34,56	1.27	3 (9%)
14	SPO	6	102	-	40,41,41	0.63	0	47,50,50	2.12	14 (29%)
14	SPO	y	105	-	40,41,41	0.66	0	47,50,50	1.91	16 (34%)
8	BCL	5	102	-	58,74,74	1.68	11 (18%)	69,115,115	1.55	13 (18%)
14	SPO	02	102	-	40,41,41	0.64	0	47,50,50	1.94	13 (27%)
8	BCL	D	101	-	58,74,74	1.63	8 (13%)	69,115,115	1.74	14 (20%)
14	SPO	g	102	-	40,41,41	0.64	0	47,50,50	1.95	11 (23%)
8	BCL	l	301	-	58,74,74	1.62	10 (17%)	69,115,115	1.70	14 (20%)
14	SPO	M	406	-	40,41,41	0.64	0	47,50,50	1.70	10 (21%)
8	BCL	s	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.79	15 (21%)
10	U10	m	406	-	59,59,63	0.68	2 (3%)	71,74,79	0.60	0
15	CDL	m	413	-	44,44,99	1.09	3 (6%)	49,54,111	1.11	3 (6%)
14	SPO	T	102	-	40,41,41	0.62	0	47,50,50	1.85	11 (23%)
9	BPH	L	302	-	51,70,70	0.62	2 (3%)	52,101,101	0.72	1 (1%)
8	BCL	3	102	-	58,74,74	1.67	9 (15%)	69,115,115	1.66	15 (21%)
15	CDL	M	410	-	78,78,99	1.02	4 (5%)	84,90,111	1.20	7 (8%)
8	BCL	08	102	-	52,68,74	1.83	11 (21%)	61,107,115	1.67	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	PGV	f	104	-	46,46,50	0.95	2 (4%)	49,52,56	1.03	2 (4%)
8	BCL	G	102	-	58,74,74	1.66	9 (15%)	69,115,115	1.67	15 (21%)
14	SPO	B	101	-	40,41,41	0.65	0	47,50,50	1.87	12 (25%)
8	BCL	g	103	-	58,74,74	1.64	10 (17%)	69,115,115	1.74	13 (18%)
8	BCL	i	103	-	58,74,74	1.64	10 (17%)	69,115,115	1.96	16 (23%)
8	BCL	07	101	-	58,74,74	1.69	11 (18%)	69,115,115	1.68	12 (17%)
12	PGV	h	806	-	25,25,50	1.29	2 (8%)	28,30,56	1.29	3 (10%)
11	LMT	3	101	-	36,36,36	0.39	0	47,47,47	0.69	0
14	SPO	j	101	-	40,41,41	0.64	0	47,50,50	1.99	12 (25%)
15	CDL	h	805	-	60,60,99	1.19	4 (6%)	66,72,111	1.14	5 (7%)
12	PGV	M	411	-	37,37,50	1.07	2 (5%)	40,43,56	1.17	3 (7%)
15	CDL	x	102	-	25,25,99	0.97	1 (4%)	28,32,111	0.87	1 (3%)
8	BCL	o	101	-	58,74,74	1.64	10 (17%)	69,115,115	1.82	17 (24%)
12	PGV	y	104	-	42,42,50	1.00	2 (4%)	44,48,56	1.07	3 (6%)
14	SPO	q	104	-	40,41,41	0.64	0	47,50,50	1.81	12 (25%)
14	SPO	s	103	-	40,41,41	0.63	0	47,50,50	1.58	10 (21%)
11	LMT	i	101	-	27,27,36	0.53	0	38,38,47	0.93	1 (2%)
12	PGV	1	201	-	42,42,50	1.01	2 (4%)	44,48,56	1.06	3 (6%)
15	CDL	X	102	-	32,32,99	1.04	2 (6%)	34,40,111	1.16	2 (5%)
11	LMT	A	701	-	36,36,36	0.43	0	47,47,47	0.76	1 (2%)
10	U10	l	304	-	35,35,63	0.79	2 (5%)	42,45,79	0.68	0
8	BCL	k	101	-	58,74,74	1.65	8 (13%)	69,115,115	1.74	13 (18%)
12	PGV	H	805	-	39,39,50	1.03	2 (5%)	42,45,56	1.11	4 (9%)
14	SPO	Y	103	-	40,41,41	0.64	0	47,50,50	1.73	14 (29%)
9	BPH	M	403	-	51,70,70	0.61	2 (3%)	52,101,101	0.74	1 (1%)
12	PGV	K	403	-	38,40,50	1.03	2 (5%)	40,42,56	1.22	4 (10%)
14	SPO	w	101	-	40,41,41	0.67	0	47,50,50	1.77	12 (25%)
14	SPO	2	102	-	40,41,41	0.64	0	47,50,50	1.83	9 (19%)
8	BCL	n	102	-	58,74,74	1.64	9 (15%)	69,115,115	1.67	15 (21%)
14	SPO	f	101	-	40,41,41	0.63	0	47,50,50	1.96	16 (34%)
11	LMT	m	409	-	34,34,36	0.50	0	45,45,47	1.02	4 (8%)
11	LMT	h	803	-	36,36,36	0.36	0	47,47,47	0.86	2 (4%)
12	PGV	l	307	-	29,29,50	1.19	2 (6%)	32,35,56	1.15	3 (9%)
14	SPO	05	102	-	40,41,41	0.64	0	47,50,50	1.76	11 (23%)
12	PGV	m	411	-	37,37,50	1.06	2 (5%)	40,43,56	1.17	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BCL	4	101	-	58,74,74	1.76	11 (18%)	69,115,115	1.71	13 (18%)
8	BCL	v	101	-	58,74,74	1.64	8 (13%)	69,115,115	1.79	17 (24%)
11	LMT	03	103	-	28,28,36	0.47	0	39,39,47	0.76	0
14	SPO	2	101	-	40,41,41	0.65	0	47,50,50	1.75	13 (27%)
14	SPO	J	101	-	40,41,41	0.63	0	47,50,50	1.77	13 (27%)
14	SPO	S	103	-	40,41,41	0.66	0	47,50,50	1.65	10 (21%)
8	BCL	04	101	-	58,74,74	1.74	11 (18%)	69,115,115	1.66	13 (18%)
8	BCL	y	103	-	58,74,74	1.63	9 (15%)	69,115,115	1.74	16 (23%)
14	SPO	V	102	-	40,41,41	0.64	0	47,50,50	1.73	12 (25%)
11	LMT	5	101	-	34,34,36	0.43	0	45,45,47	0.72	1 (2%)
11	LMT	i	102	-	36,36,36	0.36	0	47,47,47	0.79	1 (2%)
14	SPO	v	102	-	40,41,41	0.69	0	47,50,50	1.93	13 (27%)
8	BCL	e	102	-	58,74,74	1.65	9 (15%)	69,115,115	1.71	15 (21%)
14	SPO	e	101	-	40,41,41	0.67	0	47,50,50	1.83	14 (29%)
8	BCL	E	101	-	58,74,74	1.64	8 (13%)	69,115,115	1.71	16 (23%)
14	SPO	g	101	-	40,41,41	0.66	0	47,50,50	1.79	12 (25%)
14	SPO	P	101	-	40,41,41	0.63	0	47,50,50	1.76	10 (21%)
8	BCL	I	102	-	58,74,74	1.63	8 (13%)	69,115,115	1.78	17 (24%)
12	PGV	l	305	-	38,38,50	1.05	2 (5%)	41,44,56	1.16	3 (7%)
12	PGV	F	503	-	40,40,50	1.02	2 (5%)	43,46,56	1.13	3 (6%)
15	CDL	X	103	-	58,58,99	1.20	4 (6%)	64,70,111	1.35	8 (12%)
15	CDL	m	410	-	78,78,99	1.03	4 (5%)	84,90,111	1.19	6 (7%)
8	BCL	a	101	-	40,56,74	2.00	9 (22%)	47,93,115	1.83	13 (27%)
11	LMT	M	409	-	34,34,36	0.50	1 (2%)	45,45,47	1.02	4 (8%)
8	BCL	z	102	-	58,74,74	1.65	9 (15%)	69,115,115	1.72	13 (18%)
8	BCL	V	101	-	58,74,74	1.64	8 (13%)	69,115,115	1.87	18 (26%)
8	BCL	06	101	-	58,74,74	1.73	11 (18%)	69,115,115	1.66	13 (18%)
12	PGV	H	801	-	46,46,50	0.92	2 (4%)	49,52,56	1.10	4 (8%)
14	SPO	k	102	-	40,41,41	0.63	0	47,50,50	1.64	13 (27%)
8	BCL	T	101	-	58,74,74	1.65	9 (15%)	69,115,115	1.60	13 (18%)

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
15	CDL	K	401	-	-	24/71/71/110	-
11	LMT	L	305	-	-	4/13/53/61	0/2/2/2
8	BCL	m	402	-	-	18/37/137/137	-
11	LMT	H	802	-	-	7/21/61/61	0/2/2/2
11	LMT	h	802	-	-	3/19/39/61	0/1/1/2
12	PGV	L	307	-	-	15/43/43/55	-
14	SPO	01	103	-	-	5/47/47/47	-
8	BCL	02	101	-	-	17/37/137/137	-
14	SPO	m	407	-	-	7/47/47/47	-
12	PGV	L	310	-	-	10/43/43/55	-
14	SPO	R	101	-	-	3/47/47/47	-
14	SPO	3	103	-	-	6/47/47/47	-
9	BPH	l	302	-	-	4/37/105/105	0/5/6/6
8	BCL	05	101	-	-	14/37/137/137	-
14	SPO	Q	104	-	-	6/47/47/47	-
11	LMT	Q	101	-	-	4/15/35/61	0/1/1/2
8	BCL	2	103	-	-	22/37/137/137	-
12	PGV	f	103	-	-	15/44/44/55	-
14	SPO	I	103	-	-	4/47/47/47	-
12	PGV	x	101	-	-	12/43/43/55	-
8	BCL	Z	101	-	-	13/37/137/137	-
8	BCL	O	101	-	-	14/37/137/137	-
11	LMT	s	104	-	-	3/16/56/61	0/2/2/2
16	PTY	f	105	-	-	7/40/40/53	-
8	BCL	f	102	-	-	11/37/137/137	-
14	SPO	05	103	-	-	8/47/47/47	-
14	SPO	s	105	-	-	5/47/47/47	-
15	CDL	y	102	-	-	10/56/56/110	-
14	SPO	E	102	-	-	5/47/47/47	-
12	PGV	L	309	-	-	11/37/37/55	-
14	SPO	O	102	-	-	2/47/47/47	-
15	CDL	X	101	-	-	19/69/69/110	-
14	SPO	A	703	-	-	8/47/47/47	-
14	SPO	n	101	-	-	12/47/47/47	-
8	BCL	b	101	-	-	16/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LMT	M	407	-	-	3/19/39/61	0/1/1/2
14	SPO	G	101	-	-	6/47/47/47	-
12	PGV	k	103	-	-	9/40/42/55	-
8	BCL	w	102	-	-	16/37/137/137	-
12	PGV	l	308	-	-	12/28/28/55	-
12	PGV	l	306	-	-	14/55/55/55	-
8	BCL	F	502	-	-	16/37/137/137	-
14	SPO	n	103	-	-	5/47/47/47	-
14	SPO	08	101	-	-	8/47/47/47	-
14	SPO	2	104	-	-	1/47/47/47	-
8	BCL	1	202	-	-	15/37/137/137	-
8	BCL	W	101	-	-	16/37/137/137	-
11	LMT	U	101	-	-	8/18/58/61	0/2/2/2
14	SPO	z	101	-	-	9/47/47/47	-
8	BCL	S	101	-	-	15/37/137/137	-
10	U10	L	303	-	-	8/30/54/87	0/1/1/1
8	BCL	L	301	-	-	14/37/137/137	-
10	U10	M	405	-	-	15/63/87/87	0/1/1/1
8	BCL	Q	103	-	-	18/37/137/137	-
14	SPO	f	106	-	-	3/47/47/47	-
14	SPO	r	103	-	-	11/47/47/47	-
8	BCL	m	403	-	-	10/37/137/137	-
15	CDL	Y	101	-	-	17/49/49/110	-
12	PGV	h	801	-	-	7/51/51/55	-
16	PTY	F	501	-	-	6/44/44/53	-
8	BCL	B	102	-	-	16/37/137/137	-
12	PGV	m	412	-	-	12/43/43/55	-
9	BPH	m	404	-	-	7/37/105/105	0/5/6/6
8	BCL	q	103	-	-	12/37/137/137	-
11	LMT	U	102	-	-	7/21/61/61	0/2/2/2
11	LMT	U	103	-	-	6/21/61/61	0/2/2/2
8	BCL	P	102	-	-	20/37/137/137	-
14	SPO	01	102	-	-	10/47/47/47	-
14	SPO	G	103	-	-	10/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	M	402	-	-	17/37/137/137	-
8	BCL	7	101	-	-	9/37/137/137	-
14	SPO	K	404	-	-	2/47/47/47	-
17	LDA	y	101	-	-	0/9/9/13	-
8	BCL	03	102	-	-	9/37/137/137	-
8	BCL	Y	102	-	-	16/37/137/137	-
8	BCL	01	101	-	-	17/37/137/137	-
11	LMT	M	408	-	-	4/17/37/61	0/1/1/2
8	BCL	p	102	-	-	15/37/137/137	-
14	SPO	p	101	-	-	6/47/47/47	-
11	LMT	q	101	-	-	3/15/35/61	0/1/1/2
10	U10	D	102	-	-	10/26/50/87	0/1/1/1
11	LMT	L	306	-	-	4/11/51/61	0/2/2/2
8	BCL	j	102	-	-	19/37/137/137	-
10	U10	d	102	-	-	7/24/48/87	0/1/1/1
11	LMT	m	408	-	-	7/21/61/61	0/2/2/2
14	SPO	S	102	-	-	4/47/47/47	-
8	BCL	6	101	-	-	17/37/137/137	-
8	BCL	d	101	-	-	14/37/137/137	-
8	BCL	t	101	-	-	20/37/137/137	-
8	BCL	8	101	-	-	15/29/129/137	-
14	SPO	4	102	-	-	5/47/47/47	-
8	BCL	A	702	-	-	14/31/131/137	-
8	BCL	R	102	-	-	21/37/137/137	-
14	SPO	B	103	-	-	8/47/47/47	-
8	BCL	L	311	-	-	8/37/137/137	-
11	LMT	I	101	-	-	9/21/61/61	0/2/2/2
14	SPO	N	101	-	-	4/47/47/47	-
14	SPO	r	101	-	-	6/47/47/47	-
8	BCL	r	102	-	-	21/37/137/137	-
11	LMT	M	412	-	-	3/16/56/61	0/2/2/2
8	BCL	J	102	-	-	12/37/137/137	-
14	SPO	5	103	-	-	6/47/47/47	-
12	PGV	q	102	-	-	11/38/38/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SPO	a	102	-	-	4/47/47/47	-
12	PGV	L	308	-	-	7/55/55/55	-
16	PTY	H	803	-	-	9/40/40/53	-
8	BCL	N	102	-	-	15/37/137/137	-
11	LMT	3	104	-	-	3/13/53/61	0/2/2/2
11	LMT	03	101	-	-	8/21/61/61	0/2/2/2
11	LMT	s	101	-	-	7/17/37/61	0/1/1/2
10	U10	L	304	-	-	5/30/54/87	0/1/1/1
10	U10	l	303	-	-	11/30/54/87	0/1/1/1
8	BCL	m	401	-	-	11/37/137/137	-
12	PGV	H	804	-	-	11/29/29/55	-
8	BCL	K	402	-	-	9/37/137/137	-
16	PTY	h	804	-	-	8/41/41/53	-
8	BCL	M	401	-	-	13/37/137/137	-
12	PGV	Q	102	-	-	14/33/33/55	-
14	SPO	6	102	-	-	8/47/47/47	-
14	SPO	y	105	-	-	9/47/47/47	-
8	BCL	5	102	-	-	16/37/137/137	-
14	SPO	02	102	-	-	2/47/47/47	-
8	BCL	D	101	-	-	13/37/137/137	-
14	SPO	g	102	-	-	8/47/47/47	-
8	BCL	l	301	-	-	12/37/137/137	-
14	SPO	M	406	-	-	9/47/47/47	-
8	BCL	s	102	-	-	9/37/137/137	-
10	U10	m	406	-	-	16/59/83/87	0/1/1/1
15	CDL	m	413	-	-	17/51/51/110	-
14	SPO	T	102	-	-	6/47/47/47	-
9	BPH	L	302	-	-	5/37/105/105	0/5/6/6
8	BCL	3	102	-	-	8/37/137/137	-
15	CDL	M	410	-	-	29/89/89/110	-
8	BCL	08	102	-	-	13/29/129/137	-
12	PGV	f	104	-	-	11/51/51/55	-
8	BCL	G	102	-	-	17/37/137/137	-
14	SPO	B	101	-	-	8/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	g	103	-	-	16/37/137/137	-
8	BCL	i	103	-	-	11/37/137/137	-
8	BCL	07	101	-	-	14/37/137/137	-
12	PGV	h	806	-	-	13/29/29/55	-
11	LMT	3	101	-	-	5/21/61/61	0/2/2/2
14	SPO	j	101	-	-	10/47/47/47	-
15	CDL	h	805	-	-	27/71/71/110	-
12	PGV	M	411	-	-	22/42/42/55	-
15	CDL	x	102	-	-	7/29/29/110	-
8	BCL	o	101	-	-	11/37/137/137	-
12	PGV	y	104	-	-	5/47/47/55	-
14	SPO	q	104	-	-	6/47/47/47	-
14	SPO	s	103	-	-	2/47/47/47	-
11	LMT	i	101	-	-	3/11/51/61	0/2/2/2
12	PGV	1	201	-	-	9/47/47/55	-
15	CDL	X	102	-	-	19/38/38/110	-
11	LMT	A	701	-	-	5/21/61/61	0/2/2/2
10	U10	l	304	-	-	1/30/54/87	0/1/1/1
8	BCL	k	101	-	-	14/37/137/137	-
12	PGV	H	805	-	-	16/44/44/55	-
14	SPO	Y	103	-	-	5/47/47/47	-
9	BPH	M	403	-	-	2/37/105/105	0/5/6/6
12	PGV	K	403	-	-	8/40/42/55	-
14	SPO	w	101	-	-	5/47/47/47	-
14	SPO	2	102	-	-	6/47/47/47	-
8	BCL	n	102	-	-	14/37/137/137	-
14	SPO	f	101	-	-	9/47/47/47	-
11	LMT	m	409	-	-	5/19/59/61	0/2/2/2
11	LMT	h	803	-	-	5/21/61/61	0/2/2/2
12	PGV	l	307	-	-	12/34/34/55	-
14	SPO	05	102	-	-	6/47/47/47	-
12	PGV	m	411	-	-	18/42/42/55	-
8	BCL	4	101	-	-	12/37/137/137	-
8	BCL	v	101	-	-	17/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LMT	03	103	-	-	5/13/53/61	0/2/2/2
14	SPO	2	101	-	-	9/47/47/47	-
14	SPO	J	101	-	-	4/47/47/47	-
14	SPO	S	103	-	-	1/47/47/47	-
8	BCL	04	101	-	-	11/37/137/137	-
8	BCL	y	103	-	-	10/37/137/137	-
14	SPO	V	102	-	-	4/47/47/47	-
11	LMT	5	101	-	-	4/19/59/61	0/2/2/2
11	LMT	i	102	-	-	2/21/61/61	0/2/2/2
14	SPO	v	102	-	-	8/47/47/47	-
8	BCL	e	102	-	-	11/37/137/137	-
14	SPO	e	101	-	-	8/47/47/47	-
8	BCL	E	101	-	-	20/37/137/137	-
14	SPO	g	101	-	-	4/47/47/47	-
14	SPO	P	101	-	-	5/47/47/47	-
8	BCL	I	102	-	-	11/37/137/137	-
12	PGV	l	305	-	-	13/43/43/55	-
12	PGV	F	503	-	-	14/45/45/55	-
15	CDL	X	103	-	-	21/69/69/110	-
15	CDL	m	410	-	-	30/89/89/110	-
8	BCL	a	101	-	-	8/16/116/137	-
11	LMT	M	409	-	-	8/19/59/61	0/2/2/2
8	BCL	z	102	-	-	14/37/137/137	-
8	BCL	V	101	-	-	15/37/137/137	-
8	BCL	06	101	-	-	14/37/137/137	-
12	PGV	H	801	-	-	12/51/51/55	-
14	SPO	k	102	-	-	4/47/47/47	-
8	BCL	T	101	-	-	17/37/137/137	-

All (707) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	y	101	LDA	O1-N1	-7.34	1.25	1.42
8	8	101	BCL	C3B-C2B	5.24	1.48	1.39
8	4	101	BCL	C3B-C2B	5.24	1.48	1.39
8	3	102	BCL	O2D-CGD	5.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	101	BCL	O2D-CGD	5.18	1.45	1.33
8	06	101	BCL	O2D-CGD	5.17	1.45	1.33
8	T	101	BCL	O2D-CGD	5.14	1.45	1.33
8	07	101	BCL	O2D-CGD	5.14	1.45	1.33
8	6	101	BCL	C3B-C2B	5.14	1.48	1.39
8	R	102	BCL	O2D-CGD	5.13	1.45	1.33
8	4	101	BCL	O2D-CGD	5.13	1.45	1.33
8	04	101	BCL	O2D-CGD	5.13	1.45	1.33
8	L	301	BCL	O2D-CGD	5.13	1.45	1.33
8	05	101	BCL	O2D-CGD	5.12	1.45	1.33
8	J	102	BCL	O2D-CGD	5.12	1.45	1.33
8	Y	102	BCL	O2D-CGD	5.12	1.45	1.33
8	08	102	BCL	O2D-CGD	5.12	1.45	1.33
8	6	101	BCL	O2D-CGD	5.11	1.45	1.33
8	P	102	BCL	O2D-CGD	5.10	1.45	1.33
8	5	102	BCL	O2D-CGD	5.09	1.45	1.33
8	S	101	BCL	O2D-CGD	5.08	1.45	1.33
8	1	202	BCL	O2D-CGD	5.07	1.45	1.33
8	e	102	BCL	O2D-CGD	5.06	1.45	1.33
8	2	103	BCL	O2D-CGD	5.06	1.45	1.33
8	j	102	BCL	O2D-CGD	5.06	1.45	1.33
8	E	101	BCL	O2D-CGD	5.06	1.45	1.33
8	Q	103	BCL	O2D-CGD	5.06	1.45	1.33
8	W	101	BCL	O2D-CGD	5.06	1.45	1.33
8	Z	101	BCL	O2D-CGD	5.05	1.45	1.33
8	I	102	BCL	O2D-CGD	5.05	1.45	1.33
8	r	102	BCL	O2D-CGD	5.04	1.45	1.33
8	z	102	BCL	O2D-CGD	5.04	1.45	1.33
8	7	101	BCL	O2D-CGD	5.04	1.45	1.33
8	g	103	BCL	O2D-CGD	5.04	1.45	1.33
8	n	102	BCL	O2D-CGD	5.04	1.45	1.33
8	03	102	BCL	O2D-CGD	5.03	1.45	1.33
8	M	402	BCL	O2D-CGD	5.03	1.45	1.33
8	q	103	BCL	O2D-CGD	5.02	1.45	1.33
8	O	101	BCL	O2D-CGD	5.02	1.45	1.33
8	G	102	BCL	O2D-CGD	5.02	1.45	1.33
8	8	101	BCL	O2D-CGD	5.01	1.45	1.33
8	b	101	BCL	O2D-CGD	5.01	1.45	1.33
8	K	402	BCL	O2D-CGD	5.01	1.45	1.33
8	y	103	BCL	O2D-CGD	5.01	1.45	1.33
8	R	102	BCL	C3B-C2B	5.00	1.48	1.39
8	A	702	BCL	O2D-CGD	4.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	502	BCL	O2D-CGD	4.99	1.45	1.33
8	t	101	BCL	O2D-CGD	4.99	1.45	1.33
8	w	102	BCL	O2D-CGD	4.99	1.45	1.33
8	p	102	BCL	O2D-CGD	4.99	1.45	1.33
8	l	301	BCL	O2D-CGD	4.98	1.45	1.33
8	02	101	BCL	C3B-C2B	4.98	1.48	1.39
8	N	102	BCL	O2D-CGD	4.98	1.45	1.33
8	i	103	BCL	O2D-CGD	4.97	1.45	1.33
8	v	101	BCL	O2D-CGD	4.97	1.45	1.33
8	k	101	BCL	O2D-CGD	4.96	1.45	1.33
8	02	101	BCL	O2D-CGD	4.96	1.45	1.33
8	S	101	BCL	C3B-C2B	4.96	1.48	1.39
8	01	101	BCL	O2D-CGD	4.95	1.45	1.33
8	M	401	BCL	O2D-CGD	4.95	1.45	1.33
8	d	101	BCL	O2D-CGD	4.94	1.45	1.33
8	s	102	BCL	O2D-CGD	4.93	1.45	1.33
8	V	101	BCL	O2D-CGD	4.93	1.45	1.33
8	B	102	BCL	O2D-CGD	4.91	1.45	1.33
8	D	101	BCL	O2D-CGD	4.91	1.45	1.33
8	07	101	BCL	C3B-C2B	4.90	1.48	1.39
8	08	102	BCL	C3B-C2B	4.90	1.48	1.39
8	m	403	BCL	O2D-CGD	4.90	1.45	1.33
8	o	101	BCL	O2D-CGD	4.90	1.45	1.33
8	f	102	BCL	O2D-CGD	4.89	1.45	1.33
8	7	101	BCL	C3B-C2B	4.84	1.48	1.39
8	Y	102	BCL	C3B-C2B	4.80	1.48	1.39
8	P	102	BCL	C3B-C2B	4.79	1.48	1.39
8	V	101	BCL	C3B-C2B	4.77	1.48	1.39
8	r	102	BCL	C3B-C2B	4.75	1.47	1.39
8	e	102	BCL	C3B-C2B	4.75	1.47	1.39
8	N	102	BCL	C3B-C2B	4.75	1.47	1.39
8	m	402	BCL	O2D-CGD	4.72	1.44	1.33
8	5	102	BCL	OBD-CAD	4.72	1.28	1.22
8	z	102	BCL	C3B-C2B	4.71	1.47	1.39
8	G	102	BCL	C3B-C2B	4.71	1.47	1.39
8	06	101	BCL	C3B-C2B	4.70	1.47	1.39
8	04	101	BCL	C3D-C2D	4.70	1.47	1.39
8	m	402	BCL	C3B-C2B	4.69	1.47	1.39
8	m	401	BCL	C3B-C2B	4.69	1.47	1.39
8	M	402	BCL	C3B-C2B	4.69	1.47	1.39
8	l	301	BCL	C3B-C2B	4.69	1.47	1.39
8	O	101	BCL	C3B-C2B	4.69	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	101	BCL	OBD-CAD	4.68	1.28	1.22
8	06	101	BCL	C3D-C2D	4.68	1.47	1.39
8	01	101	BCL	C3B-C2B	4.68	1.47	1.39
8	04	101	BCL	C3B-C2B	4.68	1.47	1.39
8	A	702	BCL	C3B-C2B	4.68	1.47	1.39
8	j	102	BCL	C3B-C2B	4.67	1.47	1.39
8	07	101	BCL	OBD-CAD	4.67	1.28	1.22
8	8	101	BCL	OBD-CAD	4.67	1.28	1.22
8	V	101	BCL	OBD-CAD	4.66	1.28	1.22
8	03	102	BCL	C3B-C2B	4.65	1.47	1.39
8	J	102	BCL	C3B-C2B	4.65	1.47	1.39
8	D	101	BCL	C3B-C2B	4.64	1.47	1.39
8	m	401	BCL	O2D-CGD	4.64	1.44	1.33
8	4	101	BCL	C3D-C2D	4.64	1.47	1.39
8	08	102	BCL	OBD-CAD	4.64	1.28	1.22
8	04	101	BCL	OBD-CAD	4.63	1.28	1.22
8	b	101	BCL	C3B-C2B	4.63	1.47	1.39
8	05	101	BCL	C3B-C2B	4.63	1.47	1.39
8	E	101	BCL	C3B-C2B	4.63	1.47	1.39
8	m	403	BCL	C3B-C2B	4.62	1.47	1.39
8	06	101	BCL	OBD-CAD	4.62	1.28	1.22
8	Q	103	BCL	C3B-C2B	4.62	1.47	1.39
8	2	103	BCL	C3B-C2B	4.62	1.47	1.39
8	6	101	BCL	OBD-CAD	4.62	1.28	1.22
8	02	101	BCL	OBD-CAD	4.61	1.28	1.22
8	1	202	BCL	C3B-C2B	4.60	1.47	1.39
8	B	102	BCL	C3B-C2B	4.60	1.47	1.39
8	L	311	BCL	O2D-CGD	4.60	1.44	1.33
8	Y	102	BCL	OBD-CAD	4.59	1.28	1.22
8	05	101	BCL	OBD-CAD	4.58	1.28	1.22
8	v	101	BCL	C3B-C2B	4.57	1.47	1.39
8	3	102	BCL	C3B-C2B	4.57	1.47	1.39
8	1	202	BCL	OBD-CAD	4.56	1.28	1.22
8	3	102	BCL	OBD-CAD	4.56	1.28	1.22
8	2	103	BCL	C3D-C2D	4.56	1.47	1.39
8	08	102	BCL	C3D-C2D	4.55	1.47	1.39
8	Q	103	BCL	OBD-CAD	4.55	1.28	1.22
8	j	102	BCL	OBD-CAD	4.55	1.28	1.22
8	n	102	BCL	OBD-CAD	4.55	1.28	1.22
8	a	101	BCL	OBD-CAD	4.55	1.28	1.22
8	4	101	BCL	OBD-CAD	4.55	1.28	1.22
8	W	101	BCL	OBD-CAD	4.54	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	401	BCL	C3B-C2B	4.54	1.47	1.39
8	8	101	BCL	C3D-C2D	4.54	1.47	1.39
8	o	101	BCL	C3B-C2B	4.53	1.47	1.39
8	g	103	BCL	C3B-C2B	4.53	1.47	1.39
8	y	103	BCL	C3B-C2B	4.53	1.47	1.39
8	K	402	BCL	OBD-CAD	4.52	1.28	1.22
8	G	102	BCL	OBD-CAD	4.52	1.28	1.22
8	E	101	BCL	OBD-CAD	4.50	1.28	1.22
8	k	101	BCL	C3B-C2B	4.50	1.47	1.39
8	O	101	BCL	OBD-CAD	4.50	1.28	1.22
8	t	101	BCL	C3B-C2B	4.50	1.47	1.39
8	I	102	BCL	OBD-CAD	4.50	1.28	1.22
8	L	301	BCL	C3B-C2B	4.49	1.47	1.39
8	s	102	BCL	C3B-C2B	4.49	1.47	1.39
8	F	502	BCL	C3B-C2B	4.49	1.47	1.39
8	Z	101	BCL	OBD-CAD	4.48	1.28	1.22
8	R	102	BCL	OBD-CAD	4.48	1.28	1.22
8	d	101	BCL	OBD-CAD	4.48	1.28	1.22
8	p	102	BCL	C3B-C2B	4.48	1.47	1.39
8	2	103	BCL	OBD-CAD	4.48	1.28	1.22
8	i	103	BCL	C3B-C2B	4.47	1.47	1.39
8	n	102	BCL	C3B-C2B	4.47	1.47	1.39
8	03	102	BCL	OBD-CAD	4.46	1.28	1.22
8	5	102	BCL	C3B-C2B	4.46	1.47	1.39
8	6	101	BCL	C3D-C2D	4.46	1.47	1.39
8	T	101	BCL	OBD-CAD	4.46	1.28	1.22
8	N	102	BCL	OBD-CAD	4.46	1.28	1.22
8	P	102	BCL	OBD-CAD	4.46	1.28	1.22
8	a	101	BCL	C3B-C2B	4.45	1.47	1.39
8	D	101	BCL	OBD-CAD	4.45	1.28	1.22
8	02	101	BCL	C3D-C2D	4.45	1.47	1.39
8	w	102	BCL	C3B-C2B	4.44	1.47	1.39
8	e	102	BCL	OBD-CAD	4.44	1.28	1.22
8	k	101	BCL	OBD-CAD	4.44	1.28	1.22
8	q	103	BCL	C3B-C2B	4.43	1.47	1.39
8	W	101	BCL	C3D-C2D	4.43	1.47	1.39
8	J	102	BCL	OBD-CAD	4.43	1.28	1.22
8	d	101	BCL	C3B-C2B	4.43	1.47	1.39
8	T	101	BCL	C3B-C2B	4.43	1.47	1.39
15	m	410	CDL	OA8-CA7	4.43	1.46	1.33
8	S	101	BCL	OBD-CAD	4.43	1.28	1.22
15	y	102	CDL	OA8-CA7	4.41	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	o	101	BCL	OBD-CAD	4.41	1.28	1.22
8	5	102	BCL	C3D-C2D	4.41	1.47	1.39
8	03	102	BCL	C3D-C2D	4.41	1.47	1.39
8	05	101	BCL	O2A-CGA	4.41	1.46	1.33
8	s	102	BCL	OBD-CAD	4.40	1.28	1.22
15	h	805	CDL	OA8-CA7	4.40	1.46	1.33
8	f	102	BCL	OBD-CAD	4.40	1.28	1.22
8	W	101	BCL	C3B-C2B	4.39	1.47	1.39
8	v	101	BCL	OBD-CAD	4.38	1.28	1.22
8	Z	101	BCL	C3B-C2B	4.37	1.47	1.39
8	I	102	BCL	C3B-C2B	4.37	1.47	1.39
8	L	311	BCL	C3B-C2B	4.36	1.47	1.39
8	w	102	BCL	OBD-CAD	4.36	1.28	1.22
8	L	311	BCL	O2A-CGA	4.36	1.46	1.33
8	z	102	BCL	OBD-CAD	4.36	1.28	1.22
8	R	102	BCL	C3D-C2D	4.36	1.47	1.39
8	01	101	BCL	OBD-CAD	4.35	1.28	1.22
12	L	309	PGV	O03-C19	4.35	1.46	1.33
8	L	301	BCL	OBD-CAD	4.35	1.28	1.22
15	X	101	CDL	OA8-CA7	4.35	1.46	1.33
8	t	101	BCL	OBD-CAD	4.35	1.28	1.22
8	7	101	BCL	O2A-CGA	4.35	1.46	1.33
8	Z	101	BCL	C3D-C2D	4.34	1.47	1.39
8	K	402	BCL	C3B-C2B	4.34	1.47	1.39
8	07	101	BCL	C3D-C2D	4.34	1.47	1.39
12	h	806	PGV	O03-C19	4.33	1.46	1.33
8	T	101	BCL	C3D-C2D	4.33	1.47	1.39
8	Z	101	BCL	O2A-CGA	4.33	1.46	1.33
15	K	401	CDL	OA8-CA7	4.33	1.46	1.33
12	m	412	PGV	O03-C19	4.33	1.46	1.33
8	A	702	BCL	C3D-C2D	4.32	1.47	1.39
8	2	103	BCL	O2A-CGA	4.32	1.46	1.33
15	m	413	CDL	OA8-CA7	4.32	1.46	1.33
8	y	103	BCL	OBD-CAD	4.32	1.28	1.22
8	7	101	BCL	C3D-C2D	4.32	1.47	1.39
8	j	102	BCL	C3D-C2D	4.31	1.47	1.39
12	1	201	PGV	O03-C19	4.31	1.45	1.33
15	Y	101	CDL	OA8-CA7	4.31	1.45	1.33
8	A	702	BCL	OBD-CAD	4.31	1.28	1.22
8	t	101	BCL	C3D-C2D	4.31	1.47	1.39
8	W	101	BCL	O2A-CGA	4.31	1.45	1.33
12	M	411	PGV	O03-C19	4.31	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	102	BCL	OBD-CAD	4.30	1.28	1.22
8	g	103	BCL	OBD-CAD	4.30	1.28	1.22
8	3	102	BCL	C3D-C2D	4.30	1.47	1.39
8	4	101	BCL	O2A-CGA	4.30	1.45	1.33
15	X	103	CDL	OA8-CA7	4.30	1.45	1.33
8	J	102	BCL	C3D-C2D	4.30	1.47	1.39
8	N	102	BCL	C3D-C2D	4.29	1.47	1.39
15	x	102	CDL	OA6-CA5	4.29	1.45	1.33
12	K	403	PGV	O03-C19	4.29	1.45	1.33
8	F	502	BCL	C3D-C2D	4.29	1.47	1.39
8	i	103	BCL	OBD-CAD	4.29	1.28	1.22
8	k	101	BCL	C3D-C2D	4.28	1.47	1.39
8	y	103	BCL	O2A-CGA	4.28	1.45	1.33
8	D	101	BCL	O2A-CGA	4.28	1.45	1.33
8	T	101	BCL	O2A-CGA	4.28	1.45	1.33
8	B	102	BCL	O2A-CGA	4.28	1.45	1.33
8	Q	103	BCL	C3D-C2D	4.28	1.47	1.39
12	L	308	PGV	O03-C19	4.28	1.45	1.33
12	H	804	PGV	O03-C19	4.28	1.45	1.33
8	w	102	BCL	C3D-C2D	4.28	1.47	1.39
15	K	401	CDL	OA6-CA5	4.28	1.46	1.34
8	e	102	BCL	C3D-C2D	4.28	1.47	1.39
12	f	103	PGV	O03-C19	4.27	1.45	1.33
12	x	101	PGV	O03-C19	4.27	1.45	1.33
8	Q	103	BCL	O2A-CGA	4.27	1.45	1.33
8	M	402	BCL	OBD-CAD	4.27	1.28	1.22
8	q	103	BCL	OBD-CAD	4.27	1.28	1.22
8	m	401	BCL	O2A-CGA	4.27	1.45	1.33
8	b	101	BCL	OBD-CAD	4.26	1.28	1.22
15	y	102	CDL	OB8-CB7	4.26	1.45	1.33
8	p	102	BCL	C3D-C2D	4.26	1.47	1.39
8	z	102	BCL	C3D-C2D	4.26	1.47	1.39
8	r	102	BCL	OBD-CAD	4.26	1.28	1.22
8	g	103	BCL	C3D-C2D	4.26	1.47	1.39
8	B	102	BCL	OBD-CAD	4.26	1.28	1.22
15	X	101	CDL	OB8-CB7	4.25	1.45	1.33
8	K	402	BCL	C3D-C2D	4.25	1.47	1.39
15	M	410	CDL	OA8-CA7	4.25	1.45	1.33
8	f	102	BCL	O2A-CGA	4.25	1.45	1.33
8	i	103	BCL	O2A-CGA	4.25	1.45	1.33
12	m	411	PGV	O03-C19	4.25	1.45	1.33
8	J	102	BCL	O2A-CGA	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	07	101	BCL	O2A-CGA	4.25	1.45	1.33
15	K	401	CDL	OB8-CB7	4.24	1.45	1.33
15	m	413	CDL	OB6-CB5	4.24	1.46	1.34
8	N	102	BCL	O2A-CGA	4.24	1.45	1.33
12	l	307	PGV	O03-C19	4.24	1.45	1.33
12	Q	102	PGV	O03-C19	4.24	1.45	1.33
8	Y	102	BCL	O2A-CGA	4.24	1.45	1.33
8	D	101	BCL	C3D-C2D	4.23	1.47	1.39
15	h	805	CDL	OB8-CB7	4.23	1.45	1.33
8	l	301	BCL	OBD-CAD	4.23	1.28	1.22
8	F	502	BCL	O2A-CGA	4.23	1.45	1.33
8	1	202	BCL	O2A-CGA	4.23	1.45	1.33
8	M	401	BCL	OBD-CAD	4.23	1.28	1.22
15	X	103	CDL	OB8-CB7	4.23	1.45	1.33
15	Y	101	CDL	OB8-CB7	4.23	1.45	1.33
12	F	503	PGV	O03-C19	4.23	1.45	1.33
8	r	102	BCL	C3D-C2D	4.23	1.47	1.39
15	X	101	CDL	OA6-CA5	4.23	1.46	1.34
8	6	101	BCL	O2A-CGA	4.23	1.45	1.33
12	l	305	PGV	O03-C19	4.22	1.45	1.33
8	P	102	BCL	O2A-CGA	4.22	1.45	1.33
15	h	805	CDL	OA6-CA5	4.22	1.46	1.34
8	w	102	BCL	O2A-CGA	4.22	1.45	1.33
12	y	104	PGV	O03-C19	4.22	1.45	1.33
8	06	101	BCL	O2A-CGA	4.22	1.45	1.33
8	F	502	BCL	OBD-CAD	4.21	1.28	1.22
15	K	401	CDL	OB6-CB5	4.21	1.46	1.34
12	k	103	PGV	O03-C19	4.21	1.45	1.33
8	f	102	BCL	C3B-C2B	4.21	1.47	1.39
8	R	102	BCL	O2A-CGA	4.21	1.45	1.33
8	q	103	BCL	O2A-CGA	4.21	1.45	1.33
8	G	102	BCL	O2A-CGA	4.21	1.45	1.33
8	O	101	BCL	O2A-CGA	4.21	1.45	1.33
12	f	104	PGV	O03-C19	4.21	1.45	1.33
8	n	102	BCL	C3D-C2D	4.20	1.47	1.39
8	O	101	BCL	C3D-C2D	4.20	1.47	1.39
15	X	102	CDL	OA6-CA5	4.20	1.46	1.34
15	X	103	CDL	OB6-CB5	4.19	1.46	1.34
12	H	805	PGV	O03-C19	4.19	1.45	1.33
8	e	102	BCL	O2A-CGA	4.19	1.45	1.33
8	E	101	BCL	O2A-CGA	4.19	1.45	1.33
8	k	101	BCL	O2A-CGA	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	d	101	BCL	O2A-CGA	4.19	1.45	1.33
12	Q	102	PGV	O01-C1	4.18	1.46	1.34
12	l	306	PGV	O01-C1	4.18	1.46	1.34
8	o	101	BCL	O2A-CGA	4.18	1.45	1.33
12	l	305	PGV	O01-C1	4.18	1.46	1.34
8	08	102	BCL	O2A-CGA	4.18	1.45	1.33
8	S	101	BCL	C3D-C2D	4.18	1.46	1.39
8	v	101	BCL	C3D-C2D	4.17	1.46	1.39
8	z	102	BCL	O2A-CGA	4.17	1.45	1.33
12	y	104	PGV	O01-C1	4.17	1.46	1.34
8	G	102	BCL	C3D-C2D	4.17	1.46	1.39
8	a	101	BCL	O2A-CGA	4.17	1.45	1.33
8	03	102	BCL	O2A-CGA	4.17	1.45	1.33
8	K	402	BCL	O2A-CGA	4.17	1.45	1.33
8	l	301	BCL	O2A-CGA	4.17	1.45	1.33
15	m	410	CDL	OB8-CB7	4.17	1.45	1.33
8	m	401	BCL	C3D-C2D	4.17	1.46	1.39
8	04	101	BCL	O2A-CGA	4.16	1.45	1.33
12	l	308	PGV	O03-C19	4.16	1.45	1.33
8	j	102	BCL	O2A-CGA	4.16	1.45	1.33
8	A	702	BCL	O2A-CGA	4.16	1.45	1.33
8	g	103	BCL	O2A-CGA	4.16	1.45	1.33
8	3	102	BCL	O2A-CGA	4.16	1.45	1.33
8	01	101	BCL	C3D-C2D	4.16	1.46	1.39
8	L	311	BCL	C3D-C2D	4.16	1.46	1.39
15	M	410	CDL	OB8-CB7	4.15	1.45	1.33
8	l	301	BCL	C3D-C2D	4.15	1.46	1.39
8	L	301	BCL	O2A-CGA	4.15	1.45	1.33
8	M	402	BCL	O2A-CGA	4.15	1.45	1.33
8	s	102	BCL	O2A-CGA	4.15	1.45	1.33
8	01	101	BCL	O2A-CGA	4.14	1.45	1.33
8	n	102	BCL	O2A-CGA	4.14	1.45	1.33
8	t	101	BCL	O2A-CGA	4.14	1.45	1.33
8	M	401	BCL	C3D-C2D	4.13	1.46	1.39
8	V	101	BCL	O2A-CGA	4.13	1.45	1.33
8	Y	102	BCL	C3D-C2D	4.13	1.46	1.39
12	F	503	PGV	O01-C1	4.13	1.46	1.34
12	x	101	PGV	O01-C1	4.13	1.46	1.34
8	1	202	BCL	C3D-C2D	4.13	1.46	1.39
8	05	101	BCL	C3D-C2D	4.12	1.46	1.39
8	P	102	BCL	C3D-C2D	4.12	1.46	1.39
8	a	101	BCL	C3D-C2D	4.12	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	k	103	PGV	O01-C1	4.12	1.45	1.34
15	y	102	CDL	OB6-CB5	4.12	1.45	1.34
8	02	101	BCL	O2A-CGA	4.12	1.45	1.33
8	q	103	BCL	C3D-C2D	4.12	1.46	1.39
12	L	310	PGV	O03-C19	4.12	1.45	1.33
8	5	102	BCL	O2A-CGA	4.12	1.45	1.33
8	I	102	BCL	O2A-CGA	4.11	1.45	1.33
8	r	102	BCL	O2A-CGA	4.11	1.45	1.33
8	m	403	BCL	OBD-CAD	4.10	1.28	1.22
12	q	102	PGV	O03-C19	4.10	1.45	1.33
8	p	102	BCL	O2A-CGA	4.10	1.45	1.33
8	8	101	BCL	O2A-CGA	4.09	1.45	1.33
12	L	307	PGV	O01-C1	4.08	1.45	1.34
12	L	307	PGV	O03-C19	4.08	1.45	1.33
8	M	401	BCL	O2A-CGA	4.08	1.45	1.33
8	I	102	BCL	C3D-C2D	4.07	1.46	1.39
15	M	410	CDL	OA6-CA5	4.07	1.45	1.34
8	S	101	BCL	O2A-CGA	4.06	1.45	1.33
12	1	201	PGV	O01-C1	4.06	1.45	1.34
15	X	101	CDL	OB6-CB5	4.06	1.45	1.34
8	m	403	BCL	C3D-C2D	4.06	1.46	1.39
8	y	103	BCL	C3D-C2D	4.06	1.46	1.39
15	h	805	CDL	OB6-CB5	4.06	1.45	1.34
8	V	101	BCL	C3D-C2D	4.06	1.46	1.39
12	K	403	PGV	O01-C1	4.06	1.45	1.34
12	h	806	PGV	O01-C1	4.05	1.45	1.34
8	i	103	BCL	C3D-C2D	4.05	1.46	1.39
12	M	411	PGV	O01-C1	4.04	1.45	1.34
12	m	411	PGV	O01-C1	4.04	1.45	1.34
12	q	102	PGV	O01-C1	4.04	1.45	1.34
12	H	804	PGV	O01-C1	4.04	1.45	1.34
8	m	401	BCL	OBD-CAD	4.04	1.27	1.22
8	m	402	BCL	OBD-CAD	4.03	1.27	1.22
12	l	308	PGV	O01-C1	4.02	1.45	1.34
8	m	403	BCL	O2A-CGA	4.02	1.45	1.33
8	L	301	BCL	C3D-C2D	4.01	1.46	1.39
15	M	410	CDL	OB6-CB5	4.01	1.45	1.34
15	X	103	CDL	OA6-CA5	4.01	1.45	1.34
12	H	805	PGV	O01-C1	4.01	1.45	1.34
8	s	102	BCL	C3D-C2D	4.00	1.46	1.39
12	m	412	PGV	O01-C1	4.00	1.45	1.34
8	L	311	BCL	OBD-CAD	3.99	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	b	101	BCL	O2A-CGA	3.99	1.45	1.33
8	m	402	BCL	C3D-C2D	3.99	1.46	1.39
15	m	410	CDL	OA6-CA5	3.98	1.45	1.34
8	E	101	BCL	C3D-C2D	3.98	1.46	1.39
8	m	402	BCL	O2A-CGA	3.98	1.45	1.33
12	l	307	PGV	O01-C1	3.97	1.45	1.34
8	v	101	BCL	O2A-CGA	3.96	1.44	1.33
8	o	101	BCL	C3D-C2D	3.96	1.46	1.39
8	B	102	BCL	C3D-C2D	3.96	1.46	1.39
12	h	801	PGV	O01-C1	3.95	1.45	1.34
12	l	306	PGV	O03-C19	3.95	1.44	1.33
12	L	308	PGV	O01-C1	3.95	1.45	1.34
12	f	104	PGV	O01-C1	3.94	1.45	1.34
12	H	801	PGV	O03-C19	3.94	1.44	1.33
12	H	801	PGV	O01-C1	3.93	1.45	1.34
8	8	101	BCL	C2D-C1D	3.91	1.51	1.42
15	m	410	CDL	OB6-CB5	3.88	1.45	1.34
8	b	101	BCL	C3D-C2D	3.86	1.46	1.39
12	L	309	PGV	O01-C1	3.85	1.45	1.34
12	f	103	PGV	O01-C1	3.85	1.45	1.34
12	h	801	PGV	O03-C19	3.80	1.44	1.33
8	6	101	BCL	C2D-C1D	3.80	1.51	1.42
8	08	102	BCL	C2D-C1D	3.79	1.51	1.42
8	M	402	BCL	C3D-C2D	3.78	1.46	1.39
8	7	101	BCL	C2D-C1D	3.78	1.51	1.42
8	f	102	BCL	C3D-C2D	3.78	1.46	1.39
8	d	101	BCL	C3D-C2D	3.77	1.46	1.39
12	L	310	PGV	O01-C1	3.75	1.44	1.34
8	06	101	BCL	C2D-C1D	3.73	1.51	1.42
8	3	102	BCL	C2D-C1D	3.72	1.51	1.42
8	a	101	BCL	C2D-C1D	3.70	1.50	1.42
8	5	102	BCL	C2D-C1D	3.68	1.50	1.42
8	04	101	BCL	C2D-C1D	3.62	1.50	1.42
8	05	101	BCL	C2D-C1D	3.60	1.50	1.42
8	R	102	BCL	C2D-C1D	3.60	1.50	1.42
8	Y	102	BCL	C2D-C1D	3.59	1.50	1.42
8	1	202	BCL	C2D-C1D	3.55	1.50	1.42
8	07	101	BCL	C2D-C1D	3.54	1.50	1.42
8	s	102	BCL	C2D-C1D	3.54	1.50	1.42
8	o	101	BCL	C2D-C1D	3.54	1.50	1.42
8	O	101	BCL	C2D-C1D	3.52	1.50	1.42
8	03	102	BCL	C2D-C1D	3.50	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	102	BCL	C2D-C1D	3.47	1.50	1.42
8	01	101	BCL	C2D-C1D	3.44	1.50	1.42
8	v	101	BCL	C2D-C1D	3.43	1.50	1.42
8	k	101	BCL	C2D-C1D	3.42	1.50	1.42
8	i	103	BCL	C2D-C1D	3.40	1.50	1.42
8	B	102	BCL	C2D-C1D	3.39	1.50	1.42
8	d	101	BCL	C2D-C1D	3.37	1.50	1.42
8	Q	103	BCL	C2D-C1D	3.36	1.50	1.42
8	q	103	BCL	C2D-C1D	3.36	1.50	1.42
8	P	102	BCL	C2D-C1D	3.35	1.50	1.42
8	E	101	BCL	C2D-C1D	3.34	1.50	1.42
8	4	101	BCL	C2D-C1D	3.34	1.50	1.42
8	M	402	BCL	C2D-C1D	3.33	1.50	1.42
8	V	101	BCL	C2D-C1D	3.33	1.50	1.42
8	b	101	BCL	C2D-C1D	3.32	1.50	1.42
8	L	301	BCL	C2D-C1D	3.31	1.50	1.42
8	2	103	BCL	C2D-C1D	3.31	1.50	1.42
8	W	101	BCL	C2D-C1D	3.30	1.50	1.42
8	N	102	BCL	C2D-C1D	3.29	1.50	1.42
8	T	101	BCL	C2D-C1D	3.29	1.50	1.42
8	S	101	BCL	C2D-C1D	3.28	1.50	1.42
8	02	101	BCL	C2D-C1D	3.28	1.50	1.42
8	m	403	BCL	C2D-C1D	3.26	1.50	1.42
8	y	103	BCL	C2D-C1D	3.26	1.49	1.42
8	A	702	BCL	C2D-C1D	3.23	1.49	1.42
8	K	402	BCL	C2D-C1D	3.23	1.49	1.42
8	Z	101	BCL	C2D-C1D	3.21	1.49	1.42
8	z	102	BCL	C2D-C1D	3.20	1.49	1.42
8	F	502	BCL	C2D-C1D	3.20	1.49	1.42
8	G	102	BCL	C2D-C1D	3.19	1.49	1.42
8	w	102	BCL	C2D-C1D	3.17	1.49	1.42
9	m	404	BPH	C3A-C2A	-3.16	1.51	1.54
8	l	301	BCL	C2D-C1D	3.15	1.49	1.42
15	X	102	CDL	OA8-CA7	3.15	1.45	1.33
8	t	101	BCL	C2D-C1D	3.15	1.49	1.42
8	n	102	BCL	C2D-C1D	3.14	1.49	1.42
8	j	102	BCL	C2D-C1D	3.14	1.49	1.42
8	I	102	BCL	C2D-C1D	3.13	1.49	1.42
8	M	401	BCL	C2D-C1D	3.12	1.49	1.42
8	r	102	BCL	C2D-C1D	3.10	1.49	1.42
8	p	102	BCL	C2D-C1D	3.09	1.49	1.42
8	m	402	BCL	C2D-C1D	3.08	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	08	102	BCL	MG-NC	-3.07	1.99	2.06
8	D	101	BCL	C2D-C1D	3.06	1.49	1.42
8	J	102	BCL	C2D-C1D	3.06	1.49	1.42
8	7	101	BCL	MG-NC	-3.03	1.99	2.06
8	L	311	BCL	C2D-C1D	2.99	1.49	1.42
8	4	101	BCL	MG-NA	-2.99	1.99	2.06
8	04	101	BCL	MG-NC	-2.99	1.99	2.06
8	e	102	BCL	C2D-C1D	2.97	1.49	1.42
8	04	101	BCL	MG-NA	-2.97	1.99	2.06
10	l	303	U10	C3-C2	-2.96	1.40	1.48
10	L	303	U10	C3-C2	-2.95	1.40	1.48
8	g	103	BCL	C2D-C1D	2.95	1.49	1.42
8	4	101	BCL	MG-NC	-2.93	1.99	2.06
8	08	102	BCL	MG-NA	-2.93	1.99	2.06
8	i	103	BCL	MG-NA	-2.92	1.99	2.06
8	06	101	BCL	MG-NC	-2.90	1.99	2.06
8	8	101	BCL	MG-NC	-2.88	1.99	2.06
8	06	101	BCL	MG-NA	-2.82	1.99	2.06
8	6	101	BCL	MG-NC	-2.82	1.99	2.06
8	d	101	BCL	MG-NA	-2.81	1.99	2.06
10	l	304	U10	C3-C2	-2.81	1.40	1.48
10	d	102	U10	C3-C2	-2.79	1.40	1.48
10	D	102	U10	C4-C5	-2.77	1.40	1.48
8	5	102	BCL	MG-NC	-2.77	1.99	2.06
10	m	406	U10	C4-C5	-2.74	1.41	1.48
8	07	101	BCL	MG-NC	-2.73	1.99	2.06
8	m	401	BCL	C2D-C1D	2.73	1.48	1.42
8	8	101	BCL	MG-NA	-2.73	1.99	2.06
8	A	702	BCL	MG-NA	-2.72	1.99	2.06
9	M	403	BPH	C3A-C2A	-2.72	1.52	1.54
9	l	302	BPH	C3A-C2A	-2.70	1.52	1.54
8	q	103	BCL	MG-NA	-2.70	1.99	2.06
8	6	101	BCL	MG-NA	-2.69	1.99	2.06
8	m	401	BCL	MG-NA	-2.69	1.99	2.06
8	M	402	BCL	C3C-C4C	-2.68	1.48	1.51
10	l	303	U10	C4-C5	-2.68	1.41	1.48
10	L	304	U10	C3-C2	-2.68	1.41	1.48
10	m	406	U10	C3-C2	-2.67	1.41	1.48
8	I	102	BCL	MG-NA	-2.66	1.99	2.06
10	M	405	U10	C4-C5	-2.63	1.41	1.48
8	2	103	BCL	MG-NC	-2.62	2.00	2.06
8	o	101	BCL	MG-NA	-2.62	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	102	BCL	MG-NC	-2.61	2.00	2.06
9	L	302	BPH	C3A-C2A	-2.61	1.52	1.54
8	7	101	BCL	MG-NA	-2.59	2.00	2.06
8	M	401	BCL	MG-NA	-2.59	2.00	2.06
8	2	103	BCL	MG-NA	-2.59	2.00	2.06
8	3	102	BCL	MG-NC	-2.59	2.00	2.06
8	7	101	BCL	C1B-CHB	2.58	1.48	1.41
8	B	102	BCL	MG-NA	-2.58	2.00	2.06
10	M	405	U10	C3-C2	-2.57	1.41	1.48
8	D	101	BCL	MG-NA	-2.56	2.00	2.06
8	M	401	BCL	MG-NC	-2.56	2.00	2.06
8	F	502	BCL	MG-NA	-2.56	2.00	2.06
8	a	101	BCL	MG-NA	-2.56	2.00	2.06
8	5	102	BCL	MG-NA	-2.54	2.00	2.06
8	G	102	BCL	MG-NA	-2.54	2.00	2.06
8	e	102	BCL	MG-NC	-2.54	2.00	2.06
8	B	102	BCL	MG-NC	-2.51	2.00	2.06
8	g	103	BCL	MG-NA	-2.49	2.00	2.06
8	v	101	BCL	MG-NA	-2.49	2.00	2.06
8	s	102	BCL	MG-NA	-2.49	2.00	2.06
8	j	102	BCL	MG-NA	-2.48	2.00	2.06
8	L	311	BCL	MG-NC	-2.48	2.00	2.06
8	S	101	BCL	MG-NA	-2.48	2.00	2.06
8	Y	102	BCL	MG-NA	-2.48	2.00	2.06
8	g	103	BCL	MG-NC	-2.48	2.00	2.06
8	e	102	BCL	MG-NA	-2.48	2.00	2.06
8	a	101	BCL	MG-NC	-2.48	2.00	2.06
8	j	102	BCL	MG-NC	-2.48	2.00	2.06
8	04	101	BCL	C1B-CHB	2.47	1.47	1.41
15	m	413	CDL	OB8-CB7	2.47	1.45	1.33
8	m	401	BCL	MG-NC	-2.47	2.00	2.06
8	y	103	BCL	MG-NA	-2.46	2.00	2.06
8	08	102	BCL	C1B-CHB	2.46	1.47	1.41
8	07	101	BCL	MG-NA	-2.46	2.00	2.06
8	m	403	BCL	C3C-C4C	-2.46	1.48	1.51
8	06	101	BCL	C1B-CHB	2.46	1.47	1.41
8	m	402	BCL	MG-NA	-2.46	2.00	2.06
8	L	311	BCL	MG-NA	-2.45	2.00	2.06
8	02	101	BCL	MG-NC	-2.45	2.00	2.06
8	K	402	BCL	MG-NC	-2.45	2.00	2.06
8	b	101	BCL	MG-NC	-2.45	2.00	2.06
8	R	102	BCL	MG-NC	-2.44	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	m	403	BCL	MG-NC	-2.44	2.00	2.06
8	08	102	BCL	C4B-CHC	2.44	1.47	1.41
8	K	402	BCL	MG-NA	-2.43	2.00	2.06
8	O	101	BCL	MG-NA	-2.43	2.00	2.06
8	02	101	BCL	MG-NA	-2.42	2.00	2.06
8	6	101	BCL	C1B-CHB	2.42	1.47	1.41
8	k	101	BCL	MG-NA	-2.42	2.00	2.06
8	4	101	BCL	C1B-CHB	2.42	1.47	1.41
8	8	101	BCL	CHD-C4C	2.41	1.48	1.41
8	E	101	BCL	MG-NA	-2.41	2.00	2.06
8	m	402	BCL	MG-NC	-2.41	2.00	2.06
8	04	101	BCL	C4B-CHC	2.41	1.47	1.41
8	T	101	BCL	MG-NA	-2.41	2.00	2.06
8	b	101	BCL	MG-NA	-2.40	2.00	2.06
8	N	102	BCL	MG-NA	-2.40	2.00	2.06
8	k	101	BCL	MG-NC	-2.40	2.00	2.06
8	R	102	BCL	MG-NA	-2.40	2.00	2.06
8	w	102	BCL	MG-NC	-2.40	2.00	2.06
8	V	101	BCL	MG-NC	-2.40	2.00	2.06
8	w	102	BCL	MG-NA	-2.40	2.00	2.06
8	t	101	BCL	MG-NC	-2.39	2.00	2.06
8	O	101	BCL	MG-NC	-2.38	2.00	2.06
8	Q	103	BCL	MG-NA	-2.38	2.00	2.06
8	W	101	BCL	MG-NA	-2.38	2.00	2.06
8	n	102	BCL	MG-NC	-2.38	2.00	2.06
8	m	403	BCL	MG-NA	-2.38	2.00	2.06
8	o	101	BCL	MG-NC	-2.37	2.00	2.06
8	1	202	BCL	MG-NC	-2.37	2.00	2.06
8	3	102	BCL	MG-NA	-2.37	2.00	2.06
8	v	101	BCL	MG-NC	-2.37	2.00	2.06
8	f	102	BCL	MG-NA	-2.37	2.00	2.06
9	l	302	BPH	CBD-CGD	-2.37	1.49	1.52
8	Z	101	BCL	MG-NA	-2.36	2.00	2.06
8	N	102	BCL	MG-NC	-2.36	2.00	2.06
8	8	101	BCL	C4B-CHC	2.36	1.47	1.41
8	W	101	BCL	MG-NC	-2.36	2.00	2.06
8	M	402	BCL	MG-NC	-2.35	2.00	2.06
8	L	301	BCL	MG-NC	-2.35	2.00	2.06
8	r	102	BCL	MG-NC	-2.35	2.00	2.06
8	E	101	BCL	MG-NC	-2.35	2.00	2.06
10	L	303	U10	C4-C5	-2.34	1.42	1.48
8	F	502	BCL	MG-NC	-2.34	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	102	BCL	MG-NC	-2.34	2.00	2.06
8	p	102	BCL	MG-NA	-2.34	2.00	2.06
8	6	101	BCL	C4B-CHC	2.34	1.47	1.41
8	r	102	BCL	MG-NA	-2.34	2.00	2.06
8	J	102	BCL	MG-NA	-2.34	2.00	2.06
8	2	103	BCL	C1B-CHB	2.34	1.47	1.41
8	M	402	BCL	MG-NA	-2.33	2.00	2.06
8	t	101	BCL	MG-NA	-2.33	2.00	2.06
8	08	102	BCL	CHD-C4C	2.33	1.47	1.41
8	n	102	BCL	MG-NA	-2.32	2.00	2.06
8	P	102	BCL	MG-NC	-2.32	2.00	2.06
10	d	102	U10	C4-C5	-2.31	1.42	1.48
8	V	101	BCL	MG-NA	-2.31	2.00	2.06
8	03	102	BCL	MG-NC	-2.31	2.00	2.06
8	01	101	BCL	MG-NA	-2.31	2.00	2.06
8	01	101	BCL	MG-NC	-2.30	2.00	2.06
8	05	101	BCL	MG-NC	-2.30	2.00	2.06
8	6	101	BCL	CHD-C4C	2.29	1.47	1.41
8	g	103	BCL	C3C-C4C	-2.29	1.48	1.51
8	Z	101	BCL	MG-NC	-2.29	2.00	2.06
8	06	101	BCL	C4B-CHC	2.29	1.47	1.41
8	07	101	BCL	C1B-CHB	2.28	1.47	1.41
8	A	702	BCL	MG-NC	-2.28	2.00	2.06
9	M	403	BPH	CBD-CGD	-2.28	1.49	1.52
10	l	304	U10	C4-C5	-2.28	1.42	1.48
8	S	101	BCL	MG-NC	-2.27	2.00	2.06
10	D	102	U10	C3-C2	-2.27	1.42	1.48
8	4	101	BCL	C4B-CHC	2.25	1.47	1.41
8	5	102	BCL	C1B-CHB	2.25	1.47	1.41
8	03	102	BCL	MG-NA	-2.25	2.00	2.06
8	06	101	BCL	CHD-C4C	2.24	1.47	1.41
8	z	102	BCL	MG-NC	-2.24	2.00	2.06
8	z	102	BCL	MG-NA	-2.24	2.00	2.06
8	04	101	BCL	CHD-C4C	2.24	1.47	1.41
8	J	102	BCL	MG-NC	-2.23	2.01	2.06
8	I	102	BCL	MG-NC	-2.23	2.01	2.06
8	5	102	BCL	CHD-C4C	2.23	1.47	1.41
8	s	102	BCL	MG-NC	-2.22	2.01	2.06
8	8	101	BCL	C1B-CHB	2.22	1.47	1.41
8	Y	102	BCL	C1B-CHB	2.22	1.47	1.41
8	05	101	BCL	MG-NA	-2.21	2.01	2.06
8	1	202	BCL	MG-NA	-2.20	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	101	BCL	MG-NC	-2.20	2.01	2.06
8	T	101	BCL	C1B-CHB	2.20	1.47	1.41
8	q	103	BCL	MG-NC	-2.20	2.01	2.06
8	m	401	BCL	C1B-CHB	2.20	1.47	1.41
8	Q	103	BCL	MG-NC	-2.20	2.01	2.06
8	D	101	BCL	MG-NC	-2.18	2.01	2.06
8	02	101	BCL	C1B-CHB	2.18	1.47	1.41
8	W	101	BCL	C1B-CHB	2.18	1.47	1.41
8	l	301	BCL	C3C-C4C	-2.17	1.48	1.51
8	i	103	BCL	MG-NC	-2.16	2.01	2.06
8	07	101	BCL	CHD-C4C	2.16	1.47	1.41
8	d	101	BCL	C1B-CHB	2.16	1.47	1.41
8	R	102	BCL	CHD-C4C	2.15	1.47	1.41
8	R	102	BCL	C4B-CHC	2.15	1.47	1.41
8	a	101	BCL	CHD-C4C	2.15	1.47	1.41
8	f	102	BCL	MG-NC	-2.15	2.01	2.06
8	Q	103	BCL	C1B-CHB	2.14	1.46	1.41
8	P	102	BCL	MG-NA	-2.13	2.01	2.06
8	M	401	BCL	C1B-CHB	2.13	1.46	1.41
8	7	101	BCL	C4B-CHC	2.13	1.46	1.41
8	7	101	BCL	CHD-C4C	2.13	1.47	1.41
8	l	301	BCL	MG-NC	-2.13	2.01	2.06
8	Y	102	BCL	MG-NC	-2.13	2.01	2.06
8	m	403	BCL	C4B-CHC	2.12	1.46	1.41
8	S	101	BCL	C1B-CHB	2.12	1.46	1.41
8	Z	101	BCL	C1B-CHB	2.11	1.46	1.41
8	q	103	BCL	C3C-C4C	-2.11	1.48	1.51
8	y	103	BCL	C1B-CHB	2.11	1.46	1.41
8	05	101	BCL	CHD-C4C	2.11	1.47	1.41
8	i	103	BCL	C1B-CHB	2.11	1.46	1.41
8	j	102	BCL	C1B-CHB	2.10	1.46	1.41
8	e	102	BCL	C3C-C4C	-2.10	1.49	1.51
8	r	102	BCL	C1B-CHB	2.10	1.46	1.41
8	g	103	BCL	C1B-CHB	2.10	1.46	1.41
8	s	102	BCL	C3C-C4C	-2.10	1.49	1.51
8	5	102	BCL	C4B-CHC	2.10	1.46	1.41
8	q	103	BCL	C1B-CHB	2.10	1.46	1.41
8	o	101	BCL	C3C-C4C	-2.09	1.49	1.51
8	n	102	BCL	C1B-CHB	2.09	1.46	1.41
8	1	202	BCL	C3C-C4C	-2.09	1.49	1.51
8	02	101	BCL	C4B-CHC	2.09	1.46	1.41
8	m	402	BCL	C4B-NB	-2.09	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	301	BCL	MG-NA	-2.08	2.01	2.06
8	G	102	BCL	C1B-CHB	2.08	1.46	1.41
8	3	102	BCL	CHD-C4C	2.08	1.47	1.41
8	l	301	BCL	C4B-CHC	2.07	1.46	1.41
8	07	101	BCL	C4B-CHC	2.07	1.46	1.41
8	M	402	BCL	C4B-CHC	2.07	1.46	1.41
10	L	304	U10	C4-C5	-2.07	1.42	1.48
9	L	302	BPH	CBD-CGD	-2.07	1.49	1.52
8	y	103	BCL	MG-NC	-2.07	2.01	2.06
8	m	402	BCL	C3C-C4C	-2.06	1.49	1.51
8	05	101	BCL	C1B-CHB	2.06	1.46	1.41
8	4	101	BCL	CHD-C4C	2.05	1.47	1.41
8	A	702	BCL	C1B-CHB	2.05	1.46	1.41
8	w	102	BCL	C1B-CHB	2.05	1.46	1.41
8	A	702	BCL	C3C-C4C	-2.05	1.49	1.51
8	05	101	BCL	C4B-CHC	2.04	1.46	1.41
8	l	301	BCL	MG-NA	-2.04	2.01	2.06
8	03	102	BCL	C1B-CHB	2.04	1.46	1.41
8	o	101	BCL	C1B-CHB	2.04	1.46	1.41
8	t	101	BCL	C1B-CHB	2.03	1.46	1.41
11	M	409	LMT	O1'-C1'	2.03	1.43	1.40
8	m	402	BCL	C1B-CHB	2.03	1.46	1.41
8	R	102	BCL	C1B-CHB	2.03	1.46	1.41
8	K	402	BCL	C3C-C4C	-2.02	1.49	1.51
8	P	102	BCL	C1B-CHB	2.01	1.46	1.41
8	p	102	BCL	C1B-CHB	2.01	1.46	1.41
8	i	103	BCL	C3C-C4C	-2.01	1.49	1.51
8	z	102	BCL	C1B-CHB	2.01	1.46	1.41
8	O	101	BCL	C1B-CHB	2.01	1.46	1.41
8	L	301	BCL	C3C-C4C	-2.00	1.49	1.51
8	d	101	BCL	MG-NC	-2.00	2.01	2.06

All (1766) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	p	101	SPO	C21-C22-C23	-8.43	115.28	127.31
14	G	103	SPO	C20-C19-C17	-6.52	118.00	127.31
14	R	101	SPO	C21-C22-C23	-6.39	118.19	127.31
8	V	101	BCL	O2D-CGD-CBD	6.36	122.56	111.27
14	s	105	SPO	C21-C22-C23	-6.25	118.39	127.31
14	6	102	SPO	C21-C22-C23	-6.21	118.44	127.31
8	L	311	BCL	O2D-CGD-CBD	5.95	121.85	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	m	401	BCL	O2D-CGD-CBD	5.87	121.70	111.27
8	m	402	BCL	O2D-CGD-CBD	5.84	121.64	111.27
14	B	101	SPO	C21-C22-C23	-5.78	119.06	127.31
14	5	103	SPO	C21-C22-C23	-5.63	119.28	127.31
14	3	103	SPO	C21-C22-C23	-5.61	119.30	127.31
14	j	101	SPO	C5-C6-C7	-5.57	117.48	125.89
14	2	104	SPO	C5-C6-C7	-5.54	117.52	125.89
14	g	101	SPO	C21-C22-C23	-5.51	119.44	127.31
14	6	102	SPO	C15-C14-C12	-5.51	119.44	127.31
8	M	402	BCL	CHD-C4C-NC	5.51	131.19	125.08
14	2	104	SPO	C10-C9-C7	-5.46	119.51	127.31
8	06	101	BCL	C4B-CHC-C1C	-5.45	119.33	130.12
8	o	101	BCL	O2D-CGD-CBD	5.43	120.92	111.27
14	2	101	SPO	C21-C22-C23	-5.41	119.58	127.31
14	S	103	SPO	C21-C22-C23	-5.41	119.60	127.31
14	q	104	SPO	C20-C19-C17	-5.30	119.75	127.31
14	v	102	SPO	C21-C22-C23	-5.28	119.77	127.31
8	f	102	BCL	O2D-CGD-CBD	5.28	120.65	111.27
8	s	102	BCL	CHD-C4C-NC	5.26	130.92	125.08
14	I	103	SPO	C21-C22-C23	-5.26	119.80	127.31
8	i	103	BCL	CHD-C4C-NC	5.25	130.90	125.08
14	J	101	SPO	C21-C22-C23	-5.24	119.84	127.31
8	8	101	BCL	O2D-CGD-CBD	5.23	120.56	111.27
8	04	101	BCL	C4B-CHC-C1C	-5.22	119.77	130.12
8	08	102	BCL	C1B-CHB-C4A	-5.20	119.83	130.12
8	7	101	BCL	O2D-CGD-CBD	5.19	120.48	111.27
14	4	102	SPO	C10-C9-C7	-5.17	119.93	127.31
8	7	101	BCL	C4C-CHD-C1D	-5.16	118.26	125.88
8	2	103	BCL	O2D-CGD-CBD	5.16	120.43	111.27
8	Q	103	BCL	O2D-CGD-CBD	5.15	120.41	111.27
14	08	101	SPO	C10-C9-C7	-5.12	120.00	127.31
8	M	401	BCL	O2D-CGD-CBD	5.12	120.37	111.27
8	Z	101	BCL	O2D-CGD-CBD	5.12	120.36	111.27
8	m	403	BCL	CHD-C4C-NC	5.12	130.76	125.08
14	G	103	SPO	C15-C14-C12	-5.11	120.01	127.31
14	K	404	SPO	C21-C22-C23	-5.11	120.02	127.31
8	v	101	BCL	O2D-CGD-CBD	5.10	120.33	111.27
14	a	102	SPO	C21-C22-C23	-5.09	120.04	127.31
8	8	101	BCL	C1B-CHB-C4A	-5.06	120.09	130.12
8	F	502	BCL	O2D-CGD-CBD	5.06	120.26	111.27
14	p	101	SPO	C21-C20-C19	-5.03	113.18	123.47
8	i	103	BCL	O2D-CGD-CBD	5.02	120.19	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	s	102	BCL	O2D-CGD-CBD	5.02	120.19	111.27
8	05	101	BCL	O2D-CGD-CBD	5.02	120.19	111.27
8	I	102	BCL	O2D-CGD-CBD	5.01	120.17	111.27
14	r	101	SPO	C21-C22-C23	-5.00	120.17	127.31
8	K	402	BCL	O2D-CGD-CBD	4.97	120.11	111.27
8	08	102	BCL	O2D-CGD-CBD	4.95	120.06	111.27
14	V	102	SPO	C21-C22-C23	-4.95	120.25	127.31
14	4	102	SPO	C5-C6-C7	-4.94	118.42	125.89
8	m	402	BCL	CMB-C2B-C3B	4.94	133.92	124.68
8	b	101	BCL	CHD-C4C-NC	4.94	130.56	125.08
14	05	103	SPO	C15-C14-C12	-4.91	120.30	127.31
8	01	101	BCL	O2D-CGD-CBD	4.90	119.98	111.27
8	i	103	BCL	C3C-C4C-CHD	-4.90	112.92	123.39
14	m	407	SPO	C20-C19-C17	-4.89	120.33	127.31
14	g	102	SPO	C21-C22-C23	-4.86	120.37	127.31
14	n	101	SPO	C10-C9-C7	-4.86	120.37	127.31
8	1	202	BCL	CHD-C4C-NC	4.86	130.47	125.08
8	g	103	BCL	CHD-C4C-NC	4.85	130.46	125.08
14	A	703	SPO	C27-C26-C25	-4.83	108.13	123.22
8	M	402	BCL	C3C-C4C-CHD	-4.83	113.07	123.39
8	d	101	BCL	CHD-C4C-NC	4.83	130.44	125.08
14	O	102	SPO	C21-C22-C23	-4.83	120.42	127.31
8	07	101	BCL	O2D-CGD-CBD	4.83	119.84	111.27
8	r	102	BCL	CHD-C4C-NC	4.82	130.44	125.08
8	Y	102	BCL	CHD-C4C-NC	4.82	130.43	125.08
8	o	101	BCL	CHD-C4C-NC	4.81	130.42	125.08
8	z	102	BCL	O2D-CGD-CBD	4.80	119.80	111.27
8	E	101	BCL	CMB-C2B-C3B	4.80	133.66	124.68
8	q	103	BCL	CHD-C4C-NC	4.80	130.41	125.08
8	O	101	BCL	O2D-CGD-CBD	4.79	119.78	111.27
8	B	102	BCL	O2D-CGD-CBD	4.78	119.76	111.27
8	s	102	BCL	C3C-C4C-CHD	-4.77	113.20	123.39
8	e	102	BCL	CHD-C4C-NC	4.77	130.37	125.08
8	M	402	BCL	CMB-C2B-C3B	4.75	133.56	124.68
14	05	103	SPO	C21-C22-C23	-4.75	120.54	127.31
8	b	101	BCL	CMB-C2B-C3B	4.74	133.55	124.68
14	T	102	SPO	C10-C9-C7	-4.74	120.54	127.31
14	08	101	SPO	C21-C22-C23	-4.74	120.55	127.31
8	D	101	BCL	CHD-C4C-NC	4.73	130.33	125.08
8	V	101	BCL	CMB-C2B-C3B	4.73	133.52	124.68
8	02	101	BCL	O2D-CGD-CBD	4.72	119.66	111.27
8	t	101	BCL	O2D-CGD-CBD	4.72	119.65	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	m	403	BCL	CMB-C2B-C3B	4.71	133.49	124.68
12	l	306	PGV	O01-C1-C2	4.71	121.65	111.50
8	p	102	BCL	CHD-C4C-NC	4.70	130.30	125.08
14	05	103	SPO	C10-C9-C7	-4.69	120.61	127.31
8	A	702	BCL	CHD-C4C-NC	4.69	130.28	125.08
8	B	102	BCL	CMB-C2B-C3B	4.69	133.44	124.68
8	5	102	BCL	O2D-CGD-CBD	4.68	119.59	111.27
14	j	101	SPO	C10-C9-C7	-4.68	120.63	127.31
8	J	102	BCL	O2D-CGD-CBD	4.68	119.59	111.27
8	F	502	BCL	CMB-C2B-C3B	4.68	133.43	124.68
8	T	101	BCL	O2D-CGD-CBD	4.67	119.57	111.27
8	k	101	BCL	O2D-CGD-CBD	4.67	119.56	111.27
8	i	103	BCL	C4A-NA-C1A	4.67	108.80	106.71
14	R	101	SPO	C15-C14-C12	-4.66	120.66	127.31
8	1	202	BCL	CMB-C2B-C3B	4.66	133.40	124.68
8	O	101	BCL	CMB-C2B-C3B	4.66	133.39	124.68
8	z	102	BCL	CHD-C4C-NC	4.65	130.24	125.08
8	R	102	BCL	CMB-C2B-C3B	4.65	133.38	124.68
14	08	101	SPO	C5-C6-C7	-4.65	118.87	125.89
8	d	101	BCL	C4A-NA-C1A	4.65	108.80	106.71
8	g	103	BCL	C3C-C4C-CHD	-4.64	113.47	123.39
8	r	102	BCL	C3C-C4C-CHD	-4.64	113.48	123.39
8	i	103	BCL	CMB-C2B-C3B	4.64	133.36	124.68
8	v	101	BCL	CMB-C2B-C3B	4.64	133.35	124.68
14	z	101	SPO	C21-C22-C23	-4.63	120.70	127.31
8	b	101	BCL	O2D-CGD-CBD	4.63	119.49	111.27
8	t	101	BCL	CHD-C4C-NC	4.62	130.21	125.08
8	f	102	BCL	CMB-C2B-C3B	4.62	133.32	124.68
8	p	102	BCL	O2D-CGD-CBD	4.62	119.48	111.27
14	n	103	SPO	C5-C6-C7	-4.62	118.92	125.89
14	y	105	SPO	C20-C19-C17	-4.62	120.72	127.31
8	03	102	BCL	O2D-CGD-CBD	4.62	119.47	111.27
8	m	403	BCL	C3C-C4C-CHD	-4.62	113.53	123.39
8	D	101	BCL	CMB-C2B-C3B	4.61	133.31	124.68
8	D	101	BCL	C3C-C4C-CHD	-4.61	113.55	123.39
15	X	103	CDL	OA6-CA5-C11	4.61	121.43	111.50
14	08	101	SPO	C20-C19-C17	-4.60	120.74	127.31
8	m	401	BCL	CHD-C4C-NC	4.60	130.18	125.08
8	W	101	BCL	O2D-CGD-CBD	4.59	119.43	111.27
8	S	101	BCL	O2D-CGD-CBD	4.59	119.42	111.27
8	n	102	BCL	CHD-C4C-NC	4.59	130.17	125.08
8	k	101	BCL	CHD-C4C-NC	4.59	130.17	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	01	102	SPO	C5-C6-C7	-4.58	118.97	125.89
8	j	102	BCL	O2D-CGD-CBD	4.57	119.39	111.27
14	z	101	SPO	C20-C19-C17	-4.57	120.79	127.31
8	y	103	BCL	O2D-CGD-CBD	4.57	119.39	111.27
8	06	101	BCL	O2D-CGD-CBD	4.57	119.39	111.27
14	f	101	SPO	C20-C19-C17	-4.57	120.79	127.31
8	e	102	BCL	O2D-CGD-CBD	4.56	119.37	111.27
8	Y	102	BCL	CMB-C2B-C3B	4.56	133.21	124.68
8	M	402	BCL	O2D-CGD-CBD	4.56	119.36	111.27
8	N	102	BCL	O2D-CGD-CBD	4.55	119.36	111.27
8	6	101	BCL	C4B-CHC-C1C	-4.54	121.12	130.12
8	l	301	BCL	C3C-C4C-CHD	-4.54	113.69	123.39
8	L	311	BCL	CHD-C4C-NC	4.54	130.12	125.08
8	r	102	BCL	O2D-CGD-CBD	4.54	119.34	111.27
8	l	301	BCL	CMB-C2B-C3B	4.54	133.17	124.68
8	D	101	BCL	O2D-CGD-CBD	4.52	119.31	111.27
8	k	101	BCL	CMB-C2B-C3B	4.52	133.13	124.68
8	r	102	BCL	CMB-C2B-C3B	4.52	133.13	124.68
8	3	102	BCL	CHD-C4C-NC	4.52	130.09	125.08
8	j	102	BCL	CHD-C4C-NC	4.52	130.09	125.08
8	1	202	BCL	O2D-CGD-CBD	4.51	119.29	111.27
8	g	103	BCL	O2D-CGD-CBD	4.51	119.28	111.27
8	z	102	BCL	C3C-C4C-CHD	-4.51	113.76	123.39
8	N	102	BCL	CHD-C4C-NC	4.51	130.08	125.08
8	o	101	BCL	CMB-C2B-C3B	4.50	133.10	124.68
14	02	102	SPO	C21-C22-C23	-4.50	120.89	127.31
8	P	102	BCL	O2D-CGD-CBD	4.49	119.25	111.27
8	m	401	BCL	C3C-C4C-CHD	-4.49	113.80	123.39
8	m	402	BCL	CHD-C4C-NC	4.49	130.06	125.08
8	Y	102	BCL	C3C-C4C-CHD	-4.49	113.81	123.39
8	m	403	BCL	O2D-CGD-CBD	4.48	119.22	111.27
15	M	410	CDL	OB6-CB5-C51	4.47	121.14	111.50
8	w	102	BCL	CHD-C4C-NC	4.46	130.03	125.08
12	K	403	PGV	O01-C1-C2	4.46	121.12	111.50
8	L	301	BCL	CHD-C4C-NC	4.46	130.03	125.08
8	M	401	BCL	CHD-C4C-NC	4.46	130.03	125.08
8	a	101	BCL	CHD-C4C-NC	4.46	130.03	125.08
8	t	101	BCL	C3C-C4C-CHD	-4.46	113.87	123.39
8	6	101	BCL	O2D-CGD-CBD	4.46	119.19	111.27
8	N	102	BCL	CMB-C2B-C3B	4.45	133.00	124.68
8	01	101	BCL	CMB-C2B-C3B	4.44	132.99	124.68
8	l	301	BCL	CHD-C4C-NC	4.44	130.00	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Y	102	BCL	O2D-CGD-CBD	4.44	119.15	111.27
8	1	202	BCL	C3C-C4C-CHD	-4.43	113.92	123.39
8	W	101	BCL	CHD-C4C-NC	4.43	130.00	125.08
8	A	702	BCL	O2D-CGD-CBD	4.43	119.14	111.27
8	01	101	BCL	CHD-C4C-NC	4.43	129.99	125.08
8	d	101	BCL	C3C-C4C-CHD	-4.43	113.94	123.39
8	04	101	BCL	O2D-CGD-CBD	4.42	119.13	111.27
14	Y	103	SPO	C21-C22-C23	-4.42	121.00	127.31
8	A	702	BCL	C3C-C4C-CHD	-4.42	113.95	123.39
8	G	102	BCL	O2D-CGD-CBD	4.42	119.11	111.27
8	a	101	BCL	O2D-CGD-CBD	4.41	119.11	111.27
8	y	103	BCL	CHD-C4C-NC	4.41	129.98	125.08
14	w	101	SPO	C21-C22-C23	-4.41	121.02	127.31
8	B	102	BCL	CHD-C4C-NC	4.40	129.97	125.08
8	p	102	BCL	C3C-C4C-CHD	-4.40	114.00	123.39
14	j	101	SPO	C21-C22-C23	-4.39	121.04	127.31
8	n	102	BCL	O2D-CGD-CBD	4.39	119.06	111.27
15	X	103	CDL	OB6-CB5-C51	4.38	120.94	111.50
14	01	102	SPO	C10-C9-C7	-4.38	121.06	127.31
8	4	101	BCL	O2D-CGD-CBD	4.37	119.04	111.27
15	m	410	CDL	CB4-OB6-CB5	-4.36	107.05	117.79
8	R	102	BCL	O2D-CGD-CBD	4.36	119.02	111.27
8	I	102	BCL	CHD-C4C-NC	4.36	129.91	125.08
14	6	102	SPO	C10-C9-C7	-4.35	121.11	127.31
8	y	103	BCL	CMB-C2B-C3B	4.34	132.81	124.68
8	e	102	BCL	C3C-C4C-CHD	-4.34	114.11	123.39
8	03	102	BCL	CMB-C2B-C3B	4.34	132.80	124.68
12	L	308	PGV	O01-C1-C2	4.34	120.85	111.50
14	p	101	SPO	C26-C25-C23	-4.34	114.23	126.42
14	G	103	SPO	C10-C9-C7	-4.33	121.13	127.31
8	07	101	BCL	C4C-CHD-C1D	-4.33	119.49	125.88
14	R	101	SPO	C20-C19-C17	-4.33	121.13	127.31
8	G	102	BCL	CHD-C4C-NC	4.33	129.89	125.08
8	q	103	BCL	C3C-C4C-CHD	-4.33	114.14	123.39
8	f	102	BCL	CHD-C4C-NC	4.33	129.88	125.08
15	m	410	CDL	OB6-CB5-C51	4.32	120.82	111.50
8	S	101	BCL	CMB-C2B-C3B	4.32	132.77	124.68
8	Q	103	BCL	CHD-C4C-NC	4.32	129.88	125.08
8	E	101	BCL	O2D-CGD-CBD	4.32	118.94	111.27
14	T	102	SPO	C5-C6-C7	-4.32	119.37	125.89
8	M	401	BCL	CMB-C2B-C3B	4.32	132.75	124.68
8	2	103	BCL	CHD-C4C-NC	4.31	129.87	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	101	SPO	C5-C6-C7	-4.31	119.37	125.89
14	02	102	SPO	C10-C9-C7	-4.31	121.16	127.31
8	s	102	BCL	CMB-C2B-C3B	4.31	132.74	124.68
8	S	101	BCL	CHD-C4C-NC	4.31	129.86	125.08
14	4	102	SPO	C21-C22-C23	-4.30	121.17	127.31
8	L	311	BCL	C3C-C4C-CHD	-4.30	114.21	123.39
8	T	101	BCL	CHD-C4C-NC	4.30	129.85	125.08
8	L	301	BCL	CMB-C2B-C3B	4.29	132.70	124.68
8	A	702	BCL	CMB-C2B-C3B	4.29	132.70	124.68
8	b	101	BCL	C3C-C4C-CHD	-4.29	114.23	123.39
14	G	103	SPO	C5-C6-C7	-4.29	119.42	125.89
8	P	102	BCL	CHD-C4C-NC	4.28	129.83	125.08
8	p	102	BCL	CMB-C2B-C3B	4.28	132.69	124.68
8	o	101	BCL	C3C-C4C-CHD	-4.28	114.25	123.39
8	y	103	BCL	C3C-C4C-CHD	-4.28	114.25	123.39
8	I	102	BCL	CMB-C2B-C3B	4.28	132.68	124.68
8	z	102	BCL	CMB-C2B-C3B	4.27	132.68	124.68
8	n	102	BCL	C3C-C4C-CHD	-4.27	114.27	123.39
8	L	301	BCL	C3C-C4C-CHD	-4.27	114.28	123.39
15	X	101	CDL	OA6-CA5-C11	4.25	120.67	111.50
14	E	102	SPO	C21-C22-C23	-4.25	121.24	127.31
8	O	101	BCL	CHD-C4C-NC	4.25	129.80	125.08
14	4	102	SPO	C20-C19-C17	-4.25	121.24	127.31
8	N	102	BCL	C3C-C4C-CHD	-4.25	114.31	123.39
14	g	102	SPO	C5-C6-C7	-4.25	119.48	125.89
14	v	102	SPO	C20-C19-C17	-4.24	121.25	127.31
8	w	102	BCL	C3C-C4C-CHD	-4.24	114.33	123.39
8	E	101	BCL	CHD-C4C-NC	4.24	129.78	125.08
8	V	101	BCL	CHD-C4C-NC	4.24	129.78	125.08
15	X	102	CDL	OA6-CA5-C11	4.23	120.62	111.50
8	3	102	BCL	CMB-C2B-C3B	4.23	132.59	124.68
8	f	102	BCL	C3C-C4C-CHD	-4.23	114.36	123.39
14	5	103	SPO	C20-C19-C17	-4.21	121.30	127.31
8	m	401	BCL	CMB-C2B-C3B	4.21	132.56	124.68
8	7	101	BCL	C4A-NA-C1A	4.21	108.60	106.71
14	B	101	SPO	C29-C28-C30	4.20	122.34	115.27
14	Q	104	SPO	C20-C19-C17	-4.20	121.31	127.31
8	e	102	BCL	CMB-C2B-C3B	4.19	132.52	124.68
8	Q	103	BCL	C3C-C4C-CHD	-4.19	114.45	123.39
14	g	102	SPO	C10-C9-C7	-4.19	121.34	127.31
12	y	104	PGV	O01-C1-C2	4.18	120.50	111.50
8	03	102	BCL	CHD-C4C-NC	4.17	129.71	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	05	102	SPO	C21-C22-C23	-4.17	121.36	127.31
8	F	502	BCL	CHD-C4C-NC	4.16	129.70	125.08
12	m	411	PGV	O01-C1-C2	4.16	120.47	111.50
8	04	101	BCL	C1B-CHB-C4A	-4.15	121.89	130.12
8	P	102	BCL	CMB-C2B-C3B	4.14	132.43	124.68
15	m	413	CDL	OB6-CB5-C51	4.14	120.42	111.50
12	H	804	PGV	O01-C1-C2	4.14	120.42	111.50
8	P	102	BCL	C3C-C4C-CHD	-4.14	114.56	123.39
8	q	103	BCL	O2D-CGD-CBD	4.14	118.62	111.27
8	J	102	BCL	CMB-C2B-C3B	4.14	132.41	124.68
8	v	101	BCL	CHD-C4C-NC	4.13	129.67	125.08
12	M	411	PGV	O01-C1-C2	4.13	120.41	111.50
8	d	101	BCL	O2D-CGD-CBD	4.13	118.61	111.27
12	h	806	PGV	O01-C1-C2	4.13	120.40	111.50
8	R	102	BCL	CHD-C4C-NC	4.12	129.66	125.08
8	d	101	BCL	CMB-C2B-C3B	4.12	132.39	124.68
12	F	503	PGV	O01-C1-C2	4.12	120.38	111.50
14	M	406	SPO	C21-C22-C23	-4.11	121.44	127.31
14	f	101	SPO	C31-C32-C33	-4.10	117.78	127.66
14	A	703	SPO	C31-C32-C33	-4.10	117.78	127.66
8	I	102	BCL	C3C-C4C-CHD	-4.10	114.62	123.39
8	02	101	BCL	CMB-C2B-C3B	4.10	132.35	124.68
8	4	101	BCL	C1B-CHB-C4A	-4.10	122.00	130.12
8	w	102	BCL	O2D-CGD-CBD	4.10	118.55	111.27
8	j	102	BCL	C3C-C4C-CHD	-4.10	114.64	123.39
8	07	101	BCL	C4A-NA-C1A	4.09	108.55	106.71
8	4	101	BCL	CHD-C4C-NC	4.09	129.62	125.08
12	f	103	PGV	O01-C1-C2	4.08	120.30	111.50
12	Q	102	PGV	O01-C1-C2	4.08	120.29	111.50
8	t	101	BCL	CMB-C2B-C3B	4.08	132.30	124.68
8	K	402	BCL	CHD-C4C-NC	4.07	129.60	125.08
14	P	101	SPO	C21-C22-C23	-4.07	121.50	127.31
12	h	801	PGV	O01-C1-C2	4.07	120.28	111.50
12	m	412	PGV	O01-C1-C2	4.07	120.27	111.50
8	S	101	BCL	C3C-C4C-CHD	-4.07	114.70	123.39
12	L	310	PGV	O01-C1-C2	4.07	120.27	111.50
8	V	101	BCL	C3C-C4C-CHD	-4.06	114.71	123.39
14	N	101	SPO	C21-C22-C23	-4.06	121.51	127.31
8	G	102	BCL	CMB-C2B-C3B	4.06	132.28	124.68
8	01	101	BCL	C3C-C4C-CHD	-4.06	114.72	123.39
8	8	101	BCL	CHD-C4C-NC	4.06	129.58	125.08
8	q	103	BCL	CMB-C2B-C3B	4.06	132.27	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	1	201	PGV	O01-C1-C2	4.05	120.24	111.50
8	F	502	BCL	C3C-C4C-CHD	-4.05	114.73	123.39
8	K	402	BCL	CMB-C2B-C3B	4.05	132.26	124.68
8	7	101	BCL	C4B-CHC-C1C	-4.05	122.09	130.12
12	l	305	PGV	O01-C1-C2	4.05	120.23	111.50
14	m	407	SPO	C21-C22-C23	-4.05	121.53	127.31
14	S	102	SPO	C21-C22-C23	-4.05	121.53	127.31
8	8	101	BCL	CMB-C2B-C3B	4.05	132.25	124.68
8	02	101	BCL	CHD-C4C-NC	4.05	129.57	125.08
12	l	308	PGV	O01-C1-C2	4.04	120.21	111.50
8	n	102	BCL	CMB-C2B-C3B	4.04	132.24	124.68
8	T	101	BCL	C3C-C4C-CHD	-4.04	114.76	123.39
14	01	103	SPO	C21-C22-C23	-4.04	121.55	127.31
8	O	101	BCL	C3C-C4C-CHD	-4.03	114.77	123.39
8	m	402	BCL	C3C-C4C-CHD	-4.03	114.78	123.39
8	a	101	BCL	CMB-C2B-C3B	4.03	132.21	124.68
8	B	102	BCL	C3C-C4C-CHD	-4.02	114.80	123.39
14	2	102	SPO	C10-C9-C7	-4.02	121.58	127.31
8	k	101	BCL	C3C-C4C-CHD	-4.02	114.81	123.39
14	A	703	SPO	C29-C28-C30	4.01	122.02	115.27
14	E	102	SPO	C29-C28-C30	4.01	122.01	115.27
12	H	801	PGV	O01-C1-C2	4.00	120.13	111.50
8	W	101	BCL	C3C-C4C-CHD	-3.99	114.86	123.39
8	4	101	BCL	CMB-C2B-C3B	3.99	132.15	124.68
8	j	102	BCL	CMB-C2B-C3B	3.99	132.14	124.68
14	f	106	SPO	C20-C19-C17	-3.99	121.62	127.31
14	y	105	SPO	C29-C28-C30	3.99	121.98	115.27
8	05	101	BCL	CMB-C2B-C3B	3.99	132.13	124.68
8	L	311	BCL	CMB-C2B-C3B	3.98	132.13	124.68
15	K	401	CDL	OA6-CA5-C11	3.98	120.07	111.50
14	05	102	SPO	C20-C19-C17	-3.97	121.64	127.31
8	G	102	BCL	C3C-C4C-CHD	-3.96	114.92	123.39
8	05	101	BCL	CHD-C4C-NC	3.95	129.47	125.08
14	a	102	SPO	C20-C19-C17	-3.95	121.67	127.31
14	r	101	SPO	C5-C6-C7	-3.95	119.92	125.89
11	H	802	LMT	O1B-C4'-C3'	3.95	117.78	107.28
14	e	101	SPO	C20-C19-C17	-3.94	121.68	127.31
8	M	401	BCL	C3C-C4C-CHD	-3.94	114.97	123.39
14	w	101	SPO	C5-C6-C7	-3.94	119.94	125.89
14	05	103	SPO	C5-C6-C7	-3.94	119.94	125.89
14	n	101	SPO	C15-C14-C12	-3.94	121.69	127.31
8	Z	101	BCL	CHD-C4C-NC	3.94	129.45	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	m	401	BCL	C4C-CHD-C1D	-3.93	120.08	125.88
8	3	102	BCL	O2D-CGD-CBD	3.92	118.24	111.27
8	Z	101	BCL	C3C-C4C-CHD	-3.92	115.02	123.39
14	s	105	SPO	C31-C32-C33	-3.91	118.24	127.66
14	f	106	SPO	C21-C22-C23	-3.91	121.73	127.31
14	G	101	SPO	C20-C19-C17	-3.90	121.74	127.31
14	2	104	SPO	C21-C22-C23	-3.90	121.75	127.31
8	l	301	BCL	O2D-CGD-CBD	3.90	118.19	111.27
15	h	805	CDL	OA6-CA5-C11	3.89	119.89	111.50
14	j	101	SPO	C15-C14-C12	-3.89	121.76	127.31
14	2	102	SPO	C5-C6-C7	-3.89	120.02	125.89
15	M	410	CDL	OA6-CA5-C11	3.89	119.88	111.50
8	e	102	BCL	C4C-CHD-C1D	-3.88	120.15	125.88
14	01	103	SPO	C20-C19-C17	-3.88	121.78	127.31
8	Q	103	BCL	CMB-C2B-C3B	3.87	131.92	124.68
8	v	101	BCL	C3C-C4C-CHD	-3.87	115.12	123.39
14	S	102	SPO	C15-C14-C12	-3.87	121.79	127.31
8	d	101	BCL	C1C-NC-C4C	-3.86	104.97	106.71
14	O	102	SPO	C20-C19-C17	-3.86	121.81	127.31
15	M	410	CDL	CB4-OB6-CB5	-3.86	108.30	117.79
12	k	103	PGV	O01-C1-C2	3.85	119.81	111.50
14	02	102	SPO	C5-C6-C7	-3.85	120.08	125.89
12	L	309	PGV	O01-C1-C2	3.85	119.79	111.50
8	g	103	BCL	CMB-C2B-C3B	3.84	131.87	124.68
14	R	101	SPO	C10-C9-C7	-3.84	121.83	127.31
8	w	102	BCL	CMB-C2B-C3B	3.83	131.84	124.68
8	a	101	BCL	C3C-C4C-CHD	-3.82	115.22	123.39
14	2	101	SPO	C15-C14-C12	-3.82	121.86	127.31
14	E	102	SPO	C20-C19-C17	-3.82	121.86	127.31
14	K	404	SPO	C20-C19-C17	-3.81	121.87	127.31
8	A	702	BCL	C4C-CHD-C1D	-3.81	120.26	125.88
14	P	101	SPO	C10-C9-C7	-3.80	121.88	127.31
8	J	102	BCL	C3C-C4C-CHD	-3.80	115.28	123.39
8	03	102	BCL	C3C-C4C-CHD	-3.79	115.29	123.39
8	B	102	BCL	C1-C2-C3	-3.79	119.48	126.04
14	f	101	SPO	C29-C28-C30	3.79	121.65	115.27
8	K	402	BCL	C3C-C4C-CHD	-3.79	115.30	123.39
14	q	104	SPO	C29-C28-C30	3.78	121.63	115.27
8	E	101	BCL	C3C-C4C-CHD	-3.78	115.32	123.39
8	m	401	BCL	C1-C2-C3	-3.78	119.51	126.04
8	07	101	BCL	C4B-CHC-C1C	-3.78	122.64	130.12
15	h	805	CDL	OB6-CB5-C51	3.77	119.64	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	103	BCL	C4C-CHD-C1D	-3.77	120.32	125.88
8	3	102	BCL	C3C-C4C-CHD	-3.77	115.34	123.39
14	m	407	SPO	C31-C32-C33	-3.76	118.60	127.66
14	P	101	SPO	C5-C6-C7	-3.76	120.20	125.89
14	A	703	SPO	C20-C19-C17	-3.76	121.95	127.31
8	2	103	BCL	C3C-C4C-CHD	-3.75	115.37	123.39
8	4	101	BCL	C4B-CHC-C1C	-3.75	122.69	130.12
14	e	101	SPO	C5-C6-C7	-3.75	120.23	125.89
14	g	102	SPO	C15-C14-C12	-3.74	121.98	127.31
15	X	101	CDL	OB6-CB5-C51	3.73	119.55	111.50
8	02	101	BCL	C3C-C4C-CHD	-3.73	115.42	123.39
8	Y	102	BCL	C4A-NA-C1A	3.73	108.38	106.71
14	w	101	SPO	C20-C19-C17	-3.73	121.99	127.31
12	l	307	PGV	O01-C1-C2	3.72	119.52	111.50
14	e	101	SPO	C15-C14-C12	-3.72	122.00	127.31
8	J	102	BCL	CHD-C4C-NC	3.72	129.21	125.08
12	H	805	PGV	O01-C1-C2	3.72	119.51	111.50
14	Y	103	SPO	C15-C14-C12	-3.71	122.01	127.31
14	05	103	SPO	C20-C19-C17	-3.71	122.01	127.31
8	2	103	BCL	C4B-CHC-C1C	-3.71	122.77	130.12
8	I	102	BCL	C4C-CHD-C1D	-3.70	120.41	125.88
11	L	305	LMT	O1B-C4'-C5'	3.70	119.59	109.45
8	D	101	BCL	C4C-CHD-C1D	-3.70	120.42	125.88
8	L	301	BCL	O2D-CGD-CBD	3.69	117.83	111.27
8	6	101	BCL	C1B-CHB-C4A	-3.69	122.81	130.12
15	y	102	CDL	OB6-CB5-C51	3.68	119.44	111.50
8	06	101	BCL	C4C-CHD-C1D	-3.68	120.46	125.88
8	6	101	BCL	CHD-C4C-NC	3.67	129.16	125.08
12	q	102	PGV	O01-C1-C2	3.67	119.42	111.50
14	2	102	SPO	C20-C19-C17	-3.67	122.07	127.31
8	6	101	BCL	CMB-C2B-C3B	3.67	131.55	124.68
14	01	103	SPO	C15-C14-C12	-3.67	122.07	127.31
8	5	102	BCL	C4C-CHD-C1D	-3.66	120.48	125.88
8	i	103	BCL	C1C-NC-C4C	-3.66	105.06	106.71
8	07	101	BCL	CMB-C2B-C3B	3.65	131.51	124.68
14	e	101	SPO	C34-C33-C35	3.65	121.41	115.27
8	08	102	BCL	C1C-NC-C4C	3.64	108.34	106.71
14	r	101	SPO	C10-C9-C7	-3.63	122.12	127.31
8	i	103	BCL	C4C-CHD-C1D	-3.63	120.53	125.88
14	f	101	SPO	C20-C21-C22	-3.63	116.04	123.47
8	L	311	BCL	C1-C2-C3	-3.62	119.78	126.04
14	y	105	SPO	C21-C22-C23	-3.62	122.14	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	v	102	SPO	C29-C28-C30	3.62	121.36	115.27
12	f	104	PGV	O01-C1-C2	3.61	119.28	111.50
8	L	301	BCL	C4C-CHD-C1D	-3.61	120.56	125.88
8	g	103	BCL	C4C-CHD-C1D	-3.61	120.56	125.88
14	a	102	SPO	C9-C10-C11	-3.60	111.98	123.22
14	M	406	SPO	C20-C19-C17	-3.59	122.18	127.31
8	05	101	BCL	C3C-C4C-CHD	-3.59	115.72	123.39
15	K	401	CDL	OB6-CB5-C51	3.59	119.23	111.50
14	g	102	SPO	C29-C28-C30	3.59	121.30	115.27
8	R	102	BCL	C3C-C4C-CHD	-3.58	115.73	123.39
14	05	103	SPO	C29-C28-C30	3.58	121.30	115.27
8	06	101	BCL	C1B-CHB-C4A	-3.58	123.03	130.12
8	L	311	BCL	C4C-CHD-C1D	-3.58	120.61	125.88
14	05	102	SPO	C31-C32-C33	-3.57	119.05	127.66
14	r	101	SPO	C34-C33-C35	3.57	121.28	115.27
14	B	101	SPO	C20-C19-C17	-3.57	122.21	127.31
14	Q	104	SPO	C31-C32-C33	-3.57	119.06	127.66
8	Y	102	BCL	C4C-CHD-C1D	-3.57	120.62	125.88
8	Q	103	BCL	C4C-CHD-C1D	-3.56	120.63	125.88
14	2	102	SPO	C21-C22-C23	-3.56	122.23	127.31
14	02	102	SPO	C29-C28-C30	3.55	121.25	115.27
8	4	101	BCL	C4A-NA-C1A	3.55	108.30	106.71
14	6	102	SPO	C20-C19-C17	-3.55	122.24	127.31
14	B	103	SPO	C5-C6-C7	-3.55	120.53	125.89
14	s	103	SPO	C21-C22-C23	-3.54	122.25	127.31
12	L	307	PGV	O01-C1-C2	3.54	119.14	111.50
8	b	101	BCL	C4C-CHD-C1D	-3.54	120.66	125.88
14	01	102	SPO	C20-C19-C17	-3.54	122.26	127.31
14	A	703	SPO	C20-C21-C22	-3.53	116.23	123.47
15	m	410	CDL	OA6-CA5-C11	3.53	119.11	111.50
14	O	102	SPO	C15-C14-C12	-3.52	122.28	127.31
8	4	101	BCL	C3C-C4C-CHD	-3.52	115.87	123.39
14	k	102	SPO	C20-C19-C17	-3.52	122.29	127.31
14	s	103	SPO	C20-C19-C17	-3.51	122.30	127.31
8	o	101	BCL	C4C-CHD-C1D	-3.51	120.70	125.88
8	K	402	BCL	C4C-CHD-C1D	-3.50	120.71	125.88
8	08	102	BCL	CHD-C4C-NC	3.49	128.95	125.08
14	2	102	SPO	C15-C14-C12	-3.49	122.33	127.31
14	P	101	SPO	C15-C14-C12	-3.49	122.34	127.31
14	V	102	SPO	C20-C19-C17	-3.48	122.34	127.31
14	G	101	SPO	C29-C28-C30	3.48	121.13	115.27
8	l	301	BCL	C4C-CHD-C1D	-3.48	120.75	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	j	101	SPO	C29-C28-C30	3.48	121.12	115.27
14	k	102	SPO	C29-C28-C30	3.47	121.11	115.27
14	6	102	SPO	C5-C6-C7	-3.47	120.65	125.89
8	d	101	BCL	CHC-C1C-NC	3.46	129.30	124.51
14	n	101	SPO	C34-C33-C35	3.46	121.09	115.27
14	2	101	SPO	C21-C20-C19	-3.45	116.40	123.47
14	M	406	SPO	C31-C32-C33	-3.45	119.36	127.66
8	y	103	BCL	C1-C2-C3	-3.45	120.08	126.04
14	02	102	SPO	C27-C26-C25	-3.45	112.46	123.22
8	f	102	BCL	CHB-C4A-NA	3.44	129.26	124.51
8	V	101	BCL	C1-C2-C3	-3.43	120.11	126.04
8	d	101	BCL	CAD-C3D-C4D	3.43	110.38	108.47
14	N	101	SPO	C20-C19-C17	-3.43	122.42	127.31
14	J	101	SPO	C21-C20-C19	-3.43	116.46	123.47
8	L	301	BCL	O2A-CGA-CBA	3.43	122.66	111.91
8	04	101	BCL	CHD-C4C-NC	3.42	128.88	125.08
8	R	102	BCL	C1-C2-C3	-3.42	120.12	126.04
8	I	102	BCL	C1-C2-C3	-3.42	120.13	126.04
12	L	309	PGV	C02-O01-C1	-3.41	109.40	117.79
8	M	401	BCL	C4C-CHD-C1D	-3.41	120.86	125.88
12	l	306	PGV	C02-O01-C1	-3.40	109.42	117.79
14	r	103	SPO	C20-C19-C17	-3.40	122.46	127.31
14	y	105	SPO	C27-C26-C25	-3.40	112.61	123.22
14	n	101	SPO	C29-C28-C30	3.40	120.99	115.27
8	M	402	BCL	C4C-CHD-C1D	-3.40	120.87	125.88
8	5	102	BCL	C1-C2-C3	-3.40	120.17	126.04
14	S	102	SPO	C29-C28-C30	3.39	120.98	115.27
14	s	105	SPO	C21-C20-C19	-3.39	116.53	123.47
8	5	102	BCL	CMB-C2B-C3B	3.39	131.02	124.68
12	x	101	PGV	O01-C1-C2	3.38	118.79	111.50
14	T	102	SPO	C34-C33-C35	3.38	120.96	115.27
11	h	803	LMT	O1B-C4'-C3'	3.38	116.27	107.28
8	06	101	BCL	CHD-C4C-NC	3.38	128.83	125.08
14	A	703	SPO	C21-C22-C23	-3.38	122.49	127.31
8	q	103	BCL	C4A-NA-C1A	3.38	108.22	106.71
14	g	101	SPO	C34-C33-C35	3.38	120.95	115.27
8	Z	101	BCL	C4C-CHD-C1D	-3.38	120.90	125.88
8	08	102	BCL	CMB-C2B-C3B	3.37	130.99	124.68
8	s	102	BCL	C4C-CHD-C1D	-3.37	120.90	125.88
8	j	102	BCL	C4C-CHD-C1D	-3.37	120.91	125.88
8	T	101	BCL	CMB-C2B-C3B	3.37	130.98	124.68
8	05	101	BCL	C4C-CHD-C1D	-3.37	120.91	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	03	102	BCL	O2A-CGA-CBA	3.37	122.47	111.91
8	k	101	BCL	C4C-CHD-C1D	-3.36	120.92	125.88
12	L	310	PGV	C02-O01-C1	-3.36	109.51	117.79
8	S	101	BCL	C1-C2-C3	-3.36	120.23	126.04
8	y	103	BCL	C4C-CHD-C1D	-3.36	120.92	125.88
8	w	102	BCL	C4C-CHD-C1D	-3.36	120.92	125.88
8	f	102	BCL	CHC-C1C-NC	3.35	129.15	124.51
14	2	102	SPO	C31-C32-C33	-3.35	119.59	127.66
8	s	102	BCL	C4-C3-C5	3.35	120.90	115.27
15	X	103	CDL	CB4-OB6-CB5	-3.35	109.56	117.79
8	o	101	BCL	C1-C2-C3	-3.34	120.26	126.04
14	N	101	SPO	C34-C33-C35	3.34	120.89	115.27
14	O	102	SPO	C9-C10-C11	-3.34	112.79	123.22
8	1	202	BCL	C1-C2-C3	-3.34	120.27	126.04
8	Q	103	BCL	C1-C2-C3	-3.34	120.27	126.04
8	i	103	BCL	CHC-C1C-NC	3.34	129.12	124.51
8	M	401	BCL	C1-C2-C3	-3.34	120.28	126.04
8	d	101	BCL	C4C-CHD-C1D	-3.33	120.96	125.88
8	S	101	BCL	C4C-CHD-C1D	-3.33	120.97	125.88
8	m	403	BCL	C4C-CHD-C1D	-3.33	120.97	125.88
8	f	102	BCL	CAD-C3D-C4D	3.33	110.33	108.47
8	01	101	BCL	C4C-CHD-C1D	-3.33	120.97	125.88
14	T	102	SPO	C20-C19-C17	-3.32	122.57	127.31
8	p	102	BCL	C1-C2-C3	-3.32	120.30	126.04
14	4	102	SPO	C29-C28-C30	3.32	120.85	115.27
8	j	102	BCL	C4-C3-C5	3.31	120.84	115.27
14	B	103	SPO	C29-C28-C30	3.31	120.83	115.27
14	5	103	SPO	C31-C32-C33	-3.30	119.72	127.66
14	O	102	SPO	C29-C28-C30	3.30	120.82	115.27
12	Q	102	PGV	O03-C19-C20	3.29	120.02	111.38
8	m	401	BCL	O2D-CGD-O1D	-3.29	117.40	123.84
14	g	102	SPO	C34-C33-C35	3.29	120.81	115.27
8	W	101	BCL	CMB-C2B-C3B	3.29	130.83	124.68
8	y	103	BCL	C1C-NC-C4C	-3.28	105.23	106.71
8	v	101	BCL	C4-C3-C5	3.28	120.79	115.27
14	n	103	SPO	C34-C33-C35	3.28	120.79	115.27
14	k	102	SPO	C9-C10-C11	-3.28	112.98	123.22
14	f	101	SPO	C9-C10-C11	-3.27	113.01	123.22
11	H	802	LMT	C1-O1'-C1'	-3.27	108.42	113.84
14	B	103	SPO	C21-C22-C23	-3.27	122.65	127.31
14	3	103	SPO	C21-C20-C19	-3.27	116.78	123.47
8	g	103	BCL	C1-C2-C3	-3.27	120.40	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	S	102	SPO	C21-C20-C19	-3.26	116.79	123.47
8	07	101	BCL	C1-C2-C3	-3.26	120.40	126.04
8	r	102	BCL	C4C-CHD-C1D	-3.26	121.07	125.88
8	Y	102	BCL	C4-C3-C5	3.26	120.75	115.27
14	2	104	SPO	C29-C28-C30	3.25	120.74	115.27
8	6	101	BCL	C4C-CHD-C1D	-3.25	121.08	125.88
14	P	101	SPO	C34-C33-C35	3.25	120.74	115.27
8	m	402	BCL	C4C-CHD-C1D	-3.25	121.08	125.88
8	7	101	BCL	CMB-C2B-C3B	3.25	130.75	124.68
8	p	102	BCL	C4C-CHD-C1D	-3.24	121.09	125.88
14	w	101	SPO	C10-C9-C7	-3.24	122.68	127.31
14	R	101	SPO	C5-C6-C7	-3.24	120.99	125.89
8	V	101	BCL	C4-C3-C5	3.24	120.73	115.27
8	l	301	BCL	C4-C3-C5	3.23	120.71	115.27
14	k	102	SPO	C21-C22-C23	-3.23	122.69	127.31
8	B	102	BCL	CHB-C4A-NA	3.23	128.98	124.51
14	Q	104	SPO	C21-C22-C23	-3.23	122.70	127.31
14	01	103	SPO	C9-C10-C11	-3.23	113.15	123.22
8	6	101	BCL	C1-C2-C3	-3.22	120.47	126.04
8	2	103	BCL	C1B-CHB-C4A	-3.22	123.74	130.12
14	r	103	SPO	C21-C22-C23	-3.21	122.72	127.31
8	t	101	BCL	C4C-CHD-C1D	-3.21	121.14	125.88
8	8	101	BCL	C1C-NC-C4C	3.21	108.15	106.71
8	F	502	BCL	C4C-CHD-C1D	-3.20	121.16	125.88
14	f	106	SPO	C34-C33-C35	3.20	120.66	115.27
14	I	103	SPO	C21-C20-C19	-3.20	116.92	123.47
8	m	403	BCL	CAA-C2A-C3A	-3.20	104.02	112.78
8	2	103	BCL	C4C-CHD-C1D	-3.20	121.16	125.88
14	08	101	SPO	C29-C28-C30	3.20	120.65	115.27
14	05	103	SPO	C34-C33-C35	3.20	120.65	115.27
8	F	502	BCL	CHC-C1C-NC	3.20	128.93	124.51
14	v	102	SPO	C9-C10-C11	-3.19	113.26	123.22
8	k	101	BCL	CHC-C1C-NC	3.19	128.93	124.51
8	z	102	BCL	C4-C3-C5	3.19	120.64	115.27
14	J	101	SPO	C31-C32-C33	-3.19	119.99	127.66
8	01	101	BCL	C1-C2-C3	-3.19	120.53	126.04
14	n	101	SPO	C20-C19-C17	-3.19	122.76	127.31
8	G	102	BCL	C1-C2-C3	-3.19	120.53	126.04
8	Q	103	BCL	C1C-NC-C4C	-3.19	105.27	106.71
8	L	301	BCL	C4-C3-C5	3.18	120.63	115.27
8	W	101	BCL	C4C-CHD-C1D	-3.18	121.19	125.88
8	8	101	BCL	C3C-C4C-CHD	-3.18	116.61	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	O	101	BCL	C4C-CHD-C1D	-3.18	121.19	125.88
8	b	101	BCL	C2A-C1A-CHA	-3.18	118.31	123.86
14	01	103	SPO	C31-C32-C33	-3.18	120.02	127.66
14	s	105	SPO	C29-C28-C30	3.17	120.61	115.27
8	K	402	BCL	C4-C3-C5	3.17	120.61	115.27
14	w	101	SPO	C31-C32-C33	-3.17	120.04	127.66
8	E	101	BCL	CAD-C3D-C4D	3.16	110.23	108.47
8	n	102	BCL	C4C-CHD-C1D	-3.16	121.22	125.88
14	N	101	SPO	C15-C14-C12	-3.16	122.81	127.31
8	I	102	BCL	CHC-C1C-NC	3.15	128.87	124.51
8	V	101	BCL	O2D-CGD-O1D	-3.15	117.69	123.84
8	3	102	BCL	C4-C3-C5	3.15	120.56	115.27
14	R	101	SPO	C29-C28-C30	3.14	120.56	115.27
8	v	101	BCL	C1-C2-C3	-3.14	120.61	126.04
12	l	308	PGV	O03-C19-C20	3.14	119.62	111.38
8	F	502	BCL	C1C-NC-C4C	-3.14	105.30	106.71
14	E	102	SPO	C34-C33-C35	3.14	120.55	115.27
8	z	102	BCL	O2A-CGA-CBA	3.13	121.74	111.91
8	L	311	BCL	O2D-CGD-O1D	-3.13	117.72	123.84
8	02	101	BCL	C4-C3-C5	3.13	120.54	115.27
8	z	102	BCL	C4C-CHD-C1D	-3.13	121.26	125.88
14	6	102	SPO	C31-C32-C33	-3.13	120.13	127.66
8	E	101	BCL	C4-C3-C5	3.13	120.53	115.27
8	F	502	BCL	C4-C3-C5	3.13	120.53	115.27
14	g	101	SPO	C20-C19-C17	-3.13	122.85	127.31
8	03	102	BCL	C4C-CHD-C1D	-3.13	121.27	125.88
8	F	502	BCL	CHB-C4A-NA	3.12	128.83	124.51
14	E	102	SPO	C10-C9-C7	-3.12	122.86	127.31
14	f	106	SPO	C9-C10-C11	-3.12	113.48	123.22
8	P	102	BCL	C4C-CHD-C1D	-3.12	121.28	125.88
8	o	101	BCL	CHC-C1C-NC	3.12	128.82	124.51
14	6	102	SPO	C29-C28-C30	3.12	120.51	115.27
14	s	105	SPO	C9-C10-C11	-3.11	113.50	123.22
8	02	101	BCL	O2A-CGA-CBA	3.11	121.68	111.91
14	q	104	SPO	C15-C14-C12	-3.11	122.87	127.31
8	n	102	BCL	C1-C2-C3	-3.11	120.66	126.04
8	I	102	BCL	C1C-NC-C4C	-3.11	105.31	106.71
14	T	102	SPO	C21-C22-C23	-3.11	122.88	127.31
8	B	102	BCL	C4-C3-C5	3.11	120.50	115.27
14	q	104	SPO	C21-C22-C23	-3.10	122.88	127.31
8	l	301	BCL	O2A-CGA-CBA	3.10	121.64	111.91
14	6	102	SPO	C21-C20-C19	-3.10	117.12	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	p	102	BCL	C4-C3-C5	3.10	120.48	115.27
14	I	103	SPO	C29-C28-C30	3.10	120.48	115.27
8	d	101	BCL	C1-C2-C3	-3.10	120.69	126.04
8	r	102	BCL	O2A-CGA-CBA	3.09	121.62	111.91
8	d	101	BCL	CHB-C4A-NA	3.09	128.79	124.51
14	y	105	SPO	C31-C32-C33	-3.09	120.21	127.66
15	X	102	CDL	CA4-OA6-CA5	-3.09	110.18	117.79
14	E	102	SPO	C5-C6-C7	-3.09	121.23	125.89
8	W	101	BCL	C1-C2-C3	-3.09	120.70	126.04
8	1	202	BCL	C4C-CHD-C1D	-3.08	121.33	125.88
14	N	101	SPO	C10-C9-C7	-3.08	122.91	127.31
8	s	102	BCL	CHC-C1C-NC	3.08	128.77	124.51
14	P	101	SPO	C29-C28-C30	3.08	120.45	115.27
14	01	103	SPO	C29-C28-C30	3.08	120.45	115.27
8	V	101	BCL	C4C-CHD-C1D	-3.08	121.34	125.88
14	B	103	SPO	C34-C33-C35	3.08	120.45	115.27
11	L	306	LMT	O1B-C4'-C3'	3.08	115.47	107.28
14	Y	103	SPO	C31-C32-C33	-3.08	120.25	127.66
8	D	101	BCL	C1C-NC-C4C	-3.07	105.32	106.71
8	k	101	BCL	C1-C2-C3	-3.07	120.73	126.04
8	E	101	BCL	CHB-C4A-NA	3.07	128.76	124.51
8	Y	102	BCL	C1C-NC-C4C	-3.07	105.33	106.71
14	n	103	SPO	C10-C9-C7	-3.07	122.93	127.31
12	F	503	PGV	O03-C19-C20	3.07	121.53	111.91
11	L	305	LMT	C1B-C2B-C3B	3.07	116.38	110.00
14	G	101	SPO	C31-C32-C33	-3.07	120.28	127.66
14	2	104	SPO	C31-C32-C33	-3.06	120.29	127.66
14	G	101	SPO	C21-C22-C23	-3.06	122.94	127.31
14	6	102	SPO	C34-C33-C35	3.06	120.42	115.27
8	07	101	BCL	C1C-NC-C4C	-3.06	105.33	106.71
8	Z	101	BCL	C4B-CHC-C1C	-3.06	124.06	130.12
8	e	102	BCL	O2A-CGA-CBA	3.06	121.50	111.91
14	2	104	SPO	C20-C19-C17	-3.05	122.95	127.31
8	E	101	BCL	C1-C2-C3	-3.05	120.77	126.04
14	Y	103	SPO	C5-C6-C7	-3.05	121.28	125.89
8	04	101	BCL	C4A-NA-C1A	3.05	108.08	106.71
8	M	401	BCL	O2A-CGA-CBA	3.05	121.47	111.91
12	f	103	PGV	O03-C19-C20	3.05	121.46	111.91
14	T	102	SPO	C29-C28-C30	3.04	120.39	115.27
8	i	103	BCL	CAC-C3C-C4C	-3.04	105.83	112.58
8	02	101	BCL	C1-C2-C3	-3.04	120.78	126.04
8	04	101	BCL	C4C-CHD-C1D	-3.04	121.39	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	08	102	BCL	C4B-CHC-C1C	-3.04	124.09	130.12
14	g	102	SPO	C20-C19-C17	-3.04	122.97	127.31
12	K	403	PGV	C02-O01-C1	-3.04	110.31	117.79
8	e	102	BCL	CHB-C4A-NA	3.04	128.71	124.51
14	g	101	SPO	C31-C32-C33	-3.04	120.35	127.66
8	8	101	BCL	O2D-CGD-O1D	-3.04	117.90	123.84
14	02	102	SPO	C20-C19-C17	-3.03	122.98	127.31
8	4	101	BCL	C1-C2-C3	-3.03	120.80	126.04
14	N	101	SPO	C5-C6-C7	-3.03	121.31	125.89
8	p	102	BCL	O2A-CGA-CBA	3.03	121.43	111.91
14	B	101	SPO	C21-C20-C19	-3.03	117.26	123.47
8	N	102	BCL	C4C-CHD-C1D	-3.03	121.41	125.88
8	b	101	BCL	CHB-C4A-NA	3.03	128.70	124.51
8	t	101	BCL	CHB-C4A-NA	3.02	128.69	124.51
8	E	101	BCL	O2A-CGA-CBA	3.02	121.38	111.91
14	S	103	SPO	C31-C32-C33	-3.02	120.39	127.66
14	G	103	SPO	C20-C21-C22	-3.02	117.30	123.47
14	T	102	SPO	C15-C14-C12	-3.02	123.01	127.31
14	A	703	SPO	C9-C10-C11	-3.01	113.81	123.22
8	2	103	BCL	O2A-CGA-CBA	3.01	121.36	111.91
14	a	102	SPO	C29-C28-C30	3.01	120.34	115.27
8	P	102	BCL	C4-C3-C5	3.01	120.34	115.27
8	n	102	BCL	O2A-CGA-CBA	3.01	121.36	111.91
15	X	103	CDL	CA4-OA6-CA5	-3.01	110.38	117.79
8	02	101	BCL	C4C-CHD-C1D	-3.01	121.44	125.88
8	04	101	BCL	C1C-NC-C4C	3.01	108.06	106.71
8	J	102	BCL	O2A-CGA-CBA	3.01	121.34	111.91
8	v	101	BCL	C4C-CHD-C1D	-3.01	121.44	125.88
14	s	103	SPO	C29-C28-C30	3.00	120.33	115.27
8	r	102	BCL	C4-C3-C5	3.00	120.32	115.27
14	y	105	SPO	C34-C33-C35	3.00	120.32	115.27
14	08	101	SPO	C34-C33-C35	3.00	120.32	115.27
14	G	103	SPO	C29-C28-C30	3.00	120.32	115.27
8	w	102	BCL	O2A-CGA-CBA	3.00	121.31	111.91
8	D	101	BCL	CHC-C1C-NC	2.99	128.65	124.51
14	I	103	SPO	C31-C32-C33	-2.99	120.45	127.66
14	M	406	SPO	C15-C14-C12	-2.99	123.04	127.31
8	T	101	BCL	C4C-CHD-C1D	-2.99	121.47	125.88
8	3	102	BCL	C4C-CHD-C1D	-2.98	121.48	125.88
14	A	703	SPO	C34-C33-C35	2.98	120.29	115.27
8	V	101	BCL	CHB-C4A-NA	2.98	128.64	124.51
12	H	804	PGV	C02-O01-C1	-2.98	110.46	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	f	101	SPO	C27-C26-C25	-2.98	113.92	123.22
14	K	404	SPO	C34-C33-C35	2.98	120.28	115.27
14	S	102	SPO	C5-C6-C7	-2.98	121.39	125.89
8	4	101	BCL	C4C-CHD-C1D	-2.98	121.49	125.88
8	t	101	BCL	C1-C2-C3	-2.97	120.91	126.04
8	5	102	BCL	C4-C3-C5	2.97	120.27	115.27
14	Q	104	SPO	C29-C28-C30	2.97	120.27	115.27
14	02	102	SPO	C34-C33-C35	2.97	120.27	115.27
8	2	103	BCL	CMB-C2B-C3B	2.97	130.23	124.68
8	B	102	BCL	O2D-CGD-O1D	-2.97	118.04	123.84
8	04	101	BCL	C1-C2-C3	-2.96	120.92	126.04
12	f	103	PGV	C02-O01-C1	-2.96	110.50	117.79
12	H	801	PGV	O03-C19-C20	2.96	121.20	111.91
8	5	102	BCL	C4B-CHC-C1C	-2.96	124.26	130.12
8	01	101	BCL	O2A-CGA-CBA	2.96	121.19	111.91
14	p	101	SPO	C15-C14-C12	-2.96	123.09	127.31
8	Z	101	BCL	CMB-C2B-C3B	2.96	130.21	124.68
14	B	101	SPO	C9-C10-C11	-2.95	114.00	123.22
8	f	102	BCL	C4C-CHD-C1D	-2.95	121.52	125.88
8	E	101	BCL	C4C-CHD-C1D	-2.95	121.53	125.88
8	T	101	BCL	C4B-CHC-C1C	-2.95	124.28	130.12
8	b	101	BCL	CHC-C1C-NC	2.94	128.58	124.51
14	B	101	SPO	C15-C14-C12	-2.94	123.11	127.31
8	M	402	BCL	C1-C2-C3	-2.94	120.95	126.04
8	W	101	BCL	C4B-CHC-C1C	-2.94	124.30	130.12
8	4	101	BCL	O2A-CGA-CBA	2.94	121.13	111.91
8	06	101	BCL	C4-C3-C5	2.94	120.21	115.27
14	3	103	SPO	C34-C33-C35	2.93	120.20	115.27
8	02	101	BCL	C4B-CHC-C1C	-2.93	124.31	130.12
8	G	102	BCL	C4C-CHD-C1D	-2.93	121.56	125.88
11	m	409	LMT	C1B-O1B-C4'	-2.93	110.72	117.96
8	B	102	BCL	C4C-CHD-C1D	-2.92	121.57	125.88
8	i	103	BCL	C1-C2-C3	-2.92	120.99	126.04
8	q	103	BCL	CHC-C1C-NC	2.92	128.55	124.51
14	B	101	SPO	C10-C9-C7	-2.92	123.15	127.31
8	q	103	BCL	O2A-CGA-CBA	2.91	121.05	111.91
14	T	102	SPO	C31-C32-C33	-2.91	120.64	127.66
14	4	102	SPO	C15-C14-C12	-2.91	123.15	127.31
8	M	402	BCL	CHB-C4A-NA	2.91	128.54	124.51
8	D	101	BCL	O2A-CGA-CBA	2.91	121.05	111.91
8	m	402	BCL	C1-C2-C3	-2.91	121.01	126.04
12	l	305	PGV	O03-C19-C20	2.91	121.04	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	J	101	SPO	C15-C14-C12	-2.91	123.16	127.31
14	J	101	SPO	C29-C28-C30	2.91	120.17	115.27
8	g	103	BCL	C4-C3-C5	2.91	120.16	115.27
14	3	103	SPO	C20-C19-C17	-2.90	123.17	127.31
14	01	102	SPO	C29-C28-C30	2.90	120.16	115.27
14	r	103	SPO	C31-C32-C33	-2.90	120.67	127.66
8	1	202	BCL	C4-C3-C5	2.90	120.16	115.27
14	g	101	SPO	C9-C10-C11	-2.90	114.16	123.22
8	05	101	BCL	O2A-CGA-CBA	2.90	121.02	111.91
8	e	102	BCL	C4-C3-C5	2.90	120.15	115.27
8	N	102	BCL	C1-C2-C3	-2.90	121.03	126.04
8	05	101	BCL	CHB-C4A-NA	2.90	128.52	124.51
14	V	102	SPO	C34-C33-C35	2.90	120.14	115.27
14	Y	103	SPO	C20-C19-C17	-2.90	123.18	127.31
14	2	102	SPO	C29-C28-C30	2.89	120.14	115.27
14	j	101	SPO	C21-C20-C19	-2.89	117.55	123.47
8	L	311	BCL	C4-C3-C5	2.89	120.13	115.27
14	n	103	SPO	C21-C22-C23	-2.89	123.19	127.31
8	02	101	BCL	C1B-CHB-C4A	-2.88	124.41	130.12
8	g	103	BCL	CHB-C4A-NA	2.88	128.50	124.51
14	J	101	SPO	C9-C10-C11	-2.88	114.23	123.22
8	M	401	BCL	C4-C3-C5	2.88	120.11	115.27
14	G	103	SPO	C21-C22-C23	-2.88	123.20	127.31
8	S	101	BCL	C4-C3-C5	2.88	120.11	115.27
8	6	101	BCL	C3C-C4C-CHD	-2.87	117.25	123.39
8	T	101	BCL	C4-C3-C5	2.87	120.11	115.27
8	j	102	BCL	O2A-CGA-CBA	2.87	120.92	111.91
8	B	102	BCL	CAD-C3D-C4D	2.87	110.07	108.47
8	8	101	BCL	C4B-CHC-C1C	-2.87	124.44	130.12
14	08	101	SPO	C31-C32-C33	-2.87	120.75	127.66
14	3	103	SPO	C9-C10-C11	-2.87	114.27	123.22
8	4	101	BCL	C4-C3-C5	2.87	120.09	115.27
12	h	801	PGV	O03-C19-C20	2.87	120.90	111.91
8	1	202	BCL	CHC-C1C-NC	2.87	128.47	124.51
14	v	102	SPO	C31-C32-C33	-2.86	120.77	127.66
8	Q	103	BCL	O2A-CGA-CBA	2.86	120.89	111.91
8	J	102	BCL	O2D-CGD-O1D	-2.86	118.25	123.84
8	m	402	BCL	O2D-CGD-O1D	-2.86	118.25	123.84
14	5	103	SPO	C13-C12-C11	2.86	122.58	118.08
14	B	103	SPO	C20-C19-C17	-2.86	123.23	127.31
8	K	402	BCL	CHC-C1C-NC	2.86	128.46	124.51
14	02	102	SPO	C31-C32-C33	-2.85	120.79	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	j	101	SPO	C34-C33-C35	2.85	120.07	115.27
14	S	102	SPO	C13-C12-C11	2.85	122.57	118.08
14	z	101	SPO	C15-C14-C12	-2.85	123.24	127.31
14	w	101	SPO	C29-C28-C30	2.85	120.07	115.27
8	m	401	BCL	C4-C3-C5	2.85	120.07	115.27
8	t	101	BCL	C4-C3-C5	2.85	120.07	115.27
14	r	101	SPO	C14-C15-C16	-2.85	114.32	123.22
8	G	102	BCL	C4-C3-C5	2.85	120.06	115.27
8	M	402	BCL	O2A-CGA-CBA	2.85	120.85	111.91
8	b	101	BCL	CAD-C3D-C4D	2.85	110.06	108.47
8	y	103	BCL	CHC-C1C-NC	2.85	128.45	124.51
14	K	404	SPO	C9-C10-C11	-2.85	114.33	123.22
8	T	101	BCL	O2A-CGA-CBA	2.85	120.84	111.91
14	05	102	SPO	C29-C28-C30	2.85	120.06	115.27
14	q	104	SPO	C34-C33-C35	2.84	120.06	115.27
8	p	102	BCL	CHB-C4A-NA	2.84	128.44	124.51
14	5	103	SPO	C14-C15-C16	-2.84	114.35	123.22
8	M	402	BCL	CAA-C2A-C3A	-2.84	104.99	112.78
8	O	101	BCL	CHC-C1C-NC	2.84	128.44	124.51
8	a	101	BCL	C4C-CHD-C1D	-2.84	121.69	125.88
12	H	805	PGV	O03-C19-C20	2.84	120.81	111.91
14	J	101	SPO	C34-C33-C35	2.83	120.04	115.27
8	1	202	BCL	O2A-CGA-CBA	2.83	120.80	111.91
8	I	102	BCL	C4-C3-C5	2.83	120.03	115.27
8	i	103	BCL	CHB-C4A-NA	2.83	128.42	124.51
8	f	102	BCL	C1-C2-C3	-2.83	121.15	126.04
14	R	101	SPO	C13-C12-C14	-2.83	118.96	122.92
14	G	101	SPO	C9-C10-C11	-2.83	114.39	123.22
8	z	102	BCL	C1-C2-C3	-2.83	121.15	126.04
8	e	102	BCL	C2A-C1A-CHA	-2.83	118.92	123.86
8	7	101	BCL	C4-C3-C5	2.82	120.02	115.27
14	v	102	SPO	C13-C12-C11	2.82	122.53	118.08
14	2	101	SPO	C20-C19-C17	-2.82	123.28	127.31
8	Y	102	BCL	O2A-CGA-CBA	2.82	120.76	111.91
8	7	101	BCL	O2A-CGA-CBA	2.82	120.75	111.91
14	g	102	SPO	C21-C20-C19	-2.82	117.70	123.47
8	05	101	BCL	C4-C3-C5	2.82	120.01	115.27
8	2	103	BCL	C4-C3-C5	2.81	120.00	115.27
14	K	404	SPO	C29-C28-C30	2.81	120.00	115.27
14	05	102	SPO	C9-C10-C11	-2.81	114.44	123.22
8	g	103	BCL	O2A-CGA-CBA	2.81	120.74	111.91
8	D	101	BCL	CHB-C4A-NA	2.81	128.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	502	BCL	O2A-CGA-CBA	2.81	120.73	111.91
14	r	103	SPO	C14-C15-C16	-2.81	114.44	123.22
14	V	102	SPO	C31-C32-C33	-2.81	120.89	127.66
8	Q	103	BCL	CHC-C1C-NC	2.81	128.40	124.51
8	O	101	BCL	C4-C3-C5	2.81	120.00	115.27
14	p	101	SPO	C31-C32-C33	-2.81	120.90	127.66
8	v	101	BCL	CHC-C1C-NC	2.80	128.39	124.51
14	R	101	SPO	C21-C20-C19	-2.80	117.73	123.47
8	A	702	BCL	C1-C2-C3	-2.80	121.20	126.04
14	y	105	SPO	C21-C20-C19	-2.80	117.74	123.47
8	o	101	BCL	O2A-CGA-CBA	2.80	120.70	111.91
8	L	311	BCL	CHC-C1C-NC	2.80	128.38	124.51
8	I	102	BCL	O2A-CGA-CBA	2.80	120.69	111.91
8	K	402	BCL	CHB-C4A-NA	2.80	128.38	124.51
8	J	102	BCL	C4C-CHD-C1D	-2.80	121.75	125.88
14	a	102	SPO	C10-C9-C7	-2.80	123.32	127.31
14	O	102	SPO	C31-C32-C33	-2.79	120.93	127.66
8	A	702	BCL	C4-C3-C5	2.79	119.97	115.27
8	R	102	BCL	C4C-CHD-C1D	-2.79	121.76	125.88
14	3	103	SPO	C31-C32-C33	-2.79	120.94	127.66
8	n	102	BCL	CHC-C1C-NC	2.79	128.37	124.51
8	J	102	BCL	C4-C3-C5	2.79	119.96	115.27
8	S	101	BCL	C4A-NA-C1A	2.78	107.96	106.71
8	q	103	BCL	C1C-NC-C4C	-2.78	105.45	106.71
14	3	103	SPO	C15-C14-C12	-2.78	123.34	127.31
8	W	101	BCL	O2A-CGA-CBA	2.78	120.63	111.91
8	3	102	BCL	C1-C2-C3	-2.78	121.24	126.04
8	t	101	BCL	O2A-CGA-CBA	2.78	120.62	111.91
8	p	102	BCL	CHC-C1C-NC	2.78	128.35	124.51
14	v	102	SPO	C15-C14-C12	-2.78	123.35	127.31
15	X	103	CDL	OB8-CB7-C71	2.77	120.61	111.91
14	p	101	SPO	C34-C33-C35	2.77	119.94	115.27
8	03	102	BCL	C1-C2-C3	-2.77	121.25	126.04
8	01	101	BCL	CHB-C4A-NA	2.77	128.34	124.51
8	m	401	BCL	CHC-C1C-NC	2.77	128.34	124.51
14	g	101	SPO	C29-C28-C30	2.77	119.92	115.27
8	08	102	BCL	C3C-C4C-CHD	-2.77	117.48	123.39
14	q	104	SPO	C31-C32-C33	-2.77	121.00	127.66
8	Z	101	BCL	C4-C3-C5	2.76	119.92	115.27
14	f	101	SPO	C21-C22-C23	-2.76	123.36	127.31
9	M	403	BPH	CMA-C3A-C4A	-2.76	108.32	114.38
8	t	101	BCL	CHC-C1C-NC	2.76	128.33	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	05	103	SPO	C31-C32-C33	-2.76	121.01	127.66
15	x	102	CDL	OA6-CA5-C11	2.76	120.58	111.91
8	5	102	BCL	CHD-C4C-NC	2.76	128.14	125.08
14	S	103	SPO	C21-C20-C19	-2.76	117.82	123.47
8	f	102	BCL	O2D-CGD-O1D	-2.76	118.44	123.84
14	f	106	SPO	C31-C32-C33	-2.76	121.02	127.66
14	g	101	SPO	C21-C20-C19	-2.75	117.83	123.47
14	r	101	SPO	C26-C25-C23	-2.75	118.68	126.42
14	r	101	SPO	C21-C20-C19	-2.75	117.84	123.47
14	f	101	SPO	C14-C15-C16	-2.75	114.63	123.22
8	k	101	BCL	C4-C3-C5	2.75	119.90	115.27
8	6	101	BCL	O2A-CGA-CBA	2.75	120.53	111.91
14	n	103	SPO	C29-C28-C30	2.75	119.89	115.27
8	G	102	BCL	O2D-CGD-O1D	-2.75	118.47	123.84
12	h	806	PGV	O03-C19-C20	2.74	120.52	111.91
8	n	102	BCL	CHB-C4A-NA	2.74	128.31	124.51
8	6	101	BCL	C4-C3-C5	2.74	119.88	115.27
8	m	403	BCL	CHB-C4A-NA	2.74	128.30	124.51
8	P	102	BCL	C2A-C1A-CHA	-2.74	119.07	123.86
14	B	103	SPO	C10-C9-C7	-2.74	123.40	127.31
8	G	102	BCL	O2A-CGA-CBA	2.74	120.51	111.91
8	I	102	BCL	CHB-C4A-NA	2.74	128.30	124.51
8	o	101	BCL	C4A-NA-C1A	2.74	107.94	106.71
8	f	102	BCL	C4-C3-C5	2.74	119.88	115.27
12	k	103	PGV	O03-C19-C20	2.74	120.49	111.91
8	3	102	BCL	O2A-CGA-CBA	2.73	120.48	111.91
14	R	101	SPO	C34-C33-C35	2.73	119.87	115.27
8	y	103	BCL	C4A-NA-C1A	2.73	107.93	106.71
8	7	101	BCL	C1-C2-C3	-2.73	121.32	126.04
14	r	103	SPO	C10-C9-C7	-2.73	123.41	127.31
8	Y	102	BCL	CHB-C4A-NA	2.73	128.28	124.51
11	03	101	LMT	O1B-C4'-C3'	2.72	114.53	107.28
8	w	102	BCL	C4-C3-C5	2.72	119.85	115.27
14	V	102	SPO	C9-C10-C11	-2.72	114.72	123.22
14	5	103	SPO	C29-C28-C30	2.72	119.85	115.27
8	03	102	BCL	C4-C3-C5	2.72	119.85	115.27
14	2	102	SPO	C34-C33-C35	2.72	119.85	115.27
8	Y	102	BCL	CAD-C3D-C4D	2.72	109.99	108.47
8	08	102	BCL	C4C-CHD-C1D	-2.72	121.87	125.88
11	U	103	LMT	C1B-O1B-C4'	-2.72	111.24	117.96
15	y	102	CDL	OA8-CA7-C31	2.72	120.44	111.91
12	K	403	PGV	O03-C19-C20	2.71	120.43	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	703	SPO	C15-C14-C12	-2.71	123.44	127.31
8	l	301	BCL	CED-O2D-CGD	2.71	122.07	115.94
8	g	103	BCL	C2A-C1A-CHA	-2.71	119.12	123.86
12	q	102	PGV	O03-C19-C20	2.71	120.41	111.91
8	z	102	BCL	CHB-C4A-NA	2.71	128.25	124.51
14	q	104	SPO	C9-C10-C11	-2.71	114.77	123.22
14	K	404	SPO	C14-C15-C16	-2.70	114.78	123.22
8	L	311	BCL	C1-O2A-CGA	2.70	123.53	116.44
15	m	413	CDL	OA8-CA7-C31	2.70	120.38	111.91
8	L	301	BCL	CHC-C1C-NC	2.70	128.25	124.51
14	S	102	SPO	C40-C38-C39	2.70	120.57	114.60
14	B	103	SPO	C15-C14-C12	-2.70	123.46	127.31
8	r	102	BCL	CHB-C4A-NA	2.70	128.24	124.51
14	N	101	SPO	C29-C28-C30	2.70	119.81	115.27
8	P	102	BCL	O2A-CGA-CBA	2.70	120.37	111.91
8	B	102	BCL	CHC-C1C-NC	2.70	128.24	124.51
14	M	406	SPO	C9-C10-C11	-2.70	114.80	123.22
8	z	102	BCL	C2A-C1A-CHA	-2.69	119.15	123.86
14	Y	103	SPO	C21-C20-C19	-2.69	117.96	123.47
14	01	103	SPO	C34-C33-C35	2.69	119.80	115.27
8	o	101	BCL	CHB-C4A-NA	2.69	128.23	124.51
8	o	101	BCL	O2D-CGD-O1D	-2.69	118.58	123.84
14	s	105	SPO	C14-C15-C16	-2.69	114.82	123.22
8	t	101	BCL	O2D-CGD-O1D	-2.69	118.58	123.84
14	05	103	SPO	C21-C20-C19	-2.69	117.96	123.47
11	L	305	LMT	C1B-O5B-C5B	-2.69	108.41	113.69
14	a	102	SPO	C34-C33-C35	2.69	119.79	115.27
14	n	101	SPO	C27-C26-C25	-2.69	114.84	123.22
8	D	101	BCL	C4-C3-C5	2.68	119.78	115.27
8	R	102	BCL	C4-C3-C5	2.68	119.78	115.27
8	O	101	BCL	O2A-CGA-CBA	2.68	120.31	111.91
15	m	410	CDL	OB8-CB7-C71	2.68	120.31	111.91
8	S	101	BCL	CBA-CAA-C2A	-2.68	105.97	113.86
8	04	101	BCL	O2A-CGA-CBA	2.68	120.30	111.91
12	m	411	PGV	C02-O01-C1	-2.67	111.21	117.79
8	07	101	BCL	O2A-CGA-CBA	2.67	120.29	111.91
8	q	103	BCL	C4-C3-C5	2.67	119.76	115.27
14	r	103	SPO	C34-C33-C35	2.67	119.76	115.27
14	3	103	SPO	C29-C28-C30	2.66	119.75	115.27
8	08	102	BCL	O2D-CGD-O1D	-2.66	118.63	123.84
14	v	102	SPO	C27-C26-C25	-2.66	114.91	123.22
8	1	202	BCL	CAD-C3D-C4D	2.66	109.95	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	v	102	SPO	C34-C33-C35	2.66	119.75	115.27
12	m	411	PGV	O03-C19-C20	2.66	120.25	111.91
14	Q	104	SPO	C34-C33-C35	2.66	119.74	115.27
14	S	103	SPO	C34-C33-C35	2.66	119.74	115.27
8	v	101	BCL	CHB-C4A-NA	2.66	128.19	124.51
15	X	101	CDL	OB8-CB7-C71	2.66	120.24	111.91
14	q	104	SPO	C20-C21-C22	-2.66	118.03	123.47
8	O	101	BCL	C1C-NC-C4C	-2.65	105.51	106.71
15	X	103	CDL	OA8-CA7-C31	2.65	120.23	111.91
8	E	101	BCL	CHC-C1C-NC	2.65	128.18	124.51
8	04	101	BCL	C3C-C4C-CHD	-2.65	117.72	123.39
8	e	102	BCL	CHC-C1C-NC	2.65	128.18	124.51
8	G	102	BCL	CHC-C1C-NC	2.65	128.18	124.51
8	v	101	BCL	C4A-NA-C1A	2.65	107.90	106.71
8	y	103	BCL	O2A-CGA-CBA	2.65	120.21	111.91
8	A	702	BCL	CHB-C4A-NA	2.65	128.17	124.51
14	p	101	SPO	C9-C10-C11	-2.65	114.96	123.22
8	a	101	BCL	CHB-C4A-NA	2.64	128.17	124.51
14	B	101	SPO	C36-C37-C38	-2.64	118.72	127.75
14	V	102	SPO	C21-C20-C19	-2.64	118.06	123.47
8	K	402	BCL	O2A-CGA-CBA	2.64	120.19	111.91
8	3	102	BCL	CAD-C3D-C4D	2.64	109.94	108.47
8	08	102	BCL	O2A-CGA-CBA	2.64	120.19	111.91
14	G	103	SPO	C31-C32-C33	-2.64	121.31	127.66
8	Q	103	BCL	CHB-C4A-NA	2.64	128.16	124.51
14	m	407	SPO	C15-C14-C12	-2.64	123.55	127.31
14	v	102	SPO	C21-C20-C19	-2.63	118.08	123.47
8	y	103	BCL	C4-C3-C5	2.63	119.70	115.27
8	T	101	BCL	CHB-C4A-NA	2.63	128.15	124.51
12	M	411	PGV	O03-C19-C20	2.63	120.16	111.91
14	n	101	SPO	C31-C32-C33	-2.63	121.33	127.66
14	f	101	SPO	C40-C38-C39	2.63	120.41	114.60
8	O	101	BCL	CHB-C4A-NA	2.63	128.15	124.51
14	s	103	SPO	C9-C10-C11	-2.63	115.02	123.22
14	j	101	SPO	C20-C19-C17	-2.63	123.56	127.31
8	L	301	BCL	CED-O2D-CGD	2.63	121.88	115.94
14	08	101	SPO	C15-C14-C12	-2.63	123.56	127.31
14	01	102	SPO	C31-C32-C33	-2.62	121.34	127.66
8	R	102	BCL	O2A-CGA-CBA	2.62	120.14	111.91
8	1	202	BCL	CHB-C4A-NA	2.62	128.14	124.51
14	p	101	SPO	C29-C28-C30	2.62	119.68	115.27
14	4	102	SPO	C34-C33-C35	2.62	119.68	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	101	BCL	C4-C3-C5	2.62	119.68	115.27
14	p	101	SPO	C25-C23-C22	2.62	122.96	118.94
15	M	410	CDL	OA8-CA7-C31	2.62	120.12	111.91
14	e	101	SPO	C20-C21-C22	-2.62	118.12	123.47
15	M	410	CDL	OB8-CB7-C71	2.61	120.11	111.91
8	Z	101	BCL	O2D-CGD-O1D	-2.61	118.73	123.84
14	g	101	SPO	C13-C12-C11	2.61	122.19	118.08
14	s	105	SPO	C15-C14-C12	-2.61	123.59	127.31
15	Y	101	CDL	OB8-CB7-C71	2.61	120.09	111.91
8	2	103	BCL	C1-C2-C3	-2.61	121.53	126.04
8	m	403	BCL	O2A-CGA-CBA	2.61	120.09	111.91
8	i	103	BCL	O2A-CGA-CBA	2.61	120.09	111.91
8	V	101	BCL	CAD-C3D-C4D	2.61	109.92	108.47
14	5	103	SPO	C34-C33-C35	2.61	119.65	115.27
11	i	101	LMT	O1B-C4'-C3'	2.60	114.21	107.28
8	o	101	BCL	C1C-NC-C4C	-2.60	105.54	106.71
12	l	307	PGV	O03-C19-C20	2.60	120.07	111.91
8	V	101	BCL	CHC-C1C-NC	2.60	128.11	124.51
8	04	101	BCL	CMB-C2B-C3B	2.60	129.54	124.68
8	Y	102	BCL	C4B-CHC-C1C	-2.60	124.97	130.12
8	p	102	BCL	O2D-CGD-O1D	-2.60	118.76	123.84
8	s	102	BCL	CHB-C4A-NA	2.60	128.10	124.51
8	s	102	BCL	CAD-C3D-C4D	2.60	109.92	108.47
12	f	104	PGV	O03-C19-C20	2.60	120.06	111.91
12	x	101	PGV	O03-C19-C20	2.60	120.06	111.91
8	P	102	BCL	C1-C2-C3	-2.59	121.56	126.04
14	f	101	SPO	C13-C12-C11	2.59	122.17	118.08
8	5	102	BCL	O2A-CGA-CBA	2.59	120.05	111.91
8	k	101	BCL	CHB-C4A-NA	2.59	128.09	124.51
14	01	103	SPO	C13-C12-C11	2.59	122.16	118.08
14	I	103	SPO	C14-C15-C16	-2.59	115.14	123.22
14	G	103	SPO	C34-C33-C35	2.59	119.63	115.27
8	03	102	BCL	CHC-C1C-NC	2.59	128.09	124.51
8	m	403	BCL	C4-C3-C5	2.58	119.62	115.27
8	R	102	BCL	C1B-CHB-C4A	-2.58	125.00	130.12
8	D	101	BCL	O2D-CGD-O1D	-2.58	118.79	123.84
15	M	410	CDL	OB6-CB5-OB7	-2.58	117.46	123.70
12	L	309	PGV	O03-C19-C20	2.58	120.01	111.91
8	06	101	BCL	O2A-CGA-CBA	2.58	120.01	111.91
12	m	412	PGV	O03-C19-C20	2.58	120.01	111.91
8	A	702	BCL	O2A-CGA-CBA	2.58	120.01	111.91
14	q	104	SPO	C27-C26-C25	-2.58	115.17	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	101	BCL	CHC-C1C-NC	2.58	128.08	124.51
8	l	301	BCL	CHC-C1C-NC	2.58	128.08	124.51
12	l	308	PGV	C02-O01-C1	-2.58	111.44	117.79
8	f	102	BCL	O2A-CGA-CBA	2.58	120.00	111.91
8	Y	102	BCL	CHC-C1C-NC	2.58	128.08	124.51
8	s	102	BCL	C1-C2-C3	-2.58	121.59	126.04
14	V	102	SPO	C29-C28-C30	2.58	119.61	115.27
12	l	307	PGV	C02-O01-C1	-2.58	111.45	117.79
8	B	102	BCL	O2A-CGA-CBA	2.58	119.99	111.91
14	01	102	SPO	C15-C14-C12	-2.58	123.64	127.31
15	m	410	CDL	OB6-CB5-OB7	-2.57	117.48	123.70
8	05	101	BCL	C1-C2-C3	-2.57	121.59	126.04
14	z	101	SPO	C31-C32-C33	-2.57	121.46	127.66
14	r	101	SPO	C31-C32-C33	-2.57	121.47	127.66
8	V	101	BCL	C4A-NA-C1A	2.57	107.86	106.71
15	Y	101	CDL	OA8-CA7-C31	2.57	119.97	111.91
12	1	201	PGV	C02-O01-C1	-2.57	111.47	117.79
14	G	103	SPO	C18-C17-C19	-2.57	119.33	122.92
14	M	406	SPO	C5-C6-C7	-2.57	122.01	125.89
8	t	101	BCL	C2A-C1A-CHA	-2.57	119.37	123.86
8	06	101	BCL	C4A-NA-C1A	2.57	107.86	106.71
14	Y	103	SPO	C10-C9-C7	-2.57	123.65	127.31
8	m	401	BCL	O2A-CGA-CBA	2.57	119.96	111.91
8	A	702	BCL	CHC-C1C-NC	2.57	128.06	124.51
8	3	102	BCL	CHC-C1C-NC	2.56	128.06	124.51
14	05	102	SPO	C14-C15-C16	-2.56	115.22	123.22
12	q	102	PGV	C02-O01-C1	-2.56	111.48	117.79
8	o	101	BCL	CAC-C3C-C4C	-2.56	106.90	112.58
8	r	102	BCL	CHC-C1C-NC	2.56	128.05	124.51
14	z	101	SPO	C24-C23-C22	-2.56	119.34	122.92
14	p	101	SPO	C18-C17-C16	2.56	122.11	118.08
14	O	102	SPO	C34-C33-C35	2.55	119.57	115.27
8	y	103	BCL	CHB-C4A-NA	2.55	128.04	124.51
8	S	101	BCL	C4B-CHC-C1C	-2.55	125.06	130.12
8	G	102	BCL	CAD-C3D-C4D	2.55	109.89	108.47
14	r	103	SPO	C40-C38-C39	2.55	120.24	114.60
8	06	101	BCL	C1-C2-C3	-2.55	121.63	126.04
14	E	102	SPO	C14-C15-C16	-2.55	115.26	123.22
8	N	102	BCL	O2A-CGA-CBA	2.55	119.91	111.91
14	V	102	SPO	C18-C17-C16	2.55	122.09	118.08
14	s	105	SPO	C18-C17-C16	2.55	122.09	118.08
8	e	102	BCL	O2D-CGD-O1D	-2.54	118.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	05	102	SPO	C34-C33-C35	2.54	119.55	115.27
14	a	102	SPO	C14-C15-C16	-2.54	115.28	123.22
14	n	101	SPO	C21-C22-C23	-2.54	123.68	127.31
14	I	103	SPO	C34-C33-C35	2.54	119.55	115.27
8	o	101	BCL	C4-C3-C5	2.54	119.55	115.27
8	07	101	BCL	CHB-C4A-NA	2.54	128.03	124.51
8	m	403	BCL	CED-O2D-CGD	2.54	121.68	115.94
14	w	101	SPO	C34-C33-C35	2.54	119.54	115.27
14	S	102	SPO	C31-C32-C33	-2.54	121.56	127.66
14	e	101	SPO	C29-C28-C30	2.54	119.54	115.27
8	b	101	BCL	C1-C2-C3	-2.53	121.66	126.04
12	L	308	PGV	O03-C19-C20	2.53	119.86	111.91
8	K	402	BCL	C1C-NC-C4C	-2.53	105.57	106.71
14	s	105	SPO	C34-C33-C35	2.53	119.53	115.27
8	06	101	BCL	CMB-C2B-C3B	2.53	129.42	124.68
14	S	102	SPO	C20-C19-C17	-2.53	123.70	127.31
14	V	102	SPO	C14-C15-C16	-2.53	115.32	123.22
8	M	402	BCL	CHC-C1C-NC	2.53	128.01	124.51
8	w	102	BCL	CHB-C4A-NA	2.53	128.01	124.51
14	6	102	SPO	C15-C16-C17	-2.53	119.31	126.42
12	L	308	PGV	C02-O01-C1	-2.53	111.56	117.79
14	N	101	SPO	C31-C32-C33	-2.53	121.57	127.66
8	k	101	BCL	O2A-CGA-CBA	2.53	119.85	111.91
8	A	702	BCL	C1C-NC-C4C	-2.53	105.57	106.71
8	4	101	BCL	C1C-NC-C4C	2.53	107.84	106.71
8	7	101	BCL	CHB-C4A-NA	2.53	128.01	124.51
8	G	102	BCL	CHB-C4A-NA	2.53	128.00	124.51
14	A	703	SPO	C13-C12-C11	2.53	122.06	118.08
15	X	101	CDL	OA8-CA7-C31	2.53	119.83	111.91
12	M	411	PGV	C02-O01-C1	-2.52	111.58	117.79
14	p	101	SPO	C10-C9-C7	-2.52	123.71	127.31
8	01	101	BCL	C4-C3-C5	2.52	119.51	115.27
8	3	102	BCL	C4B-CHC-C1C	-2.52	125.12	130.12
8	06	101	BCL	C3C-C4C-CHD	-2.52	118.00	123.39
14	e	101	SPO	C40-C38-C39	2.52	120.17	114.60
15	K	401	CDL	OB8-CB7-C71	2.52	119.81	111.91
14	05	102	SPO	C40-C38-C39	2.52	120.17	114.60
14	p	101	SPO	C20-C19-C17	-2.52	123.72	127.31
14	A	703	SPO	C14-C15-C16	-2.52	115.37	123.22
8	J	102	BCL	CHB-C4A-NA	2.52	127.99	124.51
14	r	103	SPO	C29-C28-C30	2.51	119.50	115.27
14	M	406	SPO	C34-C33-C35	2.51	119.50	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	05	102	SPO	C5-C6-C7	-2.51	122.09	125.89
8	e	102	BCL	C1-C2-C3	-2.51	121.70	126.04
8	8	101	BCL	C4C-CHD-C1D	-2.51	122.17	125.88
8	6	101	BCL	O2D-CGD-O1D	-2.51	118.93	123.84
9	L	302	BPH	CMA-C3A-C4A	-2.51	108.88	114.38
14	01	102	SPO	C34-C33-C35	2.51	119.49	115.27
8	K	402	BCL	C1-C2-C3	-2.51	121.70	126.04
12	L	307	PGV	O03-C19-C20	2.51	119.78	111.91
8	I	102	BCL	O2D-CGD-O1D	-2.51	118.93	123.84
14	G	103	SPO	C40-C38-C39	2.51	120.14	114.60
14	5	103	SPO	C9-C10-C11	-2.51	115.39	123.22
8	l	301	BCL	CHB-C4A-NA	2.51	127.98	124.51
8	V	101	BCL	C1C-NC-C4C	-2.51	105.58	106.71
14	01	102	SPO	C20-C21-C22	-2.50	118.35	123.47
11	A	701	LMT	C1B-O1B-C4'	-2.50	111.77	117.96
14	j	101	SPO	C13-C12-C14	-2.50	119.42	122.92
8	01	101	BCL	CHC-C1C-NC	2.50	127.97	124.51
14	f	106	SPO	C29-C28-C30	2.50	119.47	115.27
14	e	101	SPO	C21-C22-C23	-2.50	123.75	127.31
8	8	101	BCL	O2A-CGA-CBA	2.50	119.75	111.91
15	y	102	CDL	OB8-CB7-C71	2.50	119.74	111.91
8	n	102	BCL	C4-C3-C5	2.50	119.47	115.27
14	02	102	SPO	C21-C20-C19	-2.50	118.36	123.47
8	n	102	BCL	C2A-C1A-CHA	-2.50	119.50	123.86
8	q	103	BCL	CHB-C4A-NA	2.49	127.96	124.51
14	O	102	SPO	C21-C20-C19	-2.49	118.37	123.47
14	G	101	SPO	C14-C15-C16	-2.49	115.44	123.22
8	N	102	BCL	C4-C3-C5	2.49	119.46	115.27
8	g	103	BCL	CHC-C1C-NC	2.49	127.96	124.51
8	k	101	BCL	CAD-C3D-C4D	2.49	109.86	108.47
8	w	102	BCL	C1-C2-C3	-2.49	121.74	126.04
11	U	101	LMT	C1B-O1B-C4'	-2.49	111.80	117.96
8	b	101	BCL	C4-C3-C5	2.49	119.46	115.27
8	z	102	BCL	O2D-CGD-O1D	-2.49	118.97	123.84
8	j	102	BCL	C4B-CHC-C1C	-2.49	125.19	130.12
8	d	101	BCL	C4-C3-C5	2.49	119.45	115.27
11	L	305	LMT	C1-O1'-C1'	-2.49	109.72	113.84
15	h	805	CDL	OA8-CA7-C31	2.48	119.70	111.91
11	M	409	LMT	O1B-C4'-C3'	2.48	113.89	107.28
11	L	305	LMT	O1B-C1B-C2B	2.48	114.53	108.10
8	p	102	BCL	C1C-NC-C4C	-2.48	105.59	106.71
8	m	402	BCL	O2A-CGA-CBA	2.48	119.69	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	101	BCL	CAC-C3C-C4C	-2.48	107.08	112.58
14	6	102	SPO	C10-C11-C12	-2.48	119.45	126.42
14	2	104	SPO	C8-C7-C9	-2.48	119.45	122.92
14	s	105	SPO	C26-C25-C23	-2.48	119.45	126.42
12	1	201	PGV	O03-C19-C20	2.48	119.68	111.91
14	05	103	SPO	C40-C38-C39	2.48	120.08	114.60
14	p	101	SPO	C8-C7-C6	2.48	121.98	118.08
14	s	105	SPO	C20-C19-C17	-2.48	123.78	127.31
8	q	103	BCL	C4B-CHC-C1C	-2.48	125.21	130.12
14	s	103	SPO	C14-C15-C16	-2.47	115.50	123.22
14	I	103	SPO	C10-C9-C7	-2.47	123.78	127.31
14	O	102	SPO	C13-C12-C11	2.47	121.97	118.08
12	y	104	PGV	O03-C19-C20	2.47	119.67	111.91
14	a	102	SPO	C31-C32-C33	-2.47	121.70	127.66
14	S	102	SPO	C34-C33-C35	2.47	119.43	115.27
14	P	101	SPO	C21-C20-C19	-2.47	118.41	123.47
15	m	410	CDL	OA8-CA7-C31	2.47	119.67	111.91
14	05	102	SPO	C13-C12-C11	2.47	121.97	118.08
11	h	803	LMT	C1-O1'-C1'	-2.47	109.74	113.84
8	s	102	BCL	O2A-CGA-CBA	2.47	119.66	111.91
14	y	105	SPO	C9-C10-C11	-2.47	115.52	123.22
8	L	301	BCL	O2A-CGA-O1A	-2.47	117.37	123.59
14	4	102	SPO	C40-C38-C39	2.46	120.05	114.60
14	2	101	SPO	C18-C17-C16	2.46	121.96	118.08
14	A	703	SPO	C24-C23-C25	2.46	121.96	118.08
14	m	407	SPO	C34-C33-C35	2.46	119.41	115.27
14	p	101	SPO	C24-C23-C22	-2.46	119.47	122.92
8	F	502	BCL	C1-C2-C3	-2.46	121.78	126.04
14	A	703	SPO	C8-C7-C6	2.46	121.95	118.08
14	g	102	SPO	C40-C38-C39	2.46	120.04	114.60
8	K	402	BCL	O2D-CGD-O1D	-2.46	119.03	123.84
8	2	103	BCL	O2D-CGD-O1D	-2.46	119.03	123.84
14	j	101	SPO	C40-C38-C39	2.46	120.04	114.60
14	a	102	SPO	C21-C20-C19	-2.46	118.43	123.47
8	m	401	BCL	C1C-NC-C4C	-2.46	105.60	106.71
14	S	103	SPO	C9-C10-C11	-2.46	115.54	123.22
8	3	102	BCL	C1B-CHB-C4A	-2.46	125.25	130.12
14	S	102	SPO	C13-C12-C14	-2.46	119.48	122.92
8	m	403	BCL	CHC-C1C-NC	2.45	127.91	124.51
8	l	301	BCL	O2A-CGA-O1A	-2.45	117.40	123.59
8	e	102	BCL	C4B-CHC-C1C	-2.45	125.26	130.12
8	M	402	BCL	C4-C3-C5	2.45	119.39	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	E	102	SPO	C13-C12-C11	2.45	121.94	118.08
8	S	101	BCL	C1C-NC-C4C	-2.45	105.61	106.71
14	G	103	SPO	C36-C37-C38	-2.45	119.39	127.75
8	06	101	BCL	O2D-CGD-O1D	-2.45	119.06	123.84
8	P	102	BCL	CHC-C1C-NC	2.45	127.89	124.51
14	y	105	SPO	C15-C14-C12	-2.44	123.82	127.31
8	r	102	BCL	O2D-CGD-O1D	-2.44	119.06	123.84
8	a	101	BCL	C1B-CHB-C4A	-2.44	125.28	130.12
8	N	102	BCL	C2A-C1A-CHA	-2.44	119.59	123.86
11	M	409	LMT	C1B-O5B-C5B	2.44	118.48	113.69
14	n	101	SPO	C10-C11-C12	-2.44	119.56	126.42
8	02	101	BCL	O2D-CGD-O1D	-2.44	119.07	123.84
14	Q	104	SPO	C14-C15-C16	-2.44	115.61	123.22
14	y	105	SPO	C8-C7-C6	2.44	121.92	118.08
8	d	101	BCL	C4B-CHC-C1C	-2.44	125.29	130.12
14	n	101	SPO	C40-C38-C39	2.44	119.99	114.60
14	02	102	SPO	C24-C23-C25	2.44	121.92	118.08
11	M	409	LMT	C1'-C2'-C3'	2.44	115.07	110.00
14	k	102	SPO	C31-C32-C33	-2.44	121.79	127.66
8	g	103	BCL	O2D-CGD-O1D	-2.44	119.08	123.84
12	h	806	PGV	C02-O01-C1	-2.43	111.80	117.79
14	m	407	SPO	C9-C10-C11	-2.43	115.62	123.22
8	q	103	BCL	C1-C2-C3	-2.43	121.84	126.04
14	I	103	SPO	C20-C19-C17	-2.43	123.84	127.31
8	v	101	BCL	O2D-CGD-O1D	-2.43	119.09	123.84
14	s	103	SPO	C34-C33-C35	2.43	119.36	115.27
8	w	102	BCL	C4B-CHC-C1C	-2.43	125.31	130.12
8	j	102	BCL	CHB-C4A-NA	2.43	127.87	124.51
8	I	102	BCL	CAD-C3D-C4D	2.43	109.82	108.47
12	H	804	PGV	O03-C19-C20	2.43	119.53	111.91
14	4	102	SPO	C31-C32-C33	-2.43	121.81	127.66
14	p	101	SPO	C40-C38-C39	2.43	119.96	114.60
14	z	101	SPO	C9-C10-C11	-2.42	115.66	123.22
8	Z	101	BCL	CHB-C4A-NA	2.42	127.86	124.51
14	N	101	SPO	C40-C38-C39	2.42	119.95	114.60
14	g	102	SPO	C13-C12-C11	2.42	121.89	118.08
8	z	102	BCL	CHC-C1C-NC	2.42	127.86	124.51
14	R	101	SPO	C40-C38-C39	2.42	119.95	114.60
8	V	101	BCL	O2A-CGA-CBA	2.42	119.50	111.91
14	S	103	SPO	C15-C14-C12	-2.42	123.86	127.31
14	n	103	SPO	C20-C19-C17	-2.42	123.86	127.31
14	f	101	SPO	C24-C23-C25	2.42	121.89	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	I	103	SPO	C27-C26-C25	-2.42	115.67	123.22
11	M	409	LMT	O5'-C1'-C2'	2.42	115.46	110.35
14	2	101	SPO	C31-C32-C33	-2.41	121.85	127.66
14	Q	104	SPO	C20-C21-C22	-2.41	118.53	123.47
14	e	101	SPO	C10-C9-C7	-2.41	123.86	127.31
8	j	102	BCL	O2D-CGD-O1D	-2.41	119.12	123.84
14	G	101	SPO	C20-C21-C22	-2.41	118.54	123.47
8	04	101	BCL	C4-C3-C5	2.41	119.32	115.27
14	08	101	SPO	C40-C38-C39	2.41	119.92	114.60
14	n	103	SPO	C21-C20-C19	-2.41	118.54	123.47
8	o	101	BCL	CAD-C3D-C4D	2.41	109.81	108.47
14	S	102	SPO	C9-C10-C11	-2.41	115.71	123.22
14	3	103	SPO	C40-C38-C39	2.41	119.92	114.60
8	N	102	BCL	CHB-C4A-NA	2.41	127.84	124.51
8	L	311	BCL	O2A-CGA-CBA	2.41	119.45	111.91
14	w	101	SPO	C40-C38-C39	2.40	119.92	114.60
14	z	101	SPO	C34-C33-C35	2.40	119.32	115.27
8	P	102	BCL	CHB-C4A-NA	2.40	127.83	124.51
14	m	407	SPO	C40-C38-C39	2.40	119.91	114.60
8	i	103	BCL	C4-C3-C5	2.40	119.31	115.27
14	P	101	SPO	C40-C38-C39	2.40	119.91	114.60
14	G	101	SPO	C27-C26-C25	-2.40	115.73	123.22
14	2	104	SPO	C40-C38-C39	2.40	119.91	114.60
14	I	103	SPO	C40-C38-C39	2.40	119.90	114.60
14	Q	104	SPO	C9-C10-C11	-2.40	115.73	123.22
14	02	102	SPO	C15-C14-C12	-2.40	123.89	127.31
8	m	402	BCL	CHC-C1C-NC	2.40	127.83	124.51
8	D	101	BCL	CAD-C3D-C4D	2.40	109.81	108.47
8	v	101	BCL	C4B-CHC-C1C	-2.40	125.37	130.12
8	05	101	BCL	CAD-C3D-C4D	2.39	109.81	108.47
8	N	102	BCL	O2D-CGD-O1D	-2.39	119.16	123.84
8	m	401	BCL	C1-O2A-CGA	2.39	122.72	116.44
14	v	102	SPO	C14-C15-C16	-2.39	115.76	123.22
11	m	409	LMT	O1B-C4'-C3'	2.39	113.64	107.28
8	m	403	BCL	C1-C2-C3	-2.39	121.91	126.04
8	a	101	BCL	CAD-C3D-C4D	2.39	109.80	108.47
14	K	404	SPO	C21-C20-C19	-2.39	118.58	123.47
14	01	103	SPO	C40-C38-C39	2.39	119.88	114.60
14	T	102	SPO	C21-C20-C19	-2.39	118.58	123.47
8	i	103	BCL	C4B-CHC-C1C	-2.39	125.39	130.12
14	O	102	SPO	C40-C38-C39	2.39	119.87	114.60
8	L	301	BCL	CAD-C3D-C4D	2.39	109.80	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	102	BCL	C2A-C1A-CHA	-2.38	119.69	123.86
8	05	101	BCL	CHC-C1C-NC	2.38	127.81	124.51
8	k	101	BCL	O2D-CGD-O1D	-2.38	119.18	123.84
8	a	101	BCL	CHC-C1C-NC	2.38	127.81	124.51
14	S	102	SPO	C27-C26-C25	-2.38	115.78	123.22
8	5	102	BCL	CHB-C4A-NA	2.38	127.80	124.51
8	q	103	BCL	CAC-C3C-C4C	-2.38	107.31	112.58
14	K	404	SPO	C13-C12-C11	2.38	121.82	118.08
14	v	102	SPO	C8-C7-C6	2.38	121.82	118.08
14	f	101	SPO	C8-C7-C6	2.37	121.82	118.08
14	y	105	SPO	C13-C12-C11	2.37	121.81	118.08
14	01	102	SPO	C40-C38-C39	2.37	119.84	114.60
14	5	103	SPO	C21-C20-C19	-2.37	118.62	123.47
14	T	102	SPO	C40-C38-C39	2.37	119.83	114.60
8	W	101	BCL	C1B-CHB-C4A	-2.37	125.43	130.12
8	f	102	BCL	C1C-NC-C4C	-2.37	105.64	106.71
14	B	103	SPO	C27-C26-C25	-2.36	115.84	123.22
8	Q	103	BCL	O2D-CGD-O1D	-2.36	119.22	123.84
14	g	101	SPO	C14-C15-C16	-2.36	115.84	123.22
8	r	102	BCL	C2A-C1A-CHA	-2.36	119.73	123.86
14	I	103	SPO	C18-C17-C16	2.36	121.80	118.08
14	f	101	SPO	C36-C37-C38	-2.36	119.68	127.75
14	e	101	SPO	C24-C23-C25	2.36	121.80	118.08
8	w	102	BCL	O2D-CGD-O1D	-2.36	119.22	123.84
14	w	101	SPO	C21-C20-C19	-2.36	118.64	123.47
8	s	102	BCL	O2D-CGD-O1D	-2.36	119.23	123.84
8	O	101	BCL	O2D-CGD-O1D	-2.36	119.23	123.84
8	04	101	BCL	O2D-CGD-O1D	-2.35	119.23	123.84
14	4	102	SPO	C8-C7-C9	-2.35	119.62	122.92
14	a	102	SPO	C40-C38-C39	2.35	119.80	114.60
8	M	402	BCL	CED-O2D-CGD	2.35	121.26	115.94
8	v	101	BCL	O2A-CGA-CBA	2.35	119.29	111.91
14	j	101	SPO	C31-C32-C33	-2.35	122.00	127.66
14	f	106	SPO	C40-C38-C39	2.35	119.80	114.60
14	G	103	SPO	C15-C16-C17	-2.35	119.81	126.42
8	Q	103	BCL	C4-C3-C5	2.35	119.22	115.27
8	L	311	BCL	CHB-C4A-NA	2.35	127.76	124.51
14	2	104	SPO	C14-C15-C16	-2.35	115.89	123.22
8	F	502	BCL	O2D-CGD-O1D	-2.34	119.25	123.84
8	M	401	BCL	CHC-C1C-NC	2.34	127.75	124.51
14	2	104	SPO	C27-C26-C25	-2.34	115.90	123.22
15	X	103	CDL	OA6-CA5-OA7	-2.34	118.04	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	y	105	SPO	C24-C23-C25	2.34	121.77	118.08
14	f	101	SPO	C34-C33-C35	2.34	119.21	115.27
14	R	101	SPO	C24-C23-C22	-2.34	119.64	122.92
14	n	103	SPO	C40-C38-C39	2.34	119.78	114.60
14	k	102	SPO	C8-C7-C6	2.34	121.77	118.08
14	5	103	SPO	C40-C38-C39	2.34	119.77	114.60
14	02	102	SPO	C14-C15-C16	-2.34	115.91	123.22
8	03	102	BCL	O2A-CGA-O1A	-2.34	117.69	123.59
12	h	801	PGV	C02-O01-C1	-2.34	112.03	117.79
15	h	805	CDL	OB8-CB7-C71	2.34	119.25	111.91
14	05	103	SPO	C10-C11-C12	-2.34	119.85	126.42
14	Y	103	SPO	C40-C38-C39	2.34	119.76	114.60
8	V	101	BCL	C4B-CHC-C1C	-2.33	125.49	130.12
8	V	101	BCL	O1D-CGD-CBD	-2.33	119.71	124.48
14	p	101	SPO	C36-C35-C33	-2.33	105.31	112.98
14	k	102	SPO	C13-C12-C11	2.32	121.74	118.08
14	V	102	SPO	C36-C37-C38	-2.32	119.81	127.75
8	j	102	BCL	C1-C2-C3	-2.32	122.03	126.04
14	08	101	SPO	C21-C20-C19	-2.32	118.72	123.47
8	m	403	BCL	O2D-CGD-O1D	-2.32	119.30	123.84
14	r	103	SPO	C13-C12-C11	2.32	121.73	118.08
14	f	101	SPO	C11-C12-C14	-2.32	115.38	118.94
14	S	103	SPO	C20-C19-C17	-2.32	124.00	127.31
14	k	102	SPO	C34-C33-C35	2.32	119.17	115.27
14	e	101	SPO	C27-C26-C25	-2.32	115.98	123.22
14	S	103	SPO	C29-C28-C30	2.32	119.17	115.27
14	01	102	SPO	C21-C22-C23	-2.31	124.01	127.31
8	01	101	BCL	O2D-CGD-O1D	-2.31	119.32	123.84
9	m	404	BPH	C1A-C2A-C3A	-2.31	100.64	102.84
8	T	101	BCL	C1-C2-C3	-2.31	122.05	126.04
12	h	801	PGV	O03-C19-O04	-2.31	117.76	123.59
8	5	102	BCL	C4A-NA-C1A	2.31	107.74	106.71
8	02	101	BCL	O2A-CGA-O1A	-2.31	117.77	123.59
14	2	104	SPO	C34-C33-C35	2.31	119.15	115.27
14	Q	104	SPO	C10-C9-C7	-2.31	124.02	127.31
12	L	310	PGV	O03-C19-C20	2.30	119.14	111.91
8	K	402	BCL	CAC-C3C-C4C	-2.30	107.47	112.58
14	01	103	SPO	C27-C26-C25	-2.30	116.03	123.22
12	H	805	PGV	O03-C19-O04	-2.30	117.78	123.59
8	i	103	BCL	O2D-CGD-O1D	-2.30	119.33	123.84
8	E	101	BCL	O2D-CGD-O1D	-2.30	119.34	123.84
8	I	102	BCL	CAC-C3C-C4C	-2.30	107.48	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	101	BCL	CED-O2D-CGD	2.30	121.14	115.94
8	K	402	BCL	C4B-CHC-C1C	-2.30	125.56	130.12
14	n	103	SPO	C14-C15-C16	-2.30	116.04	123.22
14	3	103	SPO	C13-C12-C11	2.30	121.70	118.08
8	M	401	BCL	O2D-CGD-O1D	-2.30	119.34	123.84
8	P	102	BCL	CAD-C3D-C4D	2.30	109.75	108.47
14	08	101	SPO	C18-C17-C19	-2.30	119.71	122.92
8	S	101	BCL	CHB-C4A-NA	2.29	127.68	124.51
14	M	406	SPO	C10-C9-C7	-2.29	124.04	127.31
14	5	103	SPO	C36-C37-C38	-2.29	119.91	127.75
8	7	101	BCL	O2D-CGD-O1D	-2.29	119.36	123.84
12	H	805	PGV	C02-O01-C1	-2.29	112.15	117.79
11	H	802	LMT	O1'-C1'-C2'	2.29	111.88	108.30
8	05	101	BCL	C4B-CHC-C1C	-2.29	125.58	130.12
14	w	101	SPO	C18-C17-C19	-2.29	119.72	122.92
8	n	102	BCL	O2D-CGD-O1D	-2.29	119.37	123.84
14	A	703	SPO	C40-C38-C39	2.29	119.65	114.60
14	n	103	SPO	C27-C26-C25	-2.29	116.08	123.22
8	y	103	BCL	CAC-C3C-C4C	-2.29	107.51	112.58
11	U	102	LMT	O1B-C4'-C3'	2.29	113.36	107.28
14	r	101	SPO	C40-C38-C39	2.29	119.65	114.60
8	W	101	BCL	O2D-CGD-O1D	-2.29	119.37	123.84
8	07	101	BCL	O2D-CGD-O1D	-2.28	119.37	123.84
14	G	101	SPO	C13-C12-C11	2.28	121.68	118.08
14	G	101	SPO	C40-C38-C39	2.28	119.65	114.60
8	07	101	BCL	C4-C3-C5	2.28	119.11	115.27
8	l	301	BCL	C2A-C1A-CHA	-2.28	119.87	123.86
14	K	404	SPO	C26-C25-C23	-2.28	120.00	126.42
8	w	102	BCL	C2A-C1A-CHA	-2.28	119.87	123.86
8	B	102	BCL	C2A-C1A-CHA	-2.28	119.87	123.86
9	m	404	BPH	CMA-C3A-C4A	-2.28	109.38	114.38
12	k	103	PGV	C02-O01-C1	-2.28	112.18	117.79
8	A	702	BCL	O2D-CGD-O1D	-2.28	119.38	123.84
14	B	101	SPO	C40-C38-C39	2.28	119.64	114.60
14	M	406	SPO	C40-C38-C39	2.28	119.63	114.60
8	L	311	BCL	C2A-C1A-CHA	-2.28	119.88	123.86
14	Q	104	SPO	C40-C38-C39	2.28	119.63	114.60
8	M	401	BCL	C4B-CHC-C1C	-2.27	125.61	130.12
14	z	101	SPO	C5-C6-C7	-2.27	122.45	125.89
14	V	102	SPO	C13-C12-C11	2.27	121.66	118.08
14	k	102	SPO	C14-C15-C16	-2.27	116.12	123.22
8	05	101	BCL	O2D-CGD-O1D	-2.27	119.39	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	101	SPO	C14-C15-C16	-2.27	116.13	123.22
14	p	101	SPO	C14-C15-C16	-2.27	116.13	123.22
14	2	101	SPO	C40-C38-C39	2.27	119.62	114.60
14	G	103	SPO	C13-C12-C14	-2.27	119.74	122.92
8	6	101	BCL	C1C-NC-C4C	2.27	107.73	106.71
8	n	102	BCL	C1C-NC-C4C	-2.27	105.69	106.71
8	m	402	BCL	C2A-C1A-CHA	-2.27	119.89	123.86
15	h	805	CDL	CB4-OB6-CB5	-2.27	112.20	117.79
8	5	102	BCL	C3C-C4C-CHD	-2.27	118.54	123.39
8	b	101	BCL	CED-O2D-CGD	2.27	121.07	115.94
12	l	306	PGV	O03-C19-C20	2.27	119.02	111.91
8	L	301	BCL	C11-C12-C13	-2.27	108.59	115.92
14	02	102	SPO	C40-C38-C39	2.26	119.60	114.60
8	d	101	BCL	O2D-CGD-O1D	-2.26	119.41	123.84
8	03	102	BCL	O2D-CGD-O1D	-2.26	119.42	123.84
14	z	101	SPO	C40-C38-C39	2.26	119.59	114.60
14	f	106	SPO	C20-C21-C22	-2.26	118.85	123.47
14	3	103	SPO	C8-C7-C6	2.26	121.63	118.08
12	m	412	PGV	C02-O01-C1	-2.26	112.24	117.79
8	S	101	BCL	O2A-CGA-CBA	2.26	118.99	111.91
8	01	101	BCL	C4B-CHC-C1C	-2.26	125.65	130.12
8	w	102	BCL	CHC-C1C-NC	2.25	127.63	124.51
8	01	101	BCL	CAD-C3D-C4D	2.25	109.73	108.47
14	01	103	SPO	C8-C7-C6	2.25	121.62	118.08
14	05	102	SPO	C36-C37-C38	-2.25	120.06	127.75
8	T	101	BCL	O2D-CGD-O1D	-2.25	119.44	123.84
8	05	101	BCL	CAC-C3C-C4C	-2.24	107.60	112.58
8	m	401	BCL	C2A-C1A-CHA	-2.24	119.94	123.86
12	H	801	PGV	C02-O01-C1	-2.24	112.27	117.79
14	S	103	SPO	C24-C23-C22	-2.24	119.78	122.92
8	S	101	BCL	O2D-CGD-O1D	-2.24	119.46	123.84
14	k	102	SPO	C15-C14-C12	-2.24	124.11	127.31
14	q	104	SPO	C24-C23-C25	2.24	121.60	118.08
8	L	301	BCL	CHB-C4A-NA	2.24	127.61	124.51
8	Q	103	BCL	C4B-CHC-C1C	-2.24	125.68	130.12
8	06	101	BCL	C1C-NC-C4C	2.24	107.71	106.71
14	k	102	SPO	C27-C26-C25	-2.24	116.24	123.22
14	Y	103	SPO	C29-C28-C30	2.23	119.03	115.27
11	U	102	LMT	C1B-O1B-C4'	-2.23	112.44	117.96
15	M	410	CDL	CA4-OA6-CA5	-2.23	112.30	117.79
14	f	106	SPO	C14-C15-C16	-2.23	116.26	123.22
14	A	703	SPO	C6-C7-C9	-2.23	115.52	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	O	102	SPO	C8-C7-C6	2.23	121.59	118.08
8	S	101	BCL	C2A-C1A-CHA	-2.23	119.96	123.86
14	J	101	SPO	C8-C7-C6	2.23	121.59	118.08
14	2	101	SPO	C9-C10-C11	-2.23	116.27	123.22
12	L	310	PGV	O01-C1-O02	-2.23	118.32	123.70
14	z	101	SPO	C13-C12-C11	2.23	121.59	118.08
8	I	102	BCL	C4B-CHC-C1C	-2.23	125.71	130.12
14	2	104	SPO	C36-C37-C38	-2.23	120.14	127.75
14	y	105	SPO	C20-C21-C22	-2.23	118.92	123.47
8	y	103	BCL	CAD-C3D-C4D	2.23	109.71	108.47
14	r	103	SPO	C21-C20-C19	-2.22	118.92	123.47
12	Q	102	PGV	C02-O01-C1	-2.22	112.32	117.79
14	p	101	SPO	C13-C12-C11	2.22	121.58	118.08
8	Z	101	BCL	C1B-CHB-C4A	-2.22	125.72	130.12
14	J	101	SPO	C36-C37-C38	-2.22	120.16	127.75
8	L	301	BCL	C1-C2-C3	-2.22	122.20	126.04
14	2	102	SPO	C40-C38-C39	2.22	119.51	114.60
8	j	102	BCL	C1B-CHB-C4A	-2.22	125.72	130.12
8	y	103	BCL	O2D-CGD-O1D	-2.22	119.50	123.84
8	b	101	BCL	C1-O2A-CGA	2.22	122.26	116.44
14	2	104	SPO	C21-C20-C19	-2.22	118.93	123.47
8	p	102	BCL	C2A-C1A-CHA	-2.22	119.98	123.86
14	z	101	SPO	C26-C25-C23	-2.22	120.19	126.42
8	l	301	BCL	C11-C12-C13	-2.21	108.77	115.92
8	Q	103	BCL	C4A-NA-C1A	2.21	107.70	106.71
14	y	105	SPO	C10-C9-C7	-2.21	124.15	127.31
8	I	102	BCL	C4A-NA-C1A	2.21	107.70	106.71
8	O	101	BCL	C1-C2-C3	-2.21	122.22	126.04
14	P	101	SPO	C31-C32-C33	-2.21	122.34	127.66
14	E	102	SPO	C40-C38-C39	2.21	119.48	114.60
14	a	102	SPO	C13-C12-C11	2.21	121.55	118.08
14	I	103	SPO	C9-C10-C11	-2.21	116.33	123.22
14	y	105	SPO	C40-C38-C39	2.21	119.48	114.60
14	B	103	SPO	C40-C38-C39	2.20	119.47	114.60
14	q	104	SPO	C40-C38-C39	2.20	119.47	114.60
14	q	104	SPO	C8-C7-C6	2.20	121.55	118.08
8	p	102	BCL	O2A-CGA-O1A	-2.20	118.03	123.59
14	g	102	SPO	C15-C16-C17	-2.20	120.23	126.42
14	5	103	SPO	C24-C23-C22	-2.20	119.84	122.92
8	g	103	BCL	C4B-CHC-C1C	-2.20	125.76	130.12
8	O	101	BCL	C11-C12-C13	-2.20	108.81	115.92
8	01	101	BCL	O2A-CGA-O1A	-2.20	118.04	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	102	SPO	C36-C37-C38	-2.20	120.23	127.75
14	S	102	SPO	C14-C15-C16	-2.20	116.36	123.22
14	a	102	SPO	C8-C7-C6	2.20	121.54	118.08
8	Y	102	BCL	O2A-CGA-O1A	-2.20	118.05	123.59
14	4	102	SPO	C36-C37-C38	-2.20	120.25	127.75
14	2	101	SPO	C26-C25-C23	-2.20	120.25	126.42
14	J	101	SPO	C20-C19-C17	-2.19	124.18	127.31
14	P	101	SPO	C20-C19-C17	-2.19	124.18	127.31
14	f	106	SPO	C13-C12-C11	2.19	121.53	118.08
8	q	103	BCL	CAD-C3D-C4D	2.19	109.69	108.47
14	2	101	SPO	C24-C23-C22	-2.19	119.85	122.92
14	01	103	SPO	C20-C21-C22	-2.19	118.99	123.47
8	s	102	BCL	CAC-C3C-C4C	-2.19	107.73	112.58
14	g	101	SPO	C24-C23-C22	-2.19	119.86	122.92
14	Q	104	SPO	C13-C12-C11	2.19	121.52	118.08
8	E	101	BCL	C2A-C1A-CHA	-2.19	120.03	123.86
8	d	101	BCL	C1-O2A-CGA	2.19	122.18	116.44
8	b	101	BCL	O2D-CGD-O1D	-2.19	119.56	123.84
14	e	101	SPO	C31-C32-C33	-2.19	122.40	127.66
8	N	102	BCL	CHC-C1C-NC	2.19	127.53	124.51
8	3	102	BCL	CED-O2D-CGD	2.19	120.88	115.94
8	A	702	BCL	C4B-CHC-C1C	-2.19	125.79	130.12
8	T	101	BCL	CHC-C1C-NC	2.18	127.53	124.51
14	E	102	SPO	C27-C26-C25	-2.18	116.40	123.22
15	X	101	CDL	CB4-OB6-CB5	-2.18	112.42	117.79
9	m	404	BPH	CBA-CAA-C2A	-2.18	107.44	113.81
8	A	702	BCL	C2A-C1A-CHA	-2.18	120.04	123.86
14	r	103	SPO	C9-C10-C11	-2.18	116.41	123.22
14	I	103	SPO	C15-C14-C12	-2.18	124.20	127.31
14	01	103	SPO	C21-C20-C19	-2.18	119.01	123.47
8	j	102	BCL	CHC-C1C-NC	2.18	127.52	124.51
8	M	401	BCL	O2A-CGA-O1A	-2.18	118.10	123.59
8	e	102	BCL	O2A-CGA-O1A	-2.18	118.10	123.59
8	i	103	BCL	CAD-C3D-C4D	2.18	109.68	108.47
8	f	102	BCL	C4B-CHC-C1C	-2.17	125.81	130.12
9	m	404	BPH	C1-C2-C3	-2.17	122.28	126.04
8	n	102	BCL	C4B-CHC-C1C	-2.17	125.81	130.12
8	Q	103	BCL	CAC-C3C-C4C	-2.17	107.76	112.58
8	O	101	BCL	CAD-C3D-C4D	2.17	109.68	108.47
14	z	101	SPO	C21-C20-C19	-2.17	119.03	123.47
8	D	101	BCL	C4A-NA-C1A	2.17	107.68	106.71
8	G	102	BCL	C1B-CHB-C4A	-2.17	125.82	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Y	102	BCL	C1-C2-C3	-2.17	122.29	126.04
12	f	103	PGV	C03-C02-C01	-2.17	106.66	111.79
14	s	105	SPO	C8-C7-C6	2.17	121.49	118.08
14	R	101	SPO	C31-C32-C33	-2.17	122.44	127.66
8	W	101	BCL	CHB-C4A-NA	2.17	127.51	124.51
8	M	401	BCL	C2A-C1A-CHA	-2.17	120.07	123.86
14	08	101	SPO	C14-C15-C16	-2.16	116.46	123.22
8	J	102	BCL	C2A-C1A-CHA	-2.16	120.08	123.86
8	O	101	BCL	CAC-C3C-C4C	-2.16	107.79	112.58
14	01	103	SPO	C14-C15-C16	-2.16	116.49	123.22
8	S	101	BCL	CAD-C3D-C4D	2.16	109.67	108.47
14	4	102	SPO	C21-C20-C19	-2.16	119.06	123.47
14	08	101	SPO	C8-C7-C9	-2.16	119.90	122.92
8	K	402	BCL	C11-C12-C13	-2.15	108.95	115.92
14	y	105	SPO	C14-C15-C16	-2.15	116.50	123.22
8	l	301	BCL	O2D-CGD-O1D	-2.15	119.63	123.84
11	m	408	LMT	C1B-O1B-C4'	-2.15	112.64	117.96
14	v	102	SPO	C40-C38-C39	2.15	119.35	114.60
14	T	102	SPO	C8-C7-C9	-2.15	119.91	122.92
14	01	103	SPO	C36-C37-C38	-2.15	120.41	127.75
14	2	101	SPO	C29-C28-C30	2.15	118.88	115.27
8	D	101	BCL	C1-C2-C3	-2.15	122.33	126.04
14	f	101	SPO	C18-C17-C16	2.15	121.46	118.08
14	5	103	SPO	C10-C9-C7	-2.14	124.25	127.31
8	E	101	BCL	C4B-CHC-C1C	-2.14	125.87	130.12
14	6	102	SPO	C24-C23-C22	-2.14	119.92	122.92
11	m	409	LMT	C3'-C4'-C5'	-2.14	106.02	110.93
8	N	102	BCL	C4B-CHC-C1C	-2.14	125.88	130.12
8	e	102	BCL	CED-O2D-CGD	2.14	120.78	115.94
14	A	703	SPO	C18-C17-C16	2.14	121.45	118.08
8	z	102	BCL	O2A-CGA-O1A	-2.14	118.19	123.59
14	r	101	SPO	C20-C19-C17	-2.14	124.26	127.31
8	7	101	BCL	O1D-CGD-CBD	-2.14	120.11	124.48
8	m	402	BCL	O1D-CGD-CBD	-2.14	120.11	124.48
14	O	102	SPO	C36-C37-C38	-2.14	120.45	127.75
8	L	311	BCL	C4B-CHC-C1C	-2.13	125.89	130.12
14	w	101	SPO	C36-C37-C38	-2.13	120.46	127.75
14	r	103	SPO	C20-C21-C22	-2.13	119.11	123.47
14	3	103	SPO	C14-C15-C16	-2.13	116.57	123.22
14	J	101	SPO	C14-C15-C16	-2.13	116.57	123.22
12	K	403	PGV	O01-C1-O02	-2.13	118.56	123.70
8	f	102	BCL	C4A-NA-C1A	2.13	107.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	305	LMT	C4B-C3B-C2B	2.13	114.53	110.82
8	p	102	BCL	C4B-CHC-C1C	-2.13	125.91	130.12
8	6	101	BCL	C4A-NA-C1A	2.12	107.66	106.71
14	n	101	SPO	C21-C20-C19	-2.12	119.12	123.47
14	n	101	SPO	C8-C7-C9	-2.12	119.95	122.92
14	g	101	SPO	C18-C17-C16	2.12	121.42	118.08
14	08	101	SPO	C18-C17-C16	2.12	121.42	118.08
14	Y	103	SPO	C13-C12-C14	-2.12	119.95	122.92
8	t	101	BCL	C1C-NC-C4C	-2.12	105.75	106.71
8	r	102	BCL	O2A-CGA-O1A	-2.12	118.24	123.59
8	v	101	BCL	CAD-C3D-C4D	2.12	109.65	108.47
8	J	102	BCL	CHC-C1C-NC	2.12	127.44	124.51
8	M	402	BCL	O2D-CGD-O1D	-2.12	119.70	123.84
12	y	104	PGV	C02-O01-C1	-2.12	112.58	117.79
8	07	101	BCL	CAC-C3C-C4C	-2.12	107.89	112.58
14	E	102	SPO	C21-C20-C19	-2.11	119.14	123.47
14	01	102	SPO	C36-C37-C38	-2.11	120.52	127.75
8	P	102	BCL	O2D-CGD-O1D	-2.11	119.70	123.84
14	6	102	SPO	C40-C38-C39	2.11	119.27	114.60
14	n	103	SPO	C15-C14-C12	-2.11	124.30	127.31
8	4	101	BCL	O2D-CGD-O1D	-2.11	119.71	123.84
8	m	401	BCL	CHB-C4A-NA	2.11	127.43	124.51
8	E	101	BCL	CED-O2D-CGD	2.11	120.71	115.94
8	1	202	BCL	O2D-CGD-O1D	-2.11	119.71	123.84
8	K	402	BCL	C11-C10-C8	-2.11	109.10	115.92
14	s	105	SPO	C34-C33-C32	-2.11	118.27	123.68
8	F	502	BCL	C4B-CHC-C1C	-2.11	125.94	130.12
14	B	103	SPO	C21-C20-C19	-2.11	119.16	123.47
14	s	105	SPO	C13-C12-C11	2.11	121.40	118.08
14	r	103	SPO	C36-C37-C38	-2.11	120.55	127.75
14	Y	103	SPO	C13-C12-C11	2.11	121.39	118.08
14	B	103	SPO	C9-C10-C11	-2.10	116.65	123.22
15	m	413	CDL	CB6-CB4-CB3	-2.10	106.81	111.79
14	g	101	SPO	C15-C14-C12	-2.10	124.31	127.31
8	01	101	BCL	CAC-C3C-C4C	-2.10	107.92	112.58
14	2	104	SPO	C6-C7-C9	2.10	122.16	118.94
14	3	103	SPO	C36-C37-C38	-2.10	120.57	127.75
8	Q	103	BCL	O2A-CGA-O1A	-2.10	118.29	123.59
8	b	101	BCL	CMD-C2D-C3D	-2.10	120.75	124.68
14	J	101	SPO	C13-C12-C11	2.10	121.38	118.08
12	F	503	PGV	O03-C19-O04	-2.10	118.30	123.59
8	a	101	BCL	C4B-CHC-C1C	-2.10	125.96	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	n	102	BCL	O2A-CGA-O1A	-2.10	118.30	123.59
8	f	102	BCL	CMD-C2D-C3D	-2.10	120.76	124.68
8	a	101	BCL	CBA-CAA-C2A	-2.10	107.68	113.86
8	1	202	BCL	O2A-CGA-O1A	-2.10	118.30	123.59
14	Y	103	SPO	C9-C10-C11	-2.09	116.68	123.22
14	s	103	SPO	C15-C14-C12	-2.09	124.32	127.31
8	1	202	BCL	C4B-CHC-C1C	-2.09	125.97	130.12
14	4	102	SPO	C14-C15-C16	-2.09	116.69	123.22
8	o	101	BCL	C4B-CHC-C1C	-2.09	125.97	130.12
14	B	101	SPO	C18-C17-C16	2.09	121.37	118.08
8	v	101	BCL	CBA-CAA-C2A	-2.09	107.69	113.86
14	V	102	SPO	C26-C25-C23	-2.09	120.54	126.42
14	w	101	SPO	C14-C15-C16	-2.09	116.69	123.22
14	n	103	SPO	C13-C12-C11	2.09	121.37	118.08
15	K	401	CDL	OA8-CA7-C31	2.09	118.46	111.91
8	1	202	BCL	CAC-C3C-C4C	-2.09	107.95	112.58
14	p	101	SPO	C36-C37-C38	-2.08	120.62	127.75
14	R	101	SPO	C13-C12-C11	2.08	121.36	118.08
8	01	101	BCL	C1C-NC-C4C	-2.08	105.77	106.71
14	2	101	SPO	C14-C15-C16	-2.08	116.71	123.22
8	W	101	BCL	CHC-C1C-NC	2.08	127.39	124.51
15	X	103	CDL	OB6-CB5-OB7	-2.08	118.67	123.70
14	S	102	SPO	C10-C9-C7	-2.08	124.34	127.31
8	M	401	BCL	CHB-C4A-NA	2.08	127.39	124.51
8	E	101	BCL	O2A-CGA-O1A	-2.08	118.34	123.59
8	T	101	BCL	C2A-C1A-CHA	-2.08	120.22	123.86
8	I	102	BCL	O2A-CGA-O1A	-2.08	118.35	123.59
8	3	102	BCL	CAA-C2A-C3A	-2.08	107.09	112.78
8	Y	102	BCL	O2D-CGD-O1D	-2.08	119.78	123.84
14	K	404	SPO	C40-C38-C39	2.08	119.19	114.60
14	e	101	SPO	C9-C10-C11	-2.07	116.74	123.22
12	l	308	PGV	O01-C1-O02	-2.07	118.69	123.70
8	m	402	BCL	C4B-CHC-C1C	-2.07	126.01	130.12
8	s	102	BCL	C4A-NA-C1A	2.07	107.64	106.71
14	3	103	SPO	C24-C23-C22	-2.07	120.02	122.92
14	n	103	SPO	C13-C12-C14	-2.07	120.02	122.92
14	B	101	SPO	C26-C25-C23	-2.07	120.59	126.42
8	J	102	BCL	C4B-CHC-C1C	-2.07	126.01	130.12
14	s	103	SPO	C13-C12-C11	2.07	121.34	118.08
8	J	102	BCL	C1-C2-C3	-2.07	122.47	126.04
8	m	402	BCL	C6-C5-C3	-2.06	108.04	113.45
8	q	103	BCL	CED-O2D-CGD	2.06	120.61	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	703	SPO	C25-C23-C22	-2.06	115.78	118.94
12	H	801	PGV	O03-C19-O04	-2.06	118.39	123.59
8	a	101	BCL	CMD-C2D-C3D	-2.06	120.82	124.68
8	03	102	BCL	C1B-CHB-C4A	-2.06	126.03	130.12
14	m	407	SPO	C5-C6-C7	-2.06	122.78	125.89
8	k	101	BCL	C2A-C1A-CHA	-2.06	120.26	123.86
8	M	402	BCL	O2A-CGA-O1A	-2.06	118.40	123.59
11	I	101	LMT	C1-O1'-C1'	-2.06	110.43	113.84
8	Y	102	BCL	CAC-C3C-C4C	-2.06	108.02	112.58
14	05	103	SPO	C8-C7-C9	-2.06	120.04	122.92
14	n	101	SPO	C14-C15-C16	-2.06	116.80	123.22
14	E	102	SPO	C31-C32-C33	-2.06	122.71	127.66
8	M	401	BCL	O1D-CGD-CBD	-2.05	120.29	124.48
14	S	102	SPO	C18-C17-C16	2.05	121.31	118.08
12	l	305	PGV	O03-C19-O04	-2.05	118.43	123.59
8	o	101	BCL	O2A-CGA-O1A	-2.05	118.43	123.59
14	s	103	SPO	C40-C38-C39	2.05	119.12	114.60
12	f	103	PGV	O03-C19-O04	-2.05	118.43	123.59
14	r	101	SPO	C9-C10-C11	-2.04	116.84	123.22
8	G	102	BCL	C4B-CHC-C1C	-2.04	126.07	130.12
14	k	102	SPO	C40-C38-C39	2.04	119.12	114.60
8	v	101	BCL	CAC-C3C-C2C	-2.04	109.16	114.26
8	05	101	BCL	O2A-CGA-O1A	-2.04	118.44	123.59
14	N	101	SPO	C24-C23-C22	-2.04	120.06	122.92
8	R	102	BCL	O2D-CGD-O1D	-2.04	119.85	123.84
8	2	103	BCL	O2A-CGA-O1A	-2.04	118.45	123.59
14	A	703	SPO	C30-C28-C27	-2.04	115.81	121.98
8	01	101	BCL	C4A-NA-C1A	2.04	107.62	106.71
8	7	101	BCL	CHD-C4C-NC	2.04	127.34	125.08
14	a	102	SPO	C11-C12-C14	-2.04	115.81	118.94
14	J	101	SPO	C40-C38-C39	2.03	119.10	114.60
8	Y	102	BCL	CED-O2D-CGD	2.03	120.53	115.94
14	s	103	SPO	C8-C7-C6	2.03	121.28	118.08
14	M	406	SPO	C21-C20-C19	-2.03	119.31	123.47
14	k	102	SPO	C20-C21-C22	-2.03	119.31	123.47
8	5	102	BCL	CHC-C1C-NC	2.03	127.32	124.51
8	L	301	BCL	C2A-C1A-CHA	-2.03	120.31	123.86
8	M	402	BCL	C4A-NA-C1A	2.03	107.62	106.71
8	K	402	BCL	C4A-NA-C1A	2.03	107.62	106.71
14	j	101	SPO	C27-C26-C25	-2.03	116.89	123.22
8	r	102	BCL	C4B-CHC-C1C	-2.03	126.10	130.12
14	08	101	SPO	C27-C26-C25	-2.03	116.90	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	102	BCL	CED-O2D-CGD	2.02	120.51	115.94
14	05	103	SPO	C36-C37-C38	-2.02	120.84	127.75
14	s	105	SPO	C5-C6-C7	-2.02	122.84	125.89
14	S	103	SPO	C5-C6-C7	-2.02	122.84	125.89
12	m	411	PGV	O01-C1-O02	-2.02	118.82	123.70
8	R	102	BCL	CHB-C4A-NA	2.02	127.31	124.51
8	s	102	BCL	C1C-NC-C4C	-2.02	105.80	106.71
8	3	102	BCL	CHB-C4A-NA	2.02	127.30	124.51
14	A	703	SPO	C36-C37-C38	-2.02	120.85	127.75
14	I	103	SPO	C8-C7-C6	2.02	121.26	118.08
8	m	403	BCL	C2A-C1A-CHA	-2.02	120.33	123.86
14	2	101	SPO	C8-C7-C6	2.02	121.25	118.08
8	Z	101	BCL	O2A-CGA-CBA	2.02	118.23	111.91
8	R	102	BCL	CHC-C1C-NC	2.02	127.30	124.51
8	Z	101	BCL	C11-C10-C8	-2.02	109.41	115.92
14	a	102	SPO	C18-C17-C16	2.01	121.25	118.08
14	5	103	SPO	C18-C17-C16	2.01	121.25	118.08
8	Q	103	BCL	O1D-CGD-CBD	-2.01	120.37	124.48
8	5	102	BCL	O2D-CGD-O1D	-2.01	119.91	123.84
8	05	101	BCL	O1D-CGD-CBD	-2.01	120.37	124.48
12	f	103	PGV	O01-C1-O02	-2.01	118.85	123.70
11	5	101	LMT	O1B-C4'-C3'	2.01	112.62	107.28
11	i	102	LMT	O1B-C4'-C3'	2.01	112.62	107.28
14	e	101	SPO	C15-C16-C17	-2.01	120.78	126.42
14	r	101	SPO	C13-C12-C11	2.01	121.24	118.08
8	R	102	BCL	C4B-CHC-C1C	-2.01	126.14	130.12
8	v	101	BCL	C1C-NC-C4C	-2.01	105.80	106.71
14	z	101	SPO	C10-C9-C7	-2.01	124.45	127.31
11	m	409	LMT	C1'-C2'-C3'	2.01	114.17	110.00
14	6	102	SPO	C36-C37-C38	-2.01	120.90	127.75
8	1	202	BCL	CED-O2D-CGD	2.01	120.47	115.94
14	2	104	SPO	C13-C12-C11	2.00	121.23	118.08
8	y	103	BCL	C4B-CHC-C1C	-2.00	126.15	130.12
11	M	412	LMT	C1B-O1B-C4'	-2.00	113.01	117.96
14	Y	103	SPO	C34-C33-C35	2.00	118.64	115.27
14	Y	103	SPO	C26-C25-C23	-2.00	120.79	126.42
8	V	101	BCL	C2A-C1A-CHA	-2.00	120.36	123.86

There are no chirality outliers.

All (2027) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	401	BCL	CHA-CBD-CGD-O1D
8	M	401	BCL	CHA-CBD-CGD-O2D
8	B	102	BCL	C1A-C2A-CAA-CBA
8	B	102	BCL	C3A-C2A-CAA-CBA
8	B	102	BCL	CBD-CGD-O2D-CED
8	B	102	BCL	C4-C3-C5-C6
8	E	101	BCL	C2C-C3C-CAC-CBC
8	E	101	BCL	C4C-C3C-CAC-CBC
8	E	101	BCL	C2-C3-C5-C6
8	E	101	BCL	C4-C3-C5-C6
8	F	502	BCL	C2-C3-C5-C6
8	F	502	BCL	C4-C3-C5-C6
8	G	102	BCL	C4C-C3C-CAC-CBC
8	J	102	BCL	C1A-C2A-CAA-CBA
8	J	102	BCL	C3A-C2A-CAA-CBA
8	K	402	BCL	C4-C3-C5-C6
8	N	102	BCL	C1A-C2A-CAA-CBA
8	P	102	BCL	C1A-C2A-CAA-CBA
8	P	102	BCL	C3A-C2A-CAA-CBA
8	P	102	BCL	C2C-C3C-CAC-CBC
8	P	102	BCL	C4C-C3C-CAC-CBC
8	R	102	BCL	C1A-C2A-CAA-CBA
8	R	102	BCL	C3A-C2A-CAA-CBA
8	S	101	BCL	C2-C3-C5-C6
8	S	101	BCL	C4-C3-C5-C6
8	T	101	BCL	C6-C7-C8-C9
8	Z	101	BCL	C1A-C2A-CAA-CBA
8	Z	101	BCL	C3A-C2A-CAA-CBA
8	2	103	BCL	C2C-C3C-CAC-CBC
8	2	103	BCL	C4C-C3C-CAC-CBC
8	3	102	BCL	C2-C3-C5-C6
8	3	102	BCL	C4-C3-C5-C6
8	4	101	BCL	C1A-C2A-CAA-CBA
8	4	101	BCL	CHA-CBD-CGD-O1D
8	4	101	BCL	CHA-CBD-CGD-O2D
8	5	102	BCL	C2-C3-C5-C6
8	5	102	BCL	C4-C3-C5-C6
8	6	101	BCL	C1A-C2A-CAA-CBA
8	6	101	BCL	C3A-C2A-CAA-CBA
8	8	101	BCL	C1A-C2A-CAA-CBA
8	8	101	BCL	C6-C7-C8-C9
8	a	101	BCL	C4C-C3C-CAC-CBC
8	b	101	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
8	d	101	BCL	C4C-C3C-CAC-CBC
8	f	102	BCL	C2C-C3C-CAC-CBC
8	f	102	BCL	C4C-C3C-CAC-CBC
8	f	102	BCL	CHA-CBD-CGD-O1D
8	f	102	BCL	CHA-CBD-CGD-O2D
8	g	103	BCL	C1A-C2A-CAA-CBA
8	g	103	BCL	C3A-C2A-CAA-CBA
8	g	103	BCL	C2C-C3C-CAC-CBC
8	g	103	BCL	C4C-C3C-CAC-CBC
8	j	102	BCL	C1A-C2A-CAA-CBA
8	j	102	BCL	CHA-CBD-CGD-O1D
8	k	101	BCL	C4C-C3C-CAC-CBC
8	o	101	BCL	C1A-C2A-CAA-CBA
8	p	102	BCL	C2C-C3C-CAC-CBC
8	p	102	BCL	C4C-C3C-CAC-CBC
8	q	103	BCL	C1A-C2A-CAA-CBA
8	r	102	BCL	C1A-C2A-CAA-CBA
8	r	102	BCL	C2C-C3C-CAC-CBC
8	r	102	BCL	C4C-C3C-CAC-CBC
8	s	102	BCL	C2-C3-C5-C6
8	s	102	BCL	C4-C3-C5-C6
8	t	101	BCL	C1A-C2A-CAA-CBA
8	t	101	BCL	C3A-C2A-CAA-CBA
8	v	101	BCL	C4C-C3C-CAC-CBC
8	v	101	BCL	C2-C3-C5-C6
8	v	101	BCL	C4-C3-C5-C6
8	w	102	BCL	C4-C3-C5-C6
8	z	102	BCL	C1A-C2A-CAA-CBA
8	z	102	BCL	C3A-C2A-CAA-CBA
8	01	101	BCL	C1A-C2A-CAA-CBA
8	02	101	BCL	C2C-C3C-CAC-CBC
8	02	101	BCL	C4C-C3C-CAC-CBC
8	04	101	BCL	C1A-C2A-CAA-CBA
8	04	101	BCL	C3A-C2A-CAA-CBA
8	05	101	BCL	C2C-C3C-CAC-CBC
8	05	101	BCL	C4C-C3C-CAC-CBC
8	08	102	BCL	C1A-C2A-CAA-CBA
9	m	404	BPH	C1-C2-C3-C4
10	M	405	U10	C27-C28-C29-C30
10	M	405	U10	C27-C28-C29-C31
10	M	405	U10	C47-C48-C49-C50
10	M	405	U10	C47-C48-C49-C51

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Mol	Chain	Res	Type	Atoms
10	D	102	U10	C7-C8-C9-C11
10	l	303	U10	C7-C8-C9-C11
10	m	406	U10	C23-C24-C26-C27
10	m	406	U10	C25-C24-C26-C27
10	m	406	U10	C34-C36-C37-C38
10	m	406	U10	C42-C43-C44-C45
10	m	406	U10	C42-C43-C44-C46
10	m	406	U10	C50-C49-C51-C52
10	d	102	U10	C15-C14-C16-C17
11	m	408	LMT	C2-C1-O1'-C1'
11	m	409	LMT	O5'-C1'-O1'-C1
11	m	409	LMT	C2-C1-O1'-C1'
11	03	103	LMT	O5'-C1'-O1'-C1
12	L	307	PGV	C03-O11-P-O12
12	L	307	PGV	C03-O11-P-O13
12	L	307	PGV	C03-O11-P-O14
12	L	308	PGV	C03-O11-P-O12
12	M	411	PGV	C03-O11-P-O14
12	M	411	PGV	C04-O12-P-O13
12	M	411	PGV	O01-C02-C03-O11
12	M	411	PGV	O02-C1-O01-C02
12	M	411	PGV	C2-C1-O01-C02
12	H	801	PGV	C03-O11-P-O13
12	H	801	PGV	C04-O12-P-O11
12	H	801	PGV	C04-O12-P-O13
12	H	801	PGV	C04-O12-P-O14
12	H	804	PGV	C03-O11-P-O13
12	H	805	PGV	C04-O12-P-O14
12	F	503	PGV	C03-O11-P-O12
12	F	503	PGV	C03-O11-P-O13
12	F	503	PGV	C03-O11-P-O14
12	F	503	PGV	O02-C1-O01-C02
12	F	503	PGV	C2-C1-O01-C02
12	Q	102	PGV	C03-O11-P-O13
12	Q	102	PGV	C04-O12-P-O13
12	l	305	PGV	C04-O12-P-O11
12	l	305	PGV	C04-O12-P-O13
12	l	305	PGV	C2-C1-O01-C02
12	l	306	PGV	C04-O12-P-O11
12	l	307	PGV	C03-O11-P-O13
12	l	307	PGV	C04-O12-P-O11
12	l	307	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
12	l	307	PGV	O12-C04-C05-C06
12	l	308	PGV	C03-O11-P-O13
12	l	308	PGV	C03-O11-P-O14
12	l	308	PGV	O02-C1-O01-C02
12	l	308	PGV	C2-C1-O01-C02
12	m	411	PGV	C03-O11-P-O12
12	m	411	PGV	C03-O11-P-O13
12	m	411	PGV	C03-O11-P-O14
12	m	411	PGV	O12-C04-C05-O05
12	m	411	PGV	O05-C05-C06-O06
12	m	412	PGV	C03-O11-P-O14
12	h	806	PGV	C03-O11-P-O12
12	h	806	PGV	C03-O11-P-O13
12	h	806	PGV	C03-O11-P-O14
12	h	806	PGV	C04-O12-P-O14
12	h	806	PGV	O01-C02-C03-O11
12	f	103	PGV	C04-O12-P-O14
12	f	104	PGV	C04-O12-P-O13
12	q	102	PGV	C04-O12-P-O14
12	q	102	PGV	C2-C1-O01-C02
12	x	101	PGV	C04-O12-P-O13
14	M	406	SPO	C2-C1-O1-CM1
14	M	406	SPO	O1-C1-C4-C5
14	M	406	SPO	C2-C1-C4-C5
14	M	406	SPO	C3-C1-C4-C5
14	A	703	SPO	C5-C6-C7-C8
14	A	703	SPO	C10-C11-C12-C13
14	B	101	SPO	C27-C28-C30-C31
14	B	101	SPO	C29-C28-C30-C31
14	E	102	SPO	C32-C33-C35-C36
14	E	102	SPO	C34-C33-C35-C36
14	G	103	SPO	C5-C6-C7-C8
14	G	103	SPO	C5-C6-C7-C9
14	G	103	SPO	C10-C11-C12-C13
14	G	103	SPO	C10-C11-C12-C14
14	N	101	SPO	C27-C28-C30-C31
14	N	101	SPO	C29-C28-C30-C31
14	N	101	SPO	C32-C33-C35-C36
14	N	101	SPO	C34-C33-C35-C36
14	O	102	SPO	C28-C30-C31-C32
14	Q	104	SPO	C33-C35-C36-C37
14	R	101	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
14	S	102	SPO	C5-C6-C7-C8
14	S	102	SPO	C5-C6-C7-C9
14	T	102	SPO	C22-C23-C25-C26
14	T	102	SPO	C24-C23-C25-C26
14	T	102	SPO	C29-C28-C30-C31
14	T	102	SPO	C32-C33-C35-C36
14	T	102	SPO	C34-C33-C35-C36
14	V	102	SPO	C28-C30-C31-C32
14	2	101	SPO	C5-C6-C7-C8
14	2	101	SPO	C5-C6-C7-C9
14	2	102	SPO	C5-C6-C7-C8
14	2	102	SPO	C5-C6-C7-C9
14	3	103	SPO	C15-C16-C17-C18
14	3	103	SPO	C15-C16-C17-C19
14	3	103	SPO	C33-C35-C36-C37
14	4	102	SPO	C5-C6-C7-C8
14	4	102	SPO	C5-C6-C7-C9
14	4	102	SPO	C33-C35-C36-C37
14	5	103	SPO	O1-C1-C4-C5
14	5	103	SPO	C2-C1-C4-C5
14	5	103	SPO	C3-C1-C4-C5
14	6	102	SPO	O1-C1-C4-C5
14	6	102	SPO	C2-C1-C4-C5
14	6	102	SPO	C3-C1-C4-C5
14	6	102	SPO	C27-C28-C30-C31
14	6	102	SPO	C29-C28-C30-C31
14	m	407	SPO	C2-C1-O1-CM1
14	a	102	SPO	C10-C11-C12-C13
14	a	102	SPO	C10-C11-C12-C14
14	e	101	SPO	C10-C11-C12-C13
14	e	101	SPO	C10-C11-C12-C14
14	e	101	SPO	C27-C28-C30-C31
14	e	101	SPO	C29-C28-C30-C31
14	e	101	SPO	C32-C33-C35-C36
14	e	101	SPO	C34-C33-C35-C36
14	g	101	SPO	C28-C30-C31-C32
14	g	101	SPO	C32-C33-C35-C36
14	g	101	SPO	C34-C33-C35-C36
14	g	102	SPO	C10-C11-C12-C13
14	g	102	SPO	C10-C11-C12-C14
14	j	101	SPO	C3-C1-C4-C5
14	j	101	SPO	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	j	101	SPO	C29-C28-C30-C31
14	j	101	SPO	C32-C33-C35-C36
14	j	101	SPO	C34-C33-C35-C36
14	k	102	SPO	C33-C35-C36-C37
14	n	101	SPO	O1-C1-C4-C5
14	n	101	SPO	C2-C1-C4-C5
14	n	101	SPO	C3-C1-C4-C5
14	p	101	SPO	C28-C30-C31-C32
14	r	101	SPO	C22-C23-C25-C26
14	r	101	SPO	C24-C23-C25-C26
14	r	103	SPO	C34-C33-C35-C36
14	v	102	SPO	C28-C30-C31-C32
14	v	102	SPO	C34-C33-C35-C36
14	y	105	SPO	C10-C11-C12-C13
14	y	105	SPO	C29-C28-C30-C31
14	z	101	SPO	C5-C6-C7-C8
14	z	101	SPO	C22-C23-C25-C26
14	z	101	SPO	C24-C23-C25-C26
14	01	102	SPO	O1-C1-C4-C5
14	01	102	SPO	C2-C1-C4-C5
14	01	102	SPO	C3-C1-C4-C5
14	01	102	SPO	C5-C6-C7-C8
14	01	102	SPO	C5-C6-C7-C9
14	01	102	SPO	C27-C28-C30-C31
14	01	102	SPO	C29-C28-C30-C31
14	05	102	SPO	C2-C1-C4-C5
14	05	102	SPO	C3-C1-C4-C5
14	05	103	SPO	C27-C28-C30-C31
14	05	103	SPO	C29-C28-C30-C31
14	05	103	SPO	C33-C35-C36-C37
14	08	101	SPO	C10-C11-C12-C13
15	M	410	CDL	CA2-OA2-PA1-OA3
15	M	410	CDL	CA2-OA2-PA1-OA5
15	M	410	CDL	CA3-OA5-PA1-OA2
15	M	410	CDL	CA3-OA5-PA1-OA3
15	M	410	CDL	CA3-OA5-PA1-OA4
15	M	410	CDL	CB2-OB2-PB2-OB3
15	M	410	CDL	CB2-OB2-PB2-OB4
15	M	410	CDL	CB2-OB2-PB2-OB5
15	K	401	CDL	CA3-OA5-PA1-OA2
15	K	401	CDL	CA3-OA5-PA1-OA3
15	K	401	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
15	K	401	CDL	CB2-OB2-PB2-OB4
15	K	401	CDL	CB3-OB5-PB2-OB4
15	Y	101	CDL	CA3-OA5-PA1-OA3
15	X	101	CDL	O1-C1-CB2-OB2
15	X	101	CDL	CA3-OA5-PA1-OA3
15	X	101	CDL	OA6-CA4-CA6-OA8
15	X	101	CDL	CB2-OB2-PB2-OB3
15	X	101	CDL	CB2-OB2-PB2-OB5
15	X	101	CDL	CB3-OB5-PB2-OB2
15	X	102	CDL	CA3-OA5-PA1-OA2
15	X	102	CDL	CA4-CA3-OA5-PA1
15	X	102	CDL	OA9-CA7-OA8-CA6
15	X	103	CDL	CA2-OA2-PA1-OA5
15	X	103	CDL	CA3-OA5-PA1-OA2
15	X	103	CDL	CA3-OA5-PA1-OA3
15	X	103	CDL	C11-CA5-OA6-CA4
15	X	103	CDL	CB4-CB3-OB5-PB2
15	m	410	CDL	CA3-OA5-PA1-OA2
15	m	410	CDL	CA3-OA5-PA1-OA3
15	m	410	CDL	CA3-OA5-PA1-OA4
15	m	410	CDL	CB2-OB2-PB2-OB3
15	m	410	CDL	CB2-OB2-PB2-OB4
15	m	410	CDL	CB2-OB2-PB2-OB5
15	m	413	CDL	CA2-OA2-PA1-OA5
15	m	413	CDL	CB3-OB5-PB2-OB2
15	m	413	CDL	C51-CB5-OB6-CB4
15	h	805	CDL	CA2-OA2-PA1-OA4
15	h	805	CDL	CA3-OA5-PA1-OA2
15	h	805	CDL	OA5-CA3-CA4-OA6
15	h	805	CDL	C11-CA5-OA6-CA4
15	h	805	CDL	CB2-OB2-PB2-OB4
15	h	805	CDL	CB3-OB5-PB2-OB2
15	y	102	CDL	CB3-OB5-PB2-OB3
15	x	102	CDL	CA2-OA2-PA1-OA5
15	x	102	CDL	CA3-OA5-PA1-OA3
15	x	102	CDL	CB2-OB2-PB2-OB3
16	H	803	PTY	C5-O14-P1-O11
16	H	803	PTY	C5-O14-P1-O13
16	h	804	PTY	C3-O11-P1-O13
11	L	305	LMT	C5'-C4'-O1B-C1B
11	H	802	LMT	C3'-C4'-O1B-C1B
11	h	803	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
11	03	101	LMT	C3'-C4'-O1B-C1B
8	M	402	BCL	CBD-CGD-O2D-CED
8	G	102	BCL	CBD-CGD-O2D-CED
8	N	102	BCL	CBD-CGD-O2D-CED
8	01	101	BCL	CBD-CGD-O2D-CED
8	B	102	BCL	O1D-CGD-O2D-CED
11	i	102	LMT	C3'-C4'-O1B-C1B
11	L	306	LMT	O5B-C1B-O1B-C4'
11	i	101	LMT	O5B-C1B-O1B-C4'
8	L	301	BCL	CBD-CGD-O2D-CED
8	P	102	BCL	CBD-CGD-O2D-CED
8	4	101	BCL	CBD-CGD-O2D-CED
8	6	101	BCL	CBD-CGD-O2D-CED
8	m	403	BCL	CBD-CGD-O2D-CED
8	g	103	BCL	CBD-CGD-O2D-CED
8	n	102	BCL	CBD-CGD-O2D-CED
8	t	101	BCL	CBD-CGD-O2D-CED
8	w	102	BCL	CBD-CGD-O2D-CED
8	z	102	BCL	CBD-CGD-O2D-CED
8	03	102	BCL	CBD-CGD-O2D-CED
8	06	101	BCL	CBD-CGD-O2D-CED
8	a	101	BCL	O1A-CGA-O2A-C1
11	M	409	LMT	O5B-C1B-O1B-C4'
8	2	103	BCL	CBD-CGD-O2D-CED
8	02	101	BCL	CBD-CGD-O2D-CED
12	Q	102	PGV	O02-C1-O01-C02
12	l	305	PGV	O02-C1-O01-C02
12	q	102	PGV	O02-C1-O01-C02
15	K	401	CDL	OA7-CA5-OA6-CA4
15	X	103	CDL	OA7-CA5-OA6-CA4
15	h	805	CDL	OA7-CA5-OA6-CA4
8	B	102	BCL	C3-C5-C6-C7
8	E	101	BCL	C3-C5-C6-C7
8	G	102	BCL	C3-C5-C6-C7
8	J	102	BCL	C3-C5-C6-C7
8	3	102	BCL	C3-C5-C6-C7
8	g	103	BCL	C3-C5-C6-C7
8	j	102	BCL	C3-C5-C6-C7
8	q	103	BCL	C3-C5-C6-C7
8	z	102	BCL	C3-C5-C6-C7
8	Z	101	BCL	CBA-CGA-O2A-C1
8	a	101	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	Q	102	PGV	C2-C1-O01-C02
8	r	102	BCL	CBD-CGD-O2D-CED
11	5	101	LMT	C3'-C4'-O1B-C1B
11	s	104	LMT	O5B-C5B-C6B-O6B
8	7	101	BCL	C4-C3-C5-C6
10	M	405	U10	C45-C44-C46-C47
14	G	101	SPO	C34-C33-C35-C36
14	P	101	SPO	C29-C28-C30-C31
14	g	102	SPO	C29-C28-C30-C31
14	n	101	SPO	C34-C33-C35-C36
14	s	105	SPO	C34-C33-C35-C36
14	02	102	SPO	C29-C28-C30-C31
14	08	101	SPO	C29-C28-C30-C31
8	B	102	BCL	C2-C3-C5-C6
8	K	402	BCL	C2-C3-C5-C6
8	w	102	BCL	C2-C3-C5-C6
14	R	101	SPO	C32-C33-C35-C36
14	T	102	SPO	C27-C28-C30-C31
14	g	102	SPO	C27-C28-C30-C31
14	j	101	SPO	C27-C28-C30-C31
14	n	101	SPO	C32-C33-C35-C36
14	r	103	SPO	C32-C33-C35-C36
14	y	105	SPO	C27-C28-C30-C31
14	08	101	SPO	C27-C28-C30-C31
8	8	101	BCL	CBD-CGD-O2D-CED
8	n	102	BCL	C2A-CAA-CBA-CGA
8	04	101	BCL	C2A-CAA-CBA-CGA
10	D	102	U10	C7-C8-C9-C10
8	T	101	BCL	CBD-CGD-O2D-CED
8	M	402	BCL	O1D-CGD-O2D-CED
8	01	101	BCL	O1D-CGD-O2D-CED
15	m	413	CDL	OB7-CB5-OB6-CB4
8	q	103	BCL	CBD-CGD-O2D-CED
12	H	805	PGV	O12-C04-C05-O05
15	X	102	CDL	O1-C1-CB2-OB2
8	t	101	BCL	C3-C5-C6-C7
11	I	101	LMT	C3'-C4'-O1B-C1B
8	Z	101	BCL	O1A-CGA-O2A-C1
8	G	102	BCL	O1D-CGD-O2D-CED
12	L	309	PGV	C2-C1-O01-C02
8	l	301	BCL	CBD-CGD-O2D-CED
8	v	101	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
11	3	104	LMT	O5'-C5'-C6'-O6'
8	Z	101	BCL	CBD-CGD-O2D-CED
8	T	101	BCL	C3-C5-C6-C7
8	w	102	BCL	C3-C5-C6-C7
8	O	101	BCL	C5-C6-C7-C8
8	V	101	BCL	C4-C3-C5-C6
8	Y	102	BCL	C4-C3-C5-C6
8	j	102	BCL	C4-C3-C5-C6
8	05	101	BCL	C4-C3-C5-C6
10	D	102	U10	C15-C14-C16-C17
10	d	102	U10	C20-C19-C21-C22
14	B	103	SPO	C34-C33-C35-C36
14	J	101	SPO	C34-C33-C35-C36
14	P	101	SPO	C34-C33-C35-C36
14	V	102	SPO	C34-C33-C35-C36
14	f	101	SPO	C29-C28-C30-C31
14	f	106	SPO	C34-C33-C35-C36
14	k	102	SPO	C34-C33-C35-C36
14	q	104	SPO	C29-C28-C30-C31
14	r	101	SPO	C34-C33-C35-C36
11	s	104	LMT	C4B-C5B-C6B-O6B
8	V	101	BCL	C2-C3-C5-C6
8	Y	102	BCL	C2-C3-C5-C6
8	j	102	BCL	C2-C3-C5-C6
8	05	101	BCL	C2-C3-C5-C6
10	D	102	U10	C13-C14-C16-C17
10	d	102	U10	C13-C14-C16-C17
10	d	102	U10	C18-C19-C21-C22
14	B	103	SPO	C32-C33-C35-C36
14	J	101	SPO	C32-C33-C35-C36
14	P	101	SPO	C27-C28-C30-C31
14	P	101	SPO	C32-C33-C35-C36
14	V	102	SPO	C32-C33-C35-C36
14	f	101	SPO	C27-C28-C30-C31
14	f	106	SPO	C32-C33-C35-C36
14	k	102	SPO	C32-C33-C35-C36
14	q	104	SPO	C27-C28-C30-C31
14	r	101	SPO	C32-C33-C35-C36
14	v	102	SPO	C32-C33-C35-C36
8	6	101	BCL	C2A-CAA-CBA-CGA
8	w	102	BCL	C2A-CAA-CBA-CGA
11	M	409	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
11	I	101	LMT	O5'-C1'-O1'-C1
11	U	101	LMT	O5'-C1'-O1'-C1
11	U	103	LMT	O5'-C1'-O1'-C1
11	03	101	LMT	O5'-C1'-O1'-C1
10	D	102	U10	C9-C11-C12-C13
14	B	103	SPO	C28-C30-C31-C32
14	G	101	SPO	C28-C30-C31-C32
14	G	101	SPO	C33-C35-C36-C37
14	G	103	SPO	C28-C30-C31-C32
14	I	103	SPO	C28-C30-C31-C32
14	I	103	SPO	C33-C35-C36-C37
14	O	102	SPO	C33-C35-C36-C37
14	P	101	SPO	C28-C30-C31-C32
14	Q	104	SPO	C28-C30-C31-C32
14	R	101	SPO	C28-C30-C31-C32
14	S	102	SPO	C33-C35-C36-C37
14	2	101	SPO	C28-C30-C31-C32
14	2	102	SPO	C33-C35-C36-C37
14	5	103	SPO	C28-C30-C31-C32
14	f	101	SPO	C28-C30-C31-C32
14	f	101	SPO	C33-C35-C36-C37
14	j	101	SPO	C28-C30-C31-C32
14	k	102	SPO	C28-C30-C31-C32
14	n	101	SPO	C33-C35-C36-C37
14	q	104	SPO	C28-C30-C31-C32
14	q	104	SPO	C33-C35-C36-C37
14	r	103	SPO	C33-C35-C36-C37
14	s	105	SPO	C33-C35-C36-C37
14	v	102	SPO	C33-C35-C36-C37
14	w	101	SPO	C28-C30-C31-C32
14	01	103	SPO	C28-C30-C31-C32
14	01	103	SPO	C33-C35-C36-C37
14	05	102	SPO	C33-C35-C36-C37
14	05	103	SPO	C28-C30-C31-C32
8	8	101	BCL	CBA-CGA-O2A-C1
10	l	303	U10	C7-C8-C9-C10
8	N	102	BCL	O1D-CGD-O2D-CED
8	n	102	BCL	O1D-CGD-O2D-CED
8	a	101	BCL	CBD-CGD-O2D-CED
15	X	101	CDL	CA2-C1-CB2-OB2
15	X	102	CDL	CA2-C1-CB2-OB2
10	M	405	U10	C22-C23-C24-C26

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Mol	Chain	Res	Type	Atoms
8	1	202	BCL	C3-C5-C6-C7
8	6	101	BCL	O1D-CGD-O2D-CED
8	03	102	BCL	O1D-CGD-O2D-CED
8	J	102	BCL	C5-C6-C7-C8
8	V	101	BCL	C10-C11-C12-C13
8	04	101	BCL	C8-C10-C11-C12
12	M	411	PGV	O12-C04-C05-O05
12	l	307	PGV	O12-C04-C05-O05
14	E	102	SPO	C29-C28-C30-C31
14	I	103	SPO	C34-C33-C35-C36
10	L	304	U10	C12-C11-C9-C8
14	G	101	SPO	C32-C33-C35-C36
14	02	102	SPO	C27-C28-C30-C31
8	M	402	BCL	C11-C10-C8-C9
8	A	702	BCL	C6-C7-C8-C9
8	B	102	BCL	C11-C10-C8-C9
8	D	101	BCL	C6-C7-C8-C9
8	E	101	BCL	C11-C12-C13-C14
8	G	102	BCL	C11-C10-C8-C9
8	N	102	BCL	C14-C13-C15-C16
8	P	102	BCL	C6-C7-C8-C9
8	R	102	BCL	C6-C7-C8-C9
8	S	101	BCL	C11-C12-C13-C14
8	Y	102	BCL	C6-C7-C8-C9
8	1	202	BCL	C6-C7-C8-C9
8	1	202	BCL	C11-C10-C8-C9
8	2	103	BCL	C6-C7-C8-C9
8	6	101	BCL	C6-C7-C8-C9
8	l	301	BCL	C14-C13-C15-C16
8	m	401	BCL	C11-C10-C8-C9
8	m	401	BCL	C11-C12-C13-C14
8	b	101	BCL	C11-C10-C8-C9
8	d	101	BCL	C11-C10-C8-C9
8	e	102	BCL	C11-C10-C8-C9
8	g	103	BCL	C11-C10-C8-C9
8	j	102	BCL	C11-C10-C8-C9
8	j	102	BCL	C11-C12-C13-C14
8	k	101	BCL	C14-C13-C15-C16
8	n	102	BCL	C6-C7-C8-C9
8	r	102	BCL	C6-C7-C8-C9
8	s	102	BCL	C11-C10-C8-C9
8	t	101	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	y	103	BCL	C6-C7-C8-C9
8	y	103	BCL	C11-C10-C8-C9
8	z	102	BCL	C11-C10-C8-C9
8	02	101	BCL	C6-C7-C8-C9
8	L	301	BCL	O1D-CGD-O2D-CED
8	w	102	BCL	O1D-CGD-O2D-CED
8	J	102	BCL	CBD-CGD-O2D-CED
8	06	101	BCL	C2A-CAA-CBA-CGA
14	Q	104	SPO	C10-C11-C12-C13
14	e	101	SPO	C5-C6-C7-C8
14	f	101	SPO	C10-C11-C12-C13
14	n	101	SPO	C5-C6-C7-C8
14	r	103	SPO	C5-C6-C7-C8
14	v	102	SPO	C24-C23-C25-C26
14	e	101	SPO	C5-C6-C7-C9
14	r	103	SPO	C5-C6-C7-C9
12	l	306	PGV	C19-C20-C21-C22
12	q	102	PGV	C19-C20-C21-C22
8	n	102	BCL	C13-C15-C16-C17
8	q	103	BCL	C5-C6-C7-C8
8	01	101	BCL	C5-C6-C7-C8
8	W	101	BCL	CBD-CGD-O2D-CED
11	U	101	LMT	O5'-C5'-C6'-O6'
8	P	102	BCL	C3-C5-C6-C7
8	A	702	BCL	C5-C6-C7-C8
8	B	102	BCL	C5-C6-C7-C8
8	Q	103	BCL	C8-C10-C11-C12
8	S	101	BCL	C15-C16-C17-C18
8	T	101	BCL	C10-C11-C12-C13
8	W	101	BCL	C8-C10-C11-C12
8	1	202	BCL	C15-C16-C17-C18
8	z	102	BCL	C10-C11-C12-C13
8	05	101	BCL	C5-C6-C7-C8
8	Q	103	BCL	C5-C6-C7-C8
8	R	102	BCL	C10-C11-C12-C13
8	l	301	BCL	C13-C15-C16-C17
8	d	101	BCL	C15-C16-C17-C18
8	e	102	BCL	C5-C6-C7-C8
8	f	102	BCL	C13-C15-C16-C17
8	g	103	BCL	C8-C10-C11-C12
8	01	101	BCL	C8-C10-C11-C12
8	03	102	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
8	08	102	BCL	C8-C10-C11-C12
10	M	405	U10	C22-C23-C24-C25
12	L	307	PGV	C19-C20-C21-C22
12	M	411	PGV	C1-C2-C3-C4
12	H	805	PGV	C1-C2-C3-C4
12	l	306	PGV	C1-C2-C3-C4
12	m	412	PGV	C1-C2-C3-C4
12	f	103	PGV	C19-C20-C21-C22
12	x	101	PGV	C1-C2-C3-C4
15	Y	101	CDL	CA7-C31-C32-C33
15	X	103	CDL	CB5-C51-C52-C53
8	07	101	BCL	CBD-CGD-O2D-CED
8	P	102	BCL	C8-C10-C11-C12
8	6	101	BCL	C10-C11-C12-C13
8	w	102	BCL	C8-C10-C11-C12
8	z	102	BCL	O1D-CGD-O2D-CED
8	06	101	BCL	O1D-CGD-O2D-CED
11	U	103	LMT	O5'-C5'-C6'-O6'
12	L	309	PGV	O02-C1-O01-C02
10	d	102	U10	C7-C8-C9-C11
11	3	101	LMT	O1'-C1-C2-C3
8	Z	101	BCL	C5-C6-C7-C8
8	e	102	BCL	C15-C16-C17-C18
12	L	307	PGV	C2-C1-O01-C02
12	m	411	PGV	C2-C1-O01-C02
8	l	301	BCL	C15-C16-C17-C18
8	i	103	BCL	C15-C16-C17-C18
8	S	101	BCL	C11-C10-C8-C7
8	W	101	BCL	C11-C10-C8-C7
8	Y	102	BCL	C11-C10-C8-C7
8	Y	102	BCL	C11-C12-C13-C15
8	2	103	BCL	C6-C7-C8-C10
8	6	101	BCL	C11-C10-C8-C7
8	8	101	BCL	C6-C7-C8-C10
8	l	301	BCL	C12-C13-C15-C16
8	m	402	BCL	C11-C10-C8-C7
8	e	102	BCL	C6-C7-C8-C10
8	j	102	BCL	C11-C12-C13-C15
8	k	101	BCL	C6-C7-C8-C10
8	p	102	BCL	C6-C7-C8-C10
8	03	102	BCL	C6-C7-C8-C10
8	04	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
8	Y	102	BCL	C3-C5-C6-C7
14	G	103	SPO	C11-C10-C9-C7
14	n	101	SPO	C11-C10-C9-C7
8	P	102	BCL	O1D-CGD-O2D-CED
8	4	101	BCL	O1D-CGD-O2D-CED
8	g	103	BCL	O1D-CGD-O2D-CED
8	t	101	BCL	O1D-CGD-O2D-CED
8	W	101	BCL	C10-C11-C12-C13
8	3	102	BCL	C5-C6-C7-C8
8	7	101	BCL	C10-C11-C12-C13
8	m	403	BCL	C5-C6-C7-C8
8	d	101	BCL	C8-C10-C11-C12
8	o	101	BCL	C8-C10-C11-C12
8	t	101	BCL	C10-C11-C12-C13
8	v	101	BCL	C15-C16-C17-C18
8	L	311	BCL	C13-C15-C16-C17
8	m	401	BCL	C10-C11-C12-C13
14	K	404	SPO	C28-C30-C31-C32
14	4	102	SPO	C28-C30-C31-C32
14	5	103	SPO	C33-C35-C36-C37
14	6	102	SPO	C33-C35-C36-C37
14	f	106	SPO	C33-C35-C36-C37
14	s	103	SPO	C28-C30-C31-C32
14	s	103	SPO	C33-C35-C36-C37
14	y	105	SPO	C28-C30-C31-C32
14	05	102	SPO	C28-C30-C31-C32
12	Q	102	PGV	C1-C2-C3-C4
12	l	306	PGV	O12-C04-C05-O05
8	W	101	BCL	C15-C16-C17-C18
8	4	101	BCL	C15-C16-C17-C18
8	02	101	BCL	C8-C10-C11-C12
8	S	101	BCL	CBA-CGA-O2A-C1
12	m	411	PGV	C20-C19-O03-C01
8	8	101	BCL	O1A-CGA-O2A-C1
11	U	101	LMT	C4'-C5'-C6'-O6'
8	M	401	BCL	C5-C6-C7-C8
8	M	402	BCL	C5-C6-C7-C8
8	D	101	BCL	C8-C10-C11-C12
8	D	101	BCL	C13-C15-C16-C17
8	m	402	BCL	C5-C6-C7-C8
8	m	402	BCL	C10-C11-C12-C13
8	k	101	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	2	103	BCL	O1D-CGD-O2D-CED
8	O	101	BCL	CBD-CGD-O2D-CED
15	m	410	CDL	C51-CB5-OB6-CB4
11	s	101	LMT	C3-C4-C5-C6
10	M	405	U10	C46-C47-C48-C49
8	r	102	BCL	O1D-CGD-O2D-CED
8	1	202	BCL	C5-C6-C7-C8
8	7	101	BCL	C13-C15-C16-C17
8	8	101	BCL	C8-C10-C11-C12
12	L	307	PGV	C04-O12-P-O11
12	L	309	PGV	C03-O11-P-O12
12	H	801	PGV	C03-O11-P-O12
12	H	805	PGV	C04-O12-P-O11
12	F	503	PGV	C04-O12-P-O11
12	l	305	PGV	C03-O11-P-O12
12	l	307	PGV	C03-O11-P-O12
12	l	308	PGV	C03-O11-P-O12
12	m	412	PGV	C03-O11-P-O12
12	h	801	PGV	C04-O12-P-O11
12	q	102	PGV	C04-O12-P-O11
15	M	410	CDL	CB3-OB5-PB2-OB2
15	K	401	CDL	CA2-OA2-PA1-OA5
15	K	401	CDL	CB2-OB2-PB2-OB5
15	Y	101	CDL	CB2-OB2-PB2-OB5
15	X	102	CDL	CA2-OA2-PA1-OA5
15	X	103	CDL	CB2-OB2-PB2-OB5
15	X	103	CDL	CB3-OB5-PB2-OB2
15	m	410	CDL	CB3-OB5-PB2-OB2
15	h	805	CDL	CA2-OA2-PA1-OA5
15	h	805	CDL	CB2-OB2-PB2-OB5
15	y	102	CDL	CB2-OB2-PB2-OB5
8	s	102	BCL	CBA-CGA-O2A-C1
12	h	806	PGV	C20-C19-O03-C01
15	X	101	CDL	C31-CA7-OA8-CA6
8	m	403	BCL	O1D-CGD-O2D-CED
8	02	101	BCL	O1D-CGD-O2D-CED
8	j	102	BCL	C15-C16-C17-C18
8	y	103	BCL	C5-C6-C7-C8
11	3	104	LMT	C4'-C5'-C6'-O6'
12	H	805	PGV	O12-C04-C05-C06
12	m	411	PGV	O12-C04-C05-C06
12	L	307	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
12	m	411	PGV	O02-C1-O01-C02
8	W	101	BCL	C4-C3-C5-C6
10	L	304	U10	C12-C11-C9-C10
14	G	103	SPO	C29-C28-C30-C31
14	I	103	SPO	C32-C33-C35-C36
8	O	101	BCL	C15-C16-C17-C18
8	07	101	BCL	C5-C6-C7-C8
8	A	702	BCL	C2A-CAA-CBA-CGA
8	j	102	BCL	C2A-CAA-CBA-CGA
8	p	102	BCL	C2A-CAA-CBA-CGA
8	04	101	BCL	C16-C17-C18-C19
8	R	102	BCL	C13-C15-C16-C17
8	07	101	BCL	C15-C16-C17-C18
12	y	104	PGV	C1-C2-C3-C4
11	H	802	LMT	C6-C7-C8-C9
12	f	104	PGV	C22-C23-C24-C25
8	F	502	BCL	CBD-CGD-O2D-CED
8	02	101	BCL	C10-C11-C12-C13
12	K	403	PGV	C20-C21-C22-C23
12	1	201	PGV	C2-C3-C4-C5
12	l	306	PGV	C3-C4-C5-C6
12	l	306	PGV	C6-C7-C8-C9
12	m	412	PGV	C22-C23-C24-C25
8	T	101	BCL	O1D-CGD-O2D-CED
8	L	301	BCL	C16-C17-C18-C20
8	07	101	BCL	C16-C17-C18-C19
8	b	101	BCL	CBA-CGA-O2A-C1
12	k	103	PGV	C25-C26-C27-C28
15	m	410	CDL	OB7-CB5-OB6-CB4
8	I	102	BCL	C15-C16-C17-C18
11	M	407	LMT	C7-C8-C9-C10
11	U	101	LMT	C5-C6-C7-C8
15	X	103	CDL	C33-C34-C35-C36
8	8	101	BCL	O1D-CGD-O2D-CED
12	m	411	PGV	O01-C02-C03-O11
12	l	306	PGV	C2-C3-C4-C5
12	Q	102	PGV	O12-C04-C05-O05
12	l	308	PGV	O12-C04-C05-O05
12	q	102	PGV	O12-C04-C05-O05
15	M	410	CDL	O1-C1-CA2-OA2
15	Y	101	CDL	OB5-CB3-CB4-OB6
15	X	102	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
15	m	410	CDL	O1-C1-CB2-OB2
12	H	804	PGV	C04-O12-P-O13
12	h	806	PGV	C04-O12-P-O13
11	h	803	LMT	C6-C7-C8-C9
12	x	101	PGV	C22-C23-C24-C25
15	M	410	CDL	C58-C59-C60-C61
8	7	101	BCL	C5-C6-C7-C8
8	s	102	BCL	C15-C16-C17-C18
8	S	101	BCL	O1A-CGA-O2A-C1
8	4	101	BCL	C16-C17-C18-C19
8	P	102	BCL	C4-C3-C5-C6
8	1	202	BCL	C4-C3-C5-C6
10	D	102	U10	C12-C13-C14-C15
10	d	102	U10	C7-C8-C9-C10
14	J	101	SPO	C29-C28-C30-C31
14	Y	103	SPO	C34-C33-C35-C36
8	7	101	BCL	C2-C3-C5-C6
8	L	301	BCL	C11-C10-C8-C9
8	L	311	BCL	C11-C10-C8-C9
8	M	401	BCL	C11-C10-C8-C9
8	l	301	BCL	C11-C10-C8-C9
8	j	102	BCL	C14-C13-C15-C16
8	t	101	BCL	C11-C10-C8-C9
8	q	103	BCL	O1D-CGD-O2D-CED
15	y	102	CDL	CB7-C71-C72-C73
12	K	403	PGV	C3-C4-C5-C6
15	m	410	CDL	C17-C18-C19-C20
8	T	101	BCL	C15-C16-C17-C18
8	k	101	BCL	C8-C10-C11-C12
8	r	102	BCL	C8-C10-C11-C12
8	03	102	BCL	C15-C16-C17-C18
11	3	101	LMT	O5'-C5'-C6'-O6'
8	s	102	BCL	O1A-CGA-O2A-C1
12	m	411	PGV	O04-C19-O03-C01
12	L	308	PGV	C24-C25-C26-C27
12	1	201	PGV	C7-C8-C9-C10
16	f	105	PTY	C20-C21-C22-C23
12	m	411	PGV	C04-C05-C06-O06
14	j	101	SPO	C10-C11-C12-C14
14	08	101	SPO	C10-C11-C12-C14
8	06	101	BCL	C3-C5-C6-C7
12	H	804	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
8	i	103	BCL	C8-C10-C11-C12
12	H	804	PGV	C2-C1-O01-C02
15	K	401	CDL	CB5-C51-C52-C53
11	U	102	LMT	C5-C6-C7-C8
12	1	201	PGV	C3-C4-C5-C6
8	M	401	BCL	C16-C17-C18-C19
8	O	101	BCL	C16-C17-C18-C19
8	V	101	BCL	C16-C17-C18-C19
8	F	502	BCL	C5-C6-C7-C8
16	h	804	PTY	C30-C31-C32-C33
8	r	102	BCL	C13-C15-C16-C17
8	02	101	BCL	C5-C6-C7-C8
15	X	101	CDL	OA9-CA7-OA8-CA6
12	H	805	PGV	C20-C21-C22-C23
8	07	101	BCL	C3-C5-C6-C7
11	A	701	LMT	O5B-C5B-C6B-O6B
11	L	306	LMT	C5'-C4'-O1B-C1B
8	A	702	BCL	C3A-C2A-CAA-CBA
8	G	102	BCL	C3A-C2A-CAA-CBA
8	N	102	BCL	C3A-C2A-CAA-CBA
8	O	101	BCL	C3A-C2A-CAA-CBA
8	T	101	BCL	C3A-C2A-CAA-CBA
8	2	103	BCL	C3A-C2A-CAA-CBA
8	4	101	BCL	C3A-C2A-CAA-CBA
8	8	101	BCL	C3A-C2A-CAA-CBA
8	b	101	BCL	C3A-C2A-CAA-CBA
8	j	102	BCL	C3A-C2A-CAA-CBA
8	o	101	BCL	C3A-C2A-CAA-CBA
8	p	102	BCL	C3A-C2A-CAA-CBA
8	q	103	BCL	C3A-C2A-CAA-CBA
8	r	102	BCL	C3A-C2A-CAA-CBA
8	01	101	BCL	C3A-C2A-CAA-CBA
8	02	101	BCL	C3A-C2A-CAA-CBA
8	08	102	BCL	C3A-C2A-CAA-CBA
8	R	102	BCL	C8-C10-C11-C12
8	Y	102	BCL	C15-C16-C17-C18
8	s	102	BCL	C5-C6-C7-C8
11	L	305	LMT	C2-C1-O1'-C1'
15	h	805	CDL	CB5-C51-C52-C53
8	L	301	BCL	C16-C17-C18-C19
8	V	101	BCL	C16-C17-C18-C20
8	m	402	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	M	410	CDL	C11-C12-C13-C14
9	L	302	BPH	O2A-C1-C2-C3
11	03	101	LMT	O1'-C1-C2-C3
8	G	102	BCL	C4-C3-C5-C6
14	r	103	SPO	C29-C28-C30-C31
8	1	202	BCL	C2-C3-C5-C6
14	E	102	SPO	C27-C28-C30-C31
14	J	101	SPO	C27-C28-C30-C31
14	Y	103	SPO	C32-C33-C35-C36
14	r	103	SPO	C27-C28-C30-C31
14	s	105	SPO	C32-C33-C35-C36
8	E	101	BCL	C2A-CAA-CBA-CGA
8	e	102	BCL	C2A-CAA-CBA-CGA
15	m	413	CDL	C31-C32-C33-C34
12	h	806	PGV	O04-C19-O03-C01
12	L	307	PGV	C1-C2-C3-C4
8	O	101	BCL	C16-C17-C18-C20
11	M	409	LMT	C1-C2-C3-C4
8	08	102	BCL	CBD-CGD-O2D-CED
12	x	101	PGV	O12-C04-C05-O05
8	K	402	BCL	C15-C16-C17-C18
8	V	101	BCL	C5-C6-C7-C8
8	m	402	BCL	C3-C5-C6-C7
8	R	102	BCL	CBA-CGA-O2A-C1
11	M	412	LMT	C4'-C5'-C6'-O6'
11	U	102	LMT	C3-C4-C5-C6
15	h	805	CDL	C52-C53-C54-C55
8	b	101	BCL	O1A-CGA-O2A-C1
12	l	306	PGV	O12-C04-C05-C06
15	X	102	CDL	CB2-C1-CA2-OA2
15	m	410	CDL	C58-C59-C60-C61
16	H	803	PTY	C18-C19-C20-C21
10	D	102	U10	C12-C13-C14-C16
8	01	101	BCL	C10-C11-C12-C13
12	L	310	PGV	C3-C4-C5-C6
11	5	101	LMT	O5'-C5'-C6'-O6'
8	M	402	BCL	C13-C15-C16-C17
8	m	403	BCL	C10-C11-C12-C13
8	t	101	BCL	C8-C10-C11-C12
12	f	103	PGV	C2-C1-O01-C02
12	K	403	PGV	C13-C14-C15-C16
15	X	102	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
8	P	102	BCL	C13-C15-C16-C17
8	Q	103	BCL	C4-C3-C5-C6
8	o	101	BCL	C4-C3-C5-C6
8	t	101	BCL	C4-C3-C5-C6
8	z	102	BCL	C4-C3-C5-C6
14	2	102	SPO	C29-C28-C30-C31
8	L	301	BCL	C11-C10-C8-C7
8	A	702	BCL	C6-C7-C8-C10
8	E	101	BCL	C11-C10-C8-C7
8	E	101	BCL	C11-C12-C13-C15
8	G	102	BCL	C2-C3-C5-C6
8	P	102	BCL	C2-C3-C5-C6
8	P	102	BCL	C6-C7-C8-C10
8	Q	103	BCL	C2-C3-C5-C6
8	Q	103	BCL	C11-C10-C8-C7
8	S	101	BCL	C11-C12-C13-C15
8	Y	102	BCL	C6-C7-C8-C10
8	Z	101	BCL	C2-C3-C5-C6
8	6	101	BCL	C2-C3-C5-C6
8	m	401	BCL	C11-C10-C8-C7
8	o	101	BCL	C2-C3-C5-C6
8	r	102	BCL	C6-C7-C8-C10
8	s	102	BCL	C11-C10-C8-C7
8	t	101	BCL	C2-C3-C5-C6
8	t	101	BCL	C11-C10-C8-C7
8	02	101	BCL	C11-C10-C8-C7
8	06	101	BCL	C2-C3-C5-C6
8	07	101	BCL	C11-C10-C8-C7
9	m	404	BPH	C6-C7-C8-C10
14	z	101	SPO	C27-C28-C30-C31
8	R	102	BCL	O1A-CGA-O2A-C1
12	M	411	PGV	C3-C4-C5-C6
8	I	102	BCL	C5-C6-C7-C8
8	N	102	BCL	C10-C11-C12-C13
8	06	101	BCL	C13-C15-C16-C17
8	I	102	BCL	CBD-CGD-O2D-CED
8	4	101	BCL	C16-C17-C18-C20
12	k	103	PGV	C1-C2-C3-C4
15	Y	101	CDL	C33-C34-C35-C36
8	N	102	BCL	C2A-CAA-CBA-CGA
8	T	101	BCL	C2A-CAA-CBA-CGA
8	4	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
8	p	102	BCL	C10-C11-C12-C13
8	l	301	BCL	O1D-CGD-O2D-CED
12	M	411	PGV	C2-C3-C4-C5
12	H	804	PGV	C19-C20-C21-C22
8	Z	101	BCL	O1D-CGD-O2D-CED
8	6	101	BCL	C8-C10-C11-C12
11	03	101	LMT	C7-C8-C9-C10
12	h	806	PGV	C21-C22-C23-C24
11	L	306	LMT	O1'-C1-C2-C3
11	M	412	LMT	O5'-C5'-C6'-O6'
8	2	103	BCL	CBA-CGA-O2A-C1
8	Q	103	BCL	C16-C17-C18-C19
8	Z	101	BCL	C16-C17-C18-C19
8	01	101	BCL	C16-C17-C18-C19
8	L	301	BCL	C15-C16-C17-C18
8	P	102	BCL	C10-C11-C12-C13
14	w	101	SPO	C33-C35-C36-C37
12	f	104	PGV	C1-C2-C3-C4
12	L	308	PGV	C2-C1-O01-C02
12	l	307	PGV	C2-C1-O01-C02
15	M	410	CDL	C51-CB5-OB6-CB4
11	L	306	LMT	C3'-C4'-O1B-C1B
11	m	408	LMT	O1'-C1-C2-C3
8	Y	102	BCL	CBD-CGD-O2D-CED
12	k	103	PGV	C26-C27-C28-C29
15	M	410	CDL	OB7-CB5-OB6-CB4
15	m	410	CDL	OA6-CA4-CA6-OA8
8	D	101	BCL	C16-C17-C18-C19
8	04	101	BCL	C16-C17-C18-C20
12	H	805	PGV	C22-C23-C24-C25
11	i	102	LMT	O5'-C5'-C6'-O6'
8	T	101	BCL	C8-C10-C11-C12
8	Z	101	BCL	C4-C3-C5-C6
14	n	103	SPO	C29-C28-C30-C31
14	s	105	SPO	C29-C28-C30-C31
14	z	101	SPO	C29-C28-C30-C31
8	L	301	BCL	C2-C3-C5-C6
8	W	101	BCL	C2-C3-C5-C6
8	z	102	BCL	C2-C3-C5-C6
10	M	405	U10	C43-C44-C46-C47
14	G	103	SPO	C27-C28-C30-C31
11	03	103	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	Q	103	BCL	C6-C7-C8-C9
8	Q	103	BCL	C11-C10-C8-C9
8	T	101	BCL	C11-C10-C8-C9
8	Y	102	BCL	C11-C10-C8-C9
8	Y	102	BCL	C11-C12-C13-C14
8	e	102	BCL	C6-C7-C8-C9
8	k	101	BCL	C6-C7-C8-C9
8	p	102	BCL	C11-C10-C8-C9
8	p	102	BCL	C11-C12-C13-C14
8	02	101	BCL	C11-C10-C8-C9
8	03	102	BCL	C6-C7-C8-C9
8	04	101	BCL	C6-C7-C8-C9
8	07	101	BCL	C6-C7-C8-C9
8	07	101	BCL	C11-C10-C8-C9
11	m	408	LMT	O5'-C5'-C6'-O6'
16	H	803	PTY	C19-C20-C21-C22
8	P	102	BCL	C2A-CAA-CBA-CGA
8	r	102	BCL	C2A-CAA-CBA-CGA
8	t	101	BCL	C2A-CAA-CBA-CGA
8	08	102	BCL	C2A-CAA-CBA-CGA
14	B	103	SPO	C5-C6-C7-C8
14	r	101	SPO	C10-C11-C12-C13
14	A	703	SPO	C10-C11-C12-C14
14	z	101	SPO	C5-C6-C7-C9
11	s	104	LMT	C1-C2-C3-C4
8	G	102	BCL	C1A-C2A-CAA-CBA
8	O	101	BCL	C1A-C2A-CAA-CBA
8	T	101	BCL	C1A-C2A-CAA-CBA
8	2	103	BCL	C1A-C2A-CAA-CBA
8	m	401	BCL	C1A-C2A-CAA-CBA
8	02	101	BCL	C1A-C2A-CAA-CBA
8	B	102	BCL	C16-C17-C18-C19
8	Q	103	BCL	C16-C17-C18-C20
8	Z	101	BCL	C16-C17-C18-C20
8	r	102	BCL	C16-C17-C18-C19
8	07	101	BCL	C16-C17-C18-C20
12	L	308	PGV	O02-C1-O01-C02
12	f	103	PGV	O02-C1-O01-C02
12	K	403	PGV	C22-C23-C24-C25
14	r	103	SPO	C25-C26-C27-C28
8	W	101	BCL	C5-C6-C7-C8
8	5	102	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	j	102	BCL	C5-C6-C7-C8
12	Q	102	PGV	C04-O12-P-O11
12	f	103	PGV	C04-O12-P-O11
15	K	401	CDL	C31-C32-C33-C34
16	h	804	PTY	C6-C5-O14-P1
11	U	102	LMT	C1-C2-C3-C4
12	M	411	PGV	C01-C02-C03-O11
12	l	307	PGV	C01-C02-C03-O11
12	m	411	PGV	C01-C02-C03-O11
12	h	806	PGV	C01-C02-C03-O11
15	h	805	CDL	OA5-CA3-CA4-CA6
8	W	101	BCL	O1D-CGD-O2D-CED
11	Q	101	LMT	C3-C4-C5-C6
12	L	309	PGV	C5-C6-C7-C8
12	M	411	PGV	C7-C8-C9-C10
15	m	413	CDL	C71-CB7-OB8-CB6
11	3	104	LMT	O5B-C5B-C6B-O6B
8	R	102	BCL	C16-C17-C18-C19
8	Y	102	BCL	C16-C17-C18-C19
11	U	102	LMT	O5'-C5'-C6'-O6'
8	v	101	BCL	C8-C10-C11-C12
15	X	101	CDL	CA5-C11-C12-C13
16	H	803	PTY	C13-C14-C15-C16
11	H	802	LMT	O5'-C5'-C6'-O6'
12	x	101	PGV	O12-C04-C05-C06
8	L	301	BCL	C4-C3-C5-C6
8	6	101	BCL	C4-C3-C5-C6
8	06	101	BCL	C4-C3-C5-C6
8	L	301	BCL	C2C-C3C-CAC-CBC
8	G	102	BCL	C2C-C3C-CAC-CBC
8	a	101	BCL	C2C-C3C-CAC-CBC
8	d	101	BCL	C2C-C3C-CAC-CBC
8	k	101	BCL	C2C-C3C-CAC-CBC
8	v	101	BCL	C2C-C3C-CAC-CBC
8	A	702	BCL	C8-C10-C11-C12
8	2	103	BCL	C10-C11-C12-C13
12	f	104	PGV	C5-C6-C7-C8
8	G	102	BCL	C2A-CAA-CBA-CGA
8	N	102	BCL	C16-C17-C18-C19
11	A	701	LMT	O5'-C5'-C6'-O6'
11	U	103	LMT	C4-C5-C6-C7
12	H	804	PGV	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
12	Q	102	PGV	O03-C01-C02-C03
12	h	806	PGV	O03-C01-C02-C03
12	y	104	PGV	O03-C01-C02-C03
12	x	101	PGV	O03-C01-C02-C03
15	M	410	CDL	CB3-CB4-CB6-OB8
15	m	410	CDL	CB3-CB4-CB6-OB8
8	M	402	BCL	C15-C16-C17-C18
12	H	801	PGV	C24-C25-C26-C27
8	J	102	BCL	O1D-CGD-O2D-CED
12	l	307	PGV	C20-C21-C22-C23
8	E	101	BCL	C16-C17-C18-C19
8	01	101	BCL	C16-C17-C18-C20
9	m	404	BPH	C1-C2-C3-C5
8	G	102	BCL	C5-C6-C7-C8
8	07	101	BCL	C10-C11-C12-C13
14	g	101	SPO	C33-C35-C36-C37
8	1	202	BCL	CBD-CGD-O2D-CED
8	7	101	BCL	C8-C10-C11-C12
8	7	101	BCL	C15-C16-C17-C18
8	d	101	BCL	C5-C6-C7-C8
8	2	103	BCL	O1A-CGA-O2A-C1
8	a	101	BCL	O1D-CGD-O2D-CED
8	S	101	BCL	C10-C11-C12-C13
8	j	102	BCL	C10-C11-C12-C13
11	I	101	LMT	O5'-C5'-C6'-O6'
11	m	409	LMT	O5'-C5'-C6'-O6'
11	03	101	LMT	O5'-C5'-C6'-O6'
11	03	103	LMT	O5B-C5B-C6B-O6B
11	A	701	LMT	C1-C2-C3-C4
8	N	102	BCL	C4-C3-C5-C6
9	l	302	BPH	C4-C3-C5-C6
14	Q	104	SPO	C34-C33-C35-C36
14	Y	103	SPO	C29-C28-C30-C31
14	2	101	SPO	C34-C33-C35-C36
14	w	101	SPO	C29-C28-C30-C31
14	y	105	SPO	C34-C33-C35-C36
12	l	305	PGV	C21-C22-C23-C24
14	Y	103	SPO	C27-C28-C30-C31
8	07	101	BCL	O1D-CGD-O2D-CED
8	m	402	BCL	C16-C17-C18-C19
8	g	103	BCL	C5-C6-C7-C8
8	o	101	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
11	h	803	LMT	O5'-C5'-C6'-O6'
16	H	803	PTY	C17-C18-C19-C20
8	v	101	BCL	O1D-CGD-O2D-CED
15	K	401	CDL	OA5-CA3-CA4-OA6
8	r	102	BCL	C16-C17-C18-C20
12	l	305	PGV	C3-C4-C5-C6
8	K	402	BCL	C5-C6-C7-C8
11	M	409	LMT	C2-C3-C4-C5
8	B	102	BCL	C15-C16-C17-C18
14	M	406	SPO	C3-C1-O1-CM1
14	m	407	SPO	C3-C1-O1-CM1
11	M	408	LMT	C9-C10-C11-C12
12	x	101	PGV	C2-C3-C4-C5
8	02	101	BCL	CAA-CBA-CGA-O2A
12	Q	102	PGV	O03-C01-C02-O01
15	M	410	CDL	OA6-CA4-CA6-OA8
12	l	307	PGV	O02-C1-O01-C02
8	M	402	BCL	C10-C11-C12-C13
8	R	102	BCL	C5-C6-C7-C8
8	p	102	BCL	C15-C16-C17-C18
14	B	101	SPO	C3-C1-C4-C5
14	m	407	SPO	C3-C1-C4-C5
14	j	101	SPO	C2-C1-C4-C5
14	n	103	SPO	C2-C1-C4-C5
14	n	103	SPO	C3-C1-C4-C5
14	r	103	SPO	C3-C1-C4-C5
14	y	105	SPO	C2-C1-C4-C5
14	y	105	SPO	C3-C1-C4-C5
14	05	103	SPO	C3-C1-C4-C5
14	08	101	SPO	C3-C1-C4-C5
8	d	101	BCL	C4-C3-C5-C6
14	A	703	SPO	C34-C33-C35-C36
14	2	101	SPO	C29-C28-C30-C31
8	L	311	BCL	C6-C7-C8-C10
8	D	101	BCL	C11-C10-C8-C7
8	D	101	BCL	C11-C12-C13-C15
8	F	502	BCL	C6-C7-C8-C10
8	G	102	BCL	C11-C10-C8-C7
8	N	102	BCL	C12-C13-C15-C16
8	Q	103	BCL	C6-C7-C8-C10
8	R	102	BCL	C6-C7-C8-C10
8	T	101	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
8	2	103	BCL	C11-C10-C8-C7
8	4	101	BCL	C6-C7-C8-C10
8	5	102	BCL	C12-C13-C15-C16
8	6	101	BCL	C6-C7-C8-C10
8	f	102	BCL	C6-C7-C8-C10
8	g	103	BCL	C11-C10-C8-C7
8	i	103	BCL	C6-C7-C8-C10
8	n	102	BCL	C6-C7-C8-C10
8	p	102	BCL	C11-C10-C8-C7
8	t	101	BCL	C6-C7-C8-C10
8	w	102	BCL	C11-C10-C8-C7
8	z	102	BCL	C6-C7-C8-C10
8	05	101	BCL	C6-C7-C8-C10
8	07	101	BCL	C6-C7-C8-C10
14	A	703	SPO	C32-C33-C35-C36
14	Q	104	SPO	C32-C33-C35-C36
14	2	101	SPO	C27-C28-C30-C31
14	y	105	SPO	C32-C33-C35-C36
8	D	101	BCL	C11-C10-C8-C9
8	D	101	BCL	C11-C12-C13-C14
8	K	402	BCL	C11-C10-C8-C9
8	S	101	BCL	C6-C7-C8-C9
8	S	101	BCL	C14-C13-C15-C16
8	2	103	BCL	C11-C10-C8-C9
8	6	101	BCL	C11-C10-C8-C9
8	m	402	BCL	C11-C10-C8-C9
8	f	102	BCL	C6-C7-C8-C9
8	i	103	BCL	C6-C7-C8-C9
8	o	101	BCL	C6-C7-C8-C9
8	v	101	BCL	C6-C7-C8-C9
8	08	102	BCL	C11-C10-C8-C9
11	U	101	LMT	C3'-C4'-O1B-C1B
8	A	702	BCL	CBA-CGA-O2A-C1
8	f	102	BCL	C8-C10-C11-C12
8	g	103	BCL	C2A-CAA-CBA-CGA
14	j	101	SPO	O1-C1-C4-C5
14	05	102	SPO	O1-C1-C4-C5
14	G	101	SPO	C10-C11-C12-C13
8	B	102	BCL	C16-C17-C18-C20
8	R	102	BCL	C16-C17-C18-C20
8	Y	102	BCL	C16-C17-C18-C20
14	y	105	SPO	C10-C11-C12-C14

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Mol	Chain	Res	Type	Atoms
8	W	101	BCL	C3-C5-C6-C7
12	Q	102	PGV	O12-C04-C05-C06
8	R	102	BCL	C15-C16-C17-C18
15	X	102	CDL	C11-CA5-OA6-CA4
15	h	805	CDL	C31-CA7-OA8-CA6
12	L	309	PGV	C1-C2-C3-C4
8	O	101	BCL	O1D-CGD-O2D-CED
11	Q	101	LMT	C1-C2-C3-C4
8	8	101	BCL	C2-C3-C5-C6
11	U	101	LMT	C5'-C4'-O1B-C1B
8	J	102	BCL	C13-C15-C16-C17
12	H	805	PGV	C01-C02-C03-O11
12	f	104	PGV	C01-C02-C03-O11
15	K	401	CDL	OA5-CA3-CA4-CA6
10	L	304	U10	C9-C11-C12-C13
10	m	406	U10	C24-C26-C27-C28
14	3	103	SPO	C28-C30-C31-C32
15	X	101	CDL	CB5-C51-C52-C53
8	8	101	BCL	CAA-CBA-CGA-O2A
8	y	103	BCL	C4-C3-C5-C6
8	02	101	BCL	C4-C3-C5-C6
10	L	303	U10	C15-C14-C16-C17
10	m	406	U10	C45-C44-C46-C47
14	6	102	SPO	C34-C33-C35-C36
8	N	102	BCL	C2-C3-C5-C6
8	d	101	BCL	C2-C3-C5-C6
9	l	302	BPH	C2-C3-C5-C6
14	2	101	SPO	C32-C33-C35-C36
14	2	102	SPO	C27-C28-C30-C31
15	K	401	CDL	CA7-C31-C32-C33
8	k	101	BCL	C15-C16-C17-C18
15	Y	101	CDL	O1-C1-CA2-OA2
16	F	501	PTY	C35-C36-C37-C38
8	N	102	BCL	C16-C17-C18-C20
8	5	102	BCL	CBA-CGA-O2A-C1
15	m	410	CDL	C73-C74-C75-C76
15	m	413	CDL	C53-C54-C55-C56
8	w	102	BCL	C3A-C2A-CAA-CBA
15	M	410	CDL	C18-C19-C20-C21
11	I	101	LMT	C2-C1-O1'-C1'
11	I	101	LMT	C5'-C4'-O1B-C1B
8	E	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	r	102	BCL	C5-C6-C7-C8
8	w	102	BCL	C15-C16-C17-C18
12	f	103	PGV	C2-C3-C4-C5
8	6	101	BCL	C5-C6-C7-C8
8	r	102	BCL	C10-C11-C12-C13
12	l	308	PGV	O03-C01-C02-C03
15	M	410	CDL	CA3-CA4-CA6-OA8
15	X	103	CDL	CA3-CA4-CA6-OA8
15	m	410	CDL	CA3-CA4-CA6-OA8
11	U	103	LMT	O1'-C1-C2-C3
12	f	103	PGV	C1-C2-C3-C4
15	h	805	CDL	C16-C17-C18-C19
15	X	101	CDL	C74-C75-C76-C77
8	d	101	BCL	C3-C5-C6-C7
8	Y	102	BCL	O1D-CGD-O2D-CED
14	n	101	SPO	C29-C28-C30-C31
8	m	402	BCL	C16-C17-C18-C20
8	02	101	BCL	C2-C3-C5-C6
14	s	105	SPO	C27-C28-C30-C31
12	f	104	PGV	C26-C27-C28-C29
12	Q	102	PGV	C3-C4-C5-C6
12	k	103	PGV	C5-C6-C7-C8
12	M	411	PGV	C03-O11-P-O12
12	H	804	PGV	C03-O11-P-O12
15	K	401	CDL	CB3-OB5-PB2-OB2
8	F	502	BCL	O1D-CGD-O2D-CED
8	05	101	BCL	C10-C11-C12-C13
15	Y	101	CDL	C34-C35-C36-C37
15	m	410	CDL	C35-C36-C37-C38
12	L	309	PGV	O01-C02-C03-O11
12	l	307	PGV	O01-C02-C03-O11
15	h	805	CDL	OB5-CB3-CB4-OB6
16	f	105	PTY	O14-C5-C6-O7
15	x	102	CDL	OA5-CA3-CA4-OA6
8	D	101	BCL	C16-C17-C18-C20
8	E	101	BCL	C16-C17-C18-C20
11	s	101	LMT	C2-C3-C4-C5
15	m	410	CDL	C39-C40-C41-C42
8	r	102	BCL	C15-C16-C17-C18
11	h	802	LMT	C6-C7-C8-C9
11	m	408	LMT	C4B-C5B-C6B-O6B
12	l	308	PGV	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
12	m	412	PGV	O03-C01-C02-O01
12	y	104	PGV	O03-C01-C02-O01
8	m	403	BCL	C16-C17-C18-C19
8	t	101	BCL	C16-C17-C18-C19
11	s	101	LMT	C1-C2-C3-C4
14	E	102	SPO	C28-C30-C31-C32
14	S	102	SPO	C28-C30-C31-C32
15	Y	101	CDL	CB2-C1-CA2-OA2
8	F	502	BCL	C2-C1-O2A-CGA
8	l	301	BCL	C2-C1-O2A-CGA
8	05	101	BCL	C2-C1-O2A-CGA
8	y	103	BCL	C2-C3-C5-C6
8	A	702	BCL	O1A-CGA-O2A-C1
8	J	102	BCL	C6-C7-C8-C9
8	N	102	BCL	C6-C7-C8-C9
8	P	102	BCL	C11-C12-C13-C14
8	T	101	BCL	C14-C13-C15-C16
8	5	102	BCL	C14-C13-C15-C16
8	b	101	BCL	C11-C12-C13-C14
8	p	102	BCL	C6-C7-C8-C9
8	w	102	BCL	C6-C7-C8-C9
8	01	101	BCL	C6-C7-C8-C9
8	03	102	BCL	C11-C10-C8-C9
12	M	411	PGV	C02-C03-O11-P
12	m	411	PGV	C02-C03-O11-P
12	q	102	PGV	C05-C04-O12-P
15	X	102	CDL	C1-CA2-OA2-PA1
8	A	702	BCL	C3-C5-C6-C7
8	p	102	BCL	C5-C6-C7-C8
14	g	102	SPO	C15-C16-C17-C18
8	1	202	BCL	O1D-CGD-O2D-CED
8	L	301	BCL	C4C-C3C-CAC-CBC
14	A	703	SPO	C5-C6-C7-C9
14	n	101	SPO	C5-C6-C7-C9
8	I	102	BCL	O1D-CGD-O2D-CED
8	m	402	BCL	O1D-CGD-O2D-CED
8	F	502	BCL	C16-C17-C18-C19
8	5	102	BCL	C16-C17-C18-C19
15	m	410	CDL	C16-C17-C18-C19
12	f	103	PGV	C7-C8-C9-C10
12	L	309	PGV	C01-C02-C03-O11
12	H	804	PGV	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
8	M	401	BCL	C6-C7-C8-C10
8	M	402	BCL	C11-C10-C8-C7
8	B	102	BCL	C11-C10-C8-C7
8	E	101	BCL	C6-C7-C8-C10
8	F	502	BCL	C11-C10-C8-C7
8	G	102	BCL	C6-C7-C8-C10
8	J	102	BCL	C6-C7-C8-C10
8	K	402	BCL	C11-C10-C8-C7
8	R	102	BCL	C11-C10-C8-C7
8	S	101	BCL	C6-C7-C8-C10
8	S	101	BCL	C12-C13-C15-C16
8	T	101	BCL	C6-C7-C8-C10
8	W	101	BCL	C6-C7-C8-C10
8	1	202	BCL	C6-C7-C8-C10
8	l	301	BCL	C11-C10-C8-C7
8	m	401	BCL	C6-C7-C8-C10
8	b	101	BCL	C12-C13-C15-C16
8	d	101	BCL	C6-C7-C8-C10
8	e	102	BCL	C11-C10-C8-C7
8	j	102	BCL	C6-C7-C8-C10
8	j	102	BCL	C11-C10-C8-C7
8	k	101	BCL	C12-C13-C15-C16
8	o	101	BCL	C6-C7-C8-C10
8	r	102	BCL	C11-C10-C8-C7
8	v	101	BCL	C6-C7-C8-C10
8	w	102	BCL	C6-C7-C8-C10
8	y	103	BCL	C6-C7-C8-C10
8	01	101	BCL	C6-C7-C8-C10
8	02	101	BCL	C6-C7-C8-C10
8	03	102	BCL	C11-C10-C8-C7
8	08	102	BCL	C11-C10-C8-C7
10	L	303	U10	C13-C14-C16-C17
14	a	102	SPO	C11-C10-C9-C7
8	M	401	BCL	C16-C17-C18-C20
15	h	805	CDL	OA9-CA7-OA8-CA6
8	5	102	BCL	C10-C11-C12-C13
12	h	801	PGV	C3-C4-C5-C6
8	L	311	BCL	C16-C17-C18-C19
12	M	411	PGV	C20-C19-O03-C01
12	H	801	PGV	C2-C3-C4-C5
11	h	803	LMT	C4-C5-C6-C7
12	x	101	PGV	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
8	08	102	BCL	O1D-CGD-O2D-CED
8	T	101	BCL	C5-C6-C7-C8
8	l	301	BCL	CAD-CBD-CGD-O2D
8	a	101	BCL	CAD-CBD-CGD-O2D
9	L	302	BPH	CAD-CBD-CGD-O2D
9	l	302	BPH	CAD-CBD-CGD-O2D
15	X	102	CDL	OA7-CA5-OA6-CA4
14	f	101	SPO	C34-C33-C35-C36
8	t	101	BCL	C16-C17-C18-C20
8	J	102	BCL	C15-C16-C17-C18
10	L	303	U10	C9-C11-C12-C13
14	G	103	SPO	C33-C35-C36-C37
14	01	102	SPO	C28-C30-C31-C32
12	M	411	PGV	O03-C01-C02-C03
15	X	102	CDL	CA3-CA4-CA6-OA8
15	X	103	CDL	CB3-CB4-CB6-OB8
12	H	805	PGV	O01-C02-C03-O11
15	m	413	CDL	OB5-CB3-CB4-OB6
8	2	103	BCL	CAA-CBA-CGA-O2A
8	08	102	BCL	O2A-C1-C2-C3
15	m	413	CDL	C32-C33-C34-C35
15	M	410	CDL	C59-C60-C61-C62
12	F	503	PGV	O12-C04-C05-C06
12	H	805	PGV	O02-C1-O01-C02
8	R	102	BCL	CHA-CBD-CGD-O1D
8	R	102	BCL	CHA-CBD-CGD-O2D
8	V	101	BCL	CHA-CBD-CGD-O1D
8	V	101	BCL	CHA-CBD-CGD-O2D
8	m	403	BCL	CHA-CBD-CGD-O1D
8	j	102	BCL	CHA-CBD-CGD-O2D
8	y	103	BCL	C3-C5-C6-C7
12	h	806	PGV	O03-C01-C02-O01
15	M	410	CDL	OB6-CB4-CB6-OB8
15	m	410	CDL	OB6-CB4-CB6-OB8
8	5	102	BCL	O1A-CGA-O2A-C1
16	F	501	PTY	C12-C11-C8-O7
12	m	412	PGV	C2-C3-C4-C5
8	1	202	BCL	C16-C17-C18-C19
11	5	101	LMT	C5-C6-C7-C8
8	Q	103	BCL	C3-C5-C6-C7
12	H	805	PGV	C2-C1-O01-C02
8	q	103	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	01	101	BCL	C4-C3-C5-C6
10	M	405	U10	C40-C39-C41-C42
14	p	101	SPO	C29-C28-C30-C31
15	M	410	CDL	C56-C57-C58-C59
10	M	405	U10	C38-C39-C41-C42
14	f	101	SPO	C32-C33-C35-C36
14	p	101	SPO	C27-C28-C30-C31
8	A	702	BCL	C10-C11-C12-C13
8	G	102	BCL	C6-C7-C8-C9
8	W	101	BCL	C6-C7-C8-C9
8	m	402	BCL	C11-C12-C13-C14
8	b	101	BCL	C6-C7-C8-C9
8	05	101	BCL	C14-C13-C15-C16
12	h	801	PGV	C22-C23-C24-C25
8	v	101	BCL	C5-C6-C7-C8
8	O	101	BCL	C2A-CAA-CBA-CGA
8	Z	101	BCL	C15-C16-C17-C18
12	M	411	PGV	O04-C19-O03-C01
15	M	410	CDL	C37-C38-C39-C40
16	f	105	PTY	C12-C13-C14-C15
12	Q	102	PGV	C04-C05-C06-O06
8	D	101	BCL	C10-C11-C12-C13
14	Q	104	SPO	C10-C11-C12-C14
14	f	101	SPO	C10-C11-C12-C14
8	A	702	BCL	C1A-C2A-CAA-CBA
8	p	102	BCL	C1A-C2A-CAA-CBA
8	w	102	BCL	C1A-C2A-CAA-CBA
8	f	102	BCL	C16-C17-C18-C20
8	05	101	BCL	C16-C17-C18-C19
8	g	103	BCL	C10-C11-C12-C13
8	r	102	BCL	C2-C1-O2A-CGA
9	L	302	BPH	C2-C1-O2A-CGA
12	y	104	PGV	C04-O12-P-O11
12	x	101	PGV	C04-O12-P-O11
15	Y	101	CDL	CA3-OA5-PA1-OA2
15	X	101	CDL	CA3-OA5-PA1-OA2
15	m	413	CDL	CA3-OA5-PA1-OA2
15	y	102	CDL	CA2-OA2-PA1-OA5
15	y	102	CDL	CB3-OB5-PB2-OB2
15	x	102	CDL	CB2-OB2-PB2-OB5
16	h	804	PTY	C3-O11-P1-O14
14	M	406	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
14	A	703	SPO	C29-C28-C30-C31
14	01	103	SPO	C34-C33-C35-C36
8	Z	101	BCL	C3-C5-C6-C7
14	n	103	SPO	C27-C28-C30-C31
14	w	101	SPO	C27-C28-C30-C31
12	M	411	PGV	C23-C24-C25-C26
12	L	307	PGV	C04-O12-P-O13
12	L	308	PGV	C03-O11-P-O14
12	L	309	PGV	C03-O11-P-O13
12	M	411	PGV	C03-O11-P-O13
12	H	801	PGV	C03-O11-P-O14
12	H	805	PGV	C04-O12-P-O13
12	F	503	PGV	C04-O12-P-O13
12	l	305	PGV	C03-O11-P-O13
12	l	306	PGV	C04-O12-P-O14
12	l	307	PGV	C03-O11-P-O14
12	h	801	PGV	C04-O12-P-O13
12	f	103	PGV	C04-O12-P-O13
15	M	410	CDL	CB3-OB5-PB2-OB3
15	K	401	CDL	CA2-OA2-PA1-OA4
15	K	401	CDL	CB3-OB5-PB2-OB3
15	Y	101	CDL	CB2-OB2-PB2-OB3
15	X	101	CDL	CB3-OB5-PB2-OB4
15	X	102	CDL	CA2-OA2-PA1-OA3
15	X	102	CDL	CA3-OA5-PA1-OA4
15	X	103	CDL	CA2-OA2-PA1-OA4
15	X	103	CDL	CB2-OB2-PB2-OB4
15	X	103	CDL	CB3-OB5-PB2-OB3
15	m	410	CDL	CB3-OB5-PB2-OB3
15	m	413	CDL	CA2-OA2-PA1-OA4
15	m	413	CDL	CB3-OB5-PB2-OB4
15	h	805	CDL	CA3-OA5-PA1-OA3
15	h	805	CDL	CB3-OB5-PB2-OB4
15	y	102	CDL	CB2-OB2-PB2-OB3
15	x	102	CDL	CA2-OA2-PA1-OA4
15	h	805	CDL	C12-C13-C14-C15
8	06	101	BCL	C5-C6-C7-C8
15	m	413	CDL	OB5-CB3-CB4-CB6
15	h	805	CDL	OB5-CB3-CB4-CB6
10	l	303	U10	C5-C4-O4-C4M
8	F	502	BCL	C16-C17-C18-C20
8	q	103	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	F	503	PGV	C20-C21-C22-C23
8	8	101	BCL	CAD-CBD-CGD-O1D
8	m	403	BCL	CAD-CBD-CGD-O1D
10	m	406	U10	C48-C49-C51-C52
16	H	803	PTY	C2-C3-O11-P1
16	F	501	PTY	C2-C3-O11-P1
16	f	105	PTY	C2-C3-O11-P1
12	M	411	PGV	C5-C6-C7-C8
8	N	102	BCL	C3-C5-C6-C7
11	s	101	LMT	C3'-C4'-O1B-C1B
15	m	410	CDL	CA7-C31-C32-C33
8	k	101	BCL	CBA-CGA-O2A-C1
15	Y	101	CDL	OB5-CB3-CB4-CB6
12	L	307	PGV	C23-C24-C25-C26
9	L	302	BPH	C16-C17-C18-C20
8	K	402	BCL	C6-C7-C8-C10
8	O	101	BCL	C6-C7-C8-C10
8	2	103	BCL	C11-C12-C13-C15
8	5	102	BCL	C6-C7-C8-C10
8	7	101	BCL	C6-C7-C8-C10
8	m	402	BCL	C6-C7-C8-C10
8	b	101	BCL	C11-C10-C8-C7
8	d	101	BCL	C11-C10-C8-C7
8	k	101	BCL	C11-C10-C8-C7
8	q	103	BCL	C6-C7-C8-C10
8	t	101	BCL	C2C-C3C-CAC-CBC
8	z	102	BCL	C11-C10-C8-C7
8	05	101	BCL	C12-C13-C15-C16
12	L	308	PGV	C1-C2-C3-C4
12	H	804	PGV	O01-C02-C03-O11
12	f	104	PGV	O01-C02-C03-O11
11	U	103	LMT	C11-C10-C9-C8
11	H	802	LMT	C4-C5-C6-C7
11	Q	101	LMT	C11-C10-C9-C8
11	i	101	LMT	C3'-C4'-O1B-C1B
8	k	101	BCL	O1A-CGA-O2A-C1
12	F	503	PGV	O12-C04-C05-O05
11	5	101	LMT	C5'-C4'-O1B-C1B
8	6	101	BCL	C16-C17-C18-C20
8	b	101	BCL	C16-C17-C18-C19
11	I	101	LMT	C4B-C5B-C6B-O6B
11	U	101	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
11	U	103	LMT	C4'-C5'-C6'-O6'
15	X	101	CDL	CA3-CA4-CA6-OA8
15	X	103	CDL	OA6-CA4-CA6-OA8
15	X	103	CDL	OB6-CB4-CB6-OB8
12	L	310	PGV	C4-C5-C6-C7
12	l	305	PGV	C2-C3-C4-C5
8	b	101	BCL	O2A-C1-C2-C3
8	2	103	BCL	C15-C16-C17-C18
11	H	802	LMT	C2-C3-C4-C5
8	O	101	BCL	C4-C3-C5-C6
8	2	103	BCL	C4-C3-C5-C6
15	M	410	CDL	C38-C39-C40-C41
15	h	805	CDL	C14-C15-C16-C17
8	q	103	BCL	C2-C3-C5-C6
8	V	101	BCL	C15-C16-C17-C18
8	M	401	BCL	C6-C7-C8-C9
8	M	401	BCL	C11-C12-C13-C14
8	E	101	BCL	C6-C7-C8-C9
8	F	502	BCL	C6-C7-C8-C9
8	F	502	BCL	C11-C10-C8-C9
8	O	101	BCL	C6-C7-C8-C9
8	Q	103	BCL	C14-C13-C15-C16
8	R	102	BCL	C11-C10-C8-C9
8	S	101	BCL	C11-C10-C8-C9
8	m	401	BCL	C6-C7-C8-C9
8	b	101	BCL	C14-C13-C15-C16
8	d	101	BCL	C6-C7-C8-C9
8	j	102	BCL	C6-C7-C8-C9
8	n	102	BCL	C11-C10-C8-C9
8	n	102	BCL	C14-C13-C15-C16
8	o	101	BCL	C11-C10-C8-C9
8	q	103	BCL	C6-C7-C8-C9
8	r	102	BCL	C11-C10-C8-C9
8	z	102	BCL	C6-C7-C8-C9
8	01	101	BCL	C11-C10-C8-C9
8	05	101	BCL	C6-C7-C8-C9
8	f	102	BCL	C16-C17-C18-C19
14	2	102	SPO	C28-C30-C31-C32
14	2	101	SPO	C15-C16-C17-C18
12	H	801	PGV	C12-C13-C14-C15
8	L	311	BCL	C16-C17-C18-C20
8	P	102	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
11	i	101	LMT	C5'-C4'-O1B-C1B
12	m	411	PGV	C23-C24-C25-C26
8	R	102	BCL	CAA-CBA-CGA-O2A
11	M	408	LMT	C11-C10-C9-C8
8	I	102	BCL	C4-C3-C5-C6
10	L	303	U10	C12-C11-C9-C10
14	M	406	SPO	C32-C33-C35-C36
15	h	805	CDL	CA5-C11-C12-C13
8	F	502	BCL	C13-C15-C16-C17
8	R	102	BCL	C3-C5-C6-C7
8	m	401	BCL	C13-C15-C16-C17
12	F	503	PGV	C03-C02-O01-C1
8	L	301	BCL	C2A-CAA-CBA-CGA
8	R	102	BCL	C2A-CAA-CBA-CGA
15	X	101	CDL	C71-CB7-OB8-CB6
8	B	102	BCL	C2-C1-O2A-CGA
8	V	101	BCL	C2-C1-O2A-CGA
8	1	202	BCL	C2-C1-O2A-CGA
8	2	103	BCL	C2-C1-O2A-CGA
8	k	101	BCL	C2-C1-O2A-CGA
11	m	408	LMT	O5B-C5B-C6B-O6B
11	A	701	LMT	C11-C10-C9-C8
12	K	403	PGV	C9-C10-C11-C12
11	M	409	LMT	C5'-C4'-O1B-C1B
11	I	101	LMT	O1'-C1-C2-C3
15	K	401	CDL	OA9-CA7-OA8-CA6
8	r	102	BCL	C4-C3-C5-C6
14	08	101	SPO	C34-C33-C35-C36
8	01	101	BCL	C2-C3-C5-C6
10	m	406	U10	C43-C44-C46-C47
14	6	102	SPO	C32-C33-C35-C36
8	Q	103	BCL	C13-C15-C16-C17
15	m	410	CDL	C61-C62-C63-C64
8	z	102	BCL	C2A-CAA-CBA-CGA
15	m	413	CDL	OB9-CB7-OB8-CB6
12	H	804	PGV	O03-C01-C02-O01
12	x	101	PGV	O03-C01-C02-O01
8	5	102	BCL	C13-C15-C16-C17
12	L	308	PGV	C04-O12-P-O11
12	L	309	PGV	C04-O12-P-O11
12	L	310	PGV	C03-O11-P-O12
12	L	310	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
12	M	411	PGV	C04-O12-P-O11
12	H	805	PGV	C03-O11-P-O12
12	1	201	PGV	C03-O11-P-O12
12	1	201	PGV	C04-O12-P-O11
12	l	306	PGV	C03-O11-P-O12
12	m	411	PGV	C04-O12-P-O11
12	m	412	PGV	C04-O12-P-O11
12	f	104	PGV	C03-O11-P-O12
12	f	104	PGV	C04-O12-P-O11
12	q	102	PGV	C03-O11-P-O12
12	y	104	PGV	C03-O11-P-O12
12	x	101	PGV	C03-O11-P-O12
15	Y	101	CDL	CA2-OA2-PA1-OA5
15	Y	101	CDL	CB3-OB5-PB2-OB2
15	X	101	CDL	CA2-OA2-PA1-OA5
15	X	102	CDL	CB2-OB2-PB2-OB5
15	m	410	CDL	CA2-OA2-PA1-OA5
15	m	413	CDL	CB2-OB2-PB2-OB5
15	y	102	CDL	CA3-OA5-PA1-OA2
16	F	501	PTY	C5-O14-P1-O11
16	h	804	PTY	C5-O14-P1-O11
8	i	103	BCL	C16-C17-C18-C19
8	06	101	BCL	C16-C17-C18-C20
14	3	103	SPO	C3-C1-C4-C5
14	f	101	SPO	C3-C1-C4-C5
14	r	103	SPO	C2-C1-C4-C5
14	05	103	SPO	C2-C1-C4-C5
15	K	401	CDL	CA3-CA4-CA6-OA8
14	m	407	SPO	C29-C28-C30-C31
8	M	401	BCL	C11-C10-C8-C7
8	I	102	BCL	C6-C7-C8-C10
8	J	102	BCL	C11-C10-C8-C7
8	T	101	BCL	C12-C13-C15-C16
8	l	301	BCL	C11-C12-C13-C15
8	01	101	BCL	C11-C10-C8-C7
15	m	410	CDL	C63-C64-C65-C66
11	03	101	LMT	C2-C3-C4-C5
8	L	311	BCL	C6-C7-C8-C9
8	W	101	BCL	C11-C10-C8-C9
8	7	101	BCL	C6-C7-C8-C9
8	k	101	BCL	C11-C10-C8-C9
14	n	103	SPO	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
14	05	103	SPO	C11-C10-C9-C7
8	L	301	BCL	C13-C15-C16-C17
8	Y	102	BCL	C5-C6-C7-C8
8	07	101	BCL	C13-C15-C16-C17
11	M	407	LMT	O1'-C1-C2-C3
8	01	101	BCL	C15-C16-C17-C18
8	6	101	BCL	C16-C17-C18-C19
11	H	802	LMT	C7-C8-C9-C10
12	h	801	PGV	C04-C05-C06-O06
15	h	805	CDL	CA4-CA3-OA5-PA1
8	o	101	BCL	C15-C16-C17-C18
14	v	102	SPO	C22-C23-C25-C26
15	M	410	CDL	CB2-C1-CA2-OA2
8	g	103	BCL	C4-C3-C5-C6
9	m	404	BPH	C4-C3-C5-C6
10	l	303	U10	C11-C12-C13-C14
8	g	103	BCL	C2-C3-C5-C6
14	n	101	SPO	C27-C28-C30-C31
12	H	805	PGV	C21-C22-C23-C24
15	K	401	CDL	C31-CA7-OA8-CA6
15	Y	101	CDL	C31-CA7-OA8-CA6
12	L	307	PGV	C11-C10-C9-C8
11	h	802	LMT	C1-C2-C3-C4
11	M	409	LMT	C3'-C4'-O1B-C1B
15	Y	101	CDL	OA9-CA7-OA8-CA6
15	X	101	CDL	OB9-CB7-OB8-CB6
8	q	103	BCL	C16-C17-C18-C20
14	B	101	SPO	C11-C10-C9-C7
14	p	101	SPO	C17-C19-C20-C21
14	Y	103	SPO	C28-C30-C31-C32
11	H	802	LMT	C3-C4-C5-C6
15	m	410	CDL	C64-C65-C66-C67
12	l	305	PGV	O01-C02-C03-O11
12	f	103	PGV	O01-C02-C03-O11
11	m	408	LMT	O5B-C1B-O1B-C4'
12	l	306	PGV	C24-C25-C26-C27
14	B	103	SPO	C29-C28-C30-C31
14	m	407	SPO	C34-C33-C35-C36
14	v	102	SPO	C29-C28-C30-C31
11	M	407	LMT	C1-C2-C3-C4
12	k	103	PGV	C6-C7-C8-C9
8	S	101	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
11	M	412	LMT	C2-C3-C4-C5
8	M	401	BCL	C2-C1-O2A-CGA
8	f	102	BCL	C2-C1-O2A-CGA
8	i	103	BCL	C2-C1-O2A-CGA
8	8	101	BCL	C11-C12-C13-C15
8	y	103	BCL	C16-C17-C18-C19
16	h	804	PTY	C8-C11-C12-C13
11	03	101	LMT	C9-C10-C11-C12
12	H	805	PGV	C6-C7-C8-C9
15	h	805	CDL	C31-C32-C33-C34
8	J	102	BCL	C2A-CAA-CBA-CGA
8	06	101	BCL	C3A-C2A-CAA-CBA
10	D	102	U10	C5-C4-O4-C4M
10	l	303	U10	C2-C3-O3-C3M
12	F	503	PGV	C21-C22-C23-C24
10	L	303	U10	C12-C11-C9-C8
11	M	408	LMT	C2-C3-C4-C5
8	B	102	BCL	C14-C13-C15-C16
8	G	102	BCL	C11-C12-C13-C14
8	I	102	BCL	C11-C12-C13-C14
8	O	101	BCL	C11-C10-C8-C9
8	P	102	BCL	C14-C13-C15-C16
8	2	103	BCL	C11-C12-C13-C14
8	3	102	BCL	C11-C10-C8-C9
8	5	102	BCL	C6-C7-C8-C9
8	m	403	BCL	C11-C10-C8-C9
8	t	101	BCL	C14-C13-C15-C16
8	04	101	BCL	C11-C10-C8-C9
8	06	101	BCL	C6-C7-C8-C9
8	2	103	BCL	C16-C17-C18-C19
12	m	411	PGV	O03-C01-C02-C03
12	f	103	PGV	O03-C01-C02-C03
15	X	102	CDL	CB3-OB5-PB2-OB4
12	f	104	PGV	C25-C26-C27-C28
12	L	310	PGV	C22-C23-C24-C25
8	P	102	BCL	C16-C17-C18-C20
8	06	101	BCL	C16-C17-C18-C19
9	l	302	BPH	O2A-C1-C2-C3
14	q	104	SPO	C10-C11-C12-C13
10	D	102	U10	C19-C21-C22-C23
8	i	103	BCL	C5-C6-C7-C8
11	m	409	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
14	2	101	SPO	C15-C16-C17-C19
14	g	102	SPO	C15-C16-C17-C19
15	K	401	CDL	CA6-CA4-OA6-CA5
15	h	805	CDL	CA6-CA4-OA6-CA5
10	l	303	U10	C15-C14-C16-C17
8	E	101	BCL	C1A-C2A-CAA-CBA
8	W	101	BCL	C1A-C2A-CAA-CBA
8	5	102	BCL	C1A-C2A-CAA-CBA
8	06	101	BCL	C1A-C2A-CAA-CBA
11	A	701	LMT	C7-C8-C9-C10
8	V	101	BCL	C6-C7-C8-C10
8	j	102	BCL	C12-C13-C15-C16
8	n	102	BCL	C11-C10-C8-C7
8	g	103	BCL	C15-C16-C17-C18
8	w	102	BCL	C5-C6-C7-C8
11	L	305	LMT	O5B-C5B-C6B-O6B
8	V	101	BCL	C3-C5-C6-C7
14	g	102	SPO	C25-C26-C27-C28
14	01	102	SPO	C25-C26-C27-C28
11	3	101	LMT	C5'-C4'-O1B-C1B
12	Q	102	PGV	C03-O11-P-O12
15	M	410	CDL	C17-C18-C19-C20
8	02	101	BCL	CAA-CBA-CGA-O1A
11	3	101	LMT	C3'-C4'-O1B-C1B
8	K	402	BCL	C3-C5-C6-C7
8	V	101	BCL	C2A-CAA-CBA-CGA
8	F	502	BCL	C15-C16-C17-C18
8	05	101	BCL	C15-C16-C17-C18
15	m	410	CDL	C38-C39-C40-C41
15	M	410	CDL	OB5-CB3-CB4-OB6
11	03	101	LMT	C11-C10-C9-C8
12	K	403	PGV	C2-C3-C4-C5
16	H	803	PTY	C12-C13-C14-C15
8	w	102	BCL	C10-C11-C12-C13
10	m	406	U10	C47-C48-C49-C50
11	Q	101	LMT	C2-C3-C4-C5
8	2	103	BCL	C8-C10-C11-C12
10	L	303	U10	C25-C24-C26-C27
10	l	303	U10	C25-C24-C26-C27
14	z	101	SPO	C34-C33-C35-C36
8	t	101	BCL	C15-C16-C17-C18
8	2	103	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	B	101	SPO	C32-C33-C35-C36
8	p	102	BCL	O1D-CGD-O2D-CED
8	m	403	BCL	C16-C17-C18-C20
15	x	102	CDL	CA4-CA3-OA5-PA1
12	f	103	PGV	O03-C01-C02-O01
16	F	501	PTY	O4-C1-C6-O7
8	i	103	BCL	C13-C15-C16-C17
8	v	101	BCL	C2A-CAA-CBA-CGA
14	n	101	SPO	C25-C26-C27-C28
8	08	102	BCL	C3-C5-C6-C7
10	m	406	U10	C46-C47-C48-C49
14	2	104	SPO	C1-C4-C5-C6
14	4	102	SPO	C1-C4-C5-C6
8	b	101	BCL	C16-C17-C18-C20
12	F	503	PGV	C28-C29-C30-C31
12	M	411	PGV	O12-C04-C05-C06
11	M	409	LMT	O1'-C1-C2-C3
16	h	804	PTY	C18-C19-C20-C21
14	a	102	SPO	C29-C28-C30-C31
8	M	402	BCL	C2-C1-O2A-CGA
8	Q	103	BCL	C2-C1-O2A-CGA
8	5	102	BCL	C2-C1-O2A-CGA
8	6	101	BCL	C2-C1-O2A-CGA
8	8	101	BCL	C2-C1-O2A-CGA
14	m	407	SPO	C32-C33-C35-C36
8	a	101	BCL	C2-C1-O2A-CGA
8	I	102	BCL	O1A-CGA-O2A-C1
15	y	102	CDL	C1-CB2-OB2-PB2
16	F	501	PTY	C40-C41-C42-C43
8	d	101	BCL	O1A-CGA-O2A-C1
11	s	101	LMT	C11-C10-C9-C8
14	M	406	SPO	C29-C28-C30-C31
14	p	101	SPO	C34-C33-C35-C36
14	B	103	SPO	C5-C6-C7-C9
14	G	101	SPO	C10-C11-C12-C14
14	r	101	SPO	C10-C11-C12-C14
8	z	102	BCL	C15-C16-C17-C18
8	I	102	BCL	C2-C3-C5-C6
8	O	101	BCL	C2-C3-C5-C6
8	r	102	BCL	C2-C3-C5-C6
10	l	303	U10	C13-C14-C16-C17
14	m	407	SPO	C27-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
12	1	201	PGV	C19-C20-C21-C22
8	t	101	BCL	C13-C15-C16-C17
12	h	806	PGV	C1-C2-C3-C4
11	I	101	LMT	O5B-C5B-C6B-O6B
11	U	102	LMT	C5'-C4'-O1B-C1B
16	f	105	PTY	O14-C5-C6-C1
8	W	101	BCL	CAA-CBA-CGA-O2A
8	i	103	BCL	O1A-CGA-O2A-C1
14	S	103	SPO	C29-C28-C30-C31
14	w	101	SPO	C34-C33-C35-C36
10	M	405	U10	C51-C52-C53-C54
12	L	309	PGV	C3-C4-C5-C6
8	N	102	BCL	C6-C7-C8-C10
8	P	102	BCL	C11-C12-C13-C15
8	3	102	BCL	C11-C10-C8-C7
8	b	101	BCL	C6-C7-C8-C10
8	s	102	BCL	C6-C7-C8-C10
10	L	303	U10	C23-C24-C26-C27
12	Q	102	PGV	O05-C05-C06-O06
12	l	305	PGV	C22-C23-C24-C25
9	M	403	BPH	C1-C2-C3-C4
14	G	103	SPO	C25-C26-C27-C28
8	M	401	BCL	CAA-CBA-CGA-O2A
11	03	103	LMT	C2'-C1'-O1'-C1
12	l	308	PGV	C1-C2-C3-C4
15	X	101	CDL	CB2-C1-CA2-OA2
8	I	102	BCL	CBA-CGA-O2A-C1
8	8	101	BCL	CAA-CBA-CGA-O1A
8	v	101	BCL	C3-C5-C6-C7
8	Q	103	BCL	C2A-CAA-CBA-CGA
8	i	103	BCL	CBA-CGA-O2A-C1
8	v	101	BCL	CBA-CGA-O2A-C1
8	07	101	BCL	C8-C10-C11-C12
12	f	104	PGV	C7-C8-C9-C10
15	X	102	CDL	C11-C12-C13-C14
8	M	402	BCL	C4-C3-C5-C6
8	D	101	BCL	C4-C3-C5-C6
8	R	102	BCL	C4-C3-C5-C6
8	b	101	BCL	C4-C3-C5-C6
8	n	102	BCL	C4-C3-C5-C6
8	i	103	BCL	C10-C11-C12-C13
8	v	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
11	3	101	LMT	C4B-C5B-C6B-O6B
10	l	303	U10	C23-C24-C26-C27
14	A	703	SPO	C27-C28-C30-C31
14	B	103	SPO	C27-C28-C30-C31
14	08	101	SPO	C32-C33-C35-C36
12	m	411	PGV	C5-C6-C7-C8
8	E	101	BCL	C11-C10-C8-C9
8	K	402	BCL	C6-C7-C8-C9
8	l	301	BCL	C11-C12-C13-C14
8	p	102	BCL	C14-C13-C15-C16
9	m	404	BPH	C6-C7-C8-C9
8	01	101	BCL	C3-C5-C6-C7
8	E	101	BCL	C3A-C2A-CAA-CBA
8	W	101	BCL	C3A-C2A-CAA-CBA
12	k	103	PGV	C9-C10-C11-C12
8	06	101	BCL	CAD-CBD-CGD-O2D
8	08	102	BCL	CAD-CBD-CGD-O2D
9	M	403	BPH	CAD-CBD-CGD-O2D
9	m	404	BPH	CAD-CBD-CGD-O2D
15	K	401	CDL	CA3-CA4-OA6-CA5
10	D	102	U10	C16-C17-C18-C19
12	l	305	PGV	O03-C19-C20-C21
12	h	801	PGV	O01-C1-C2-C3
10	m	406	U10	C35-C34-C36-C37
14	K	404	SPO	C29-C28-C30-C31
8	D	101	BCL	C2-C3-C5-C6
9	m	404	BPH	C2-C3-C5-C6
10	m	406	U10	C33-C34-C36-C37
14	p	101	SPO	C32-C33-C35-C36
14	z	101	SPO	C32-C33-C35-C36
15	m	413	CDL	OA9-CA7-OA8-CA6
14	V	102	SPO	C15-C16-C17-C19
14	q	104	SPO	C10-C11-C12-C14
10	L	304	U10	C2-C3-O3-C3M
10	d	102	U10	C5-C4-O4-C4M
12	m	412	PGV	O03-C01-C02-C03
15	K	401	CDL	CA4-CA3-OA5-PA1
11	s	101	LMT	O1'-C1-C2-C3
12	l	308	PGV	O01-C02-C03-O11
15	X	103	CDL	OB5-CB3-CB4-OB6
16	H	803	PTY	O14-C5-C6-O7
10	m	406	U10	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
8	m	402	BCL	CAA-CBA-CGA-O2A
15	y	102	CDL	C72-C73-C74-C75
8	T	101	BCL	O2A-C1-C2-C3
8	m	402	BCL	O2A-C1-C2-C3
11	U	102	LMT	C3'-C4'-O1B-C1B
11	h	802	LMT	O1'-C1-C2-C3
12	L	307	PGV	C21-C22-C23-C24
12	q	102	PGV	C20-C19-O03-C01
16	f	105	PTY	O4-C30-C31-C32
12	H	805	PGV	C9-C10-C11-C12
12	H	801	PGV	C22-C23-C24-C25
15	h	805	CDL	C11-C12-C13-C14
11	m	408	LMT	C2B-C1B-O1B-C4'
12	L	307	PGV	C2-C3-C4-C5
8	L	311	BCL	CHA-CBD-CGD-O1D
8	L	311	BCL	CHA-CBD-CGD-O2D
8	M	402	BCL	CHA-CBD-CGD-O1D
8	M	402	BCL	CHA-CBD-CGD-O2D
8	A	702	BCL	CHA-CBD-CGD-O1D
8	A	702	BCL	CHA-CBD-CGD-O2D
8	E	101	BCL	CHA-CBD-CGD-O1D
8	E	101	BCL	CHA-CBD-CGD-O2D
8	F	502	BCL	CHA-CBD-CGD-O2D
8	3	102	BCL	CHA-CBD-CGD-O1D
8	3	102	BCL	CHA-CBD-CGD-O2D
8	m	401	BCL	CHA-CBD-CGD-O1D
8	m	401	BCL	CHA-CBD-CGD-O2D
8	m	402	BCL	CHA-CBD-CGD-O1D
8	m	402	BCL	CHA-CBD-CGD-O2D
8	e	102	BCL	CHA-CBD-CGD-O1D
8	e	102	BCL	CHA-CBD-CGD-O2D
8	v	101	BCL	CHA-CBD-CGD-O1D
8	04	101	BCL	CHA-CBD-CGD-O1D
8	04	101	BCL	CHA-CBD-CGD-O2D
8	05	101	BCL	CHA-CBD-CGD-O1D
14	3	103	SPO	C25-C26-C27-C28
14	05	102	SPO	C17-C19-C20-C21
14	M	406	SPO	C27-C28-C30-C31
14	01	103	SPO	C32-C33-C35-C36
14	z	101	SPO	C3-C1-O1-CM1
11	I	101	LMT	C7-C8-C9-C10
12	l	306	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	L	310	PGV	O01-C1-C2-C3
12	L	310	PGV	O03-C19-C20-C21
11	M	408	LMT	C1-C2-C3-C4
11	03	103	LMT	C4'-C5'-C6'-O6'
8	B	102	BCL	C2A-CAA-CBA-CGA
14	B	101	SPO	C2-C1-C4-C5
14	08	101	SPO	C2-C1-C4-C5
12	m	412	PGV	O01-C1-C2-C3
12	k	103	PGV	C21-C22-C23-C24
8	M	402	BCL	C2-C3-C5-C6
8	1	202	BCL	C11-C10-C8-C7
8	b	101	BCL	C11-C12-C13-C15
8	03	102	BCL	C16-C17-C18-C19
15	y	102	CDL	C31-C32-C33-C34
12	H	801	PGV	O02-C1-O01-C02
15	K	401	CDL	OB7-CB5-OB6-CB4
8	I	102	BCL	C6-C7-C8-C9
8	V	101	BCL	C6-C7-C8-C9
8	4	101	BCL	C6-C7-C8-C9
8	m	402	BCL	C6-C7-C8-C9
8	n	102	BCL	C11-C12-C13-C14
8	w	102	BCL	C11-C10-C8-C9
12	f	103	PGV	O01-C1-C2-C3
12	k	103	PGV	O03-C19-C20-C21
15	X	103	CDL	C72-C71-CB7-OB8
8	y	103	BCL	C16-C17-C18-C20
10	M	405	U10	C5-C4-O4-C4M
10	l	304	U10	C2-C3-O3-C3M
12	L	309	PGV	C2-C3-C4-C5
10	M	405	U10	C36-C37-C38-C39
10	M	405	U10	C41-C42-C43-C44
10	l	303	U10	C16-C17-C18-C19
10	m	406	U10	C31-C32-C33-C34
12	L	307	PGV	C20-C21-C22-C23
14	r	103	SPO	O1-C1-C4-C5
14	05	103	SPO	O1-C1-C4-C5
11	M	409	LMT	C4'-C5'-C6'-O6'
11	q	101	LMT	C5-C6-C7-C8
8	d	101	BCL	CBA-CGA-O2A-C1
14	B	101	SPO	C15-C16-C17-C18
8	5	102	BCL	C16-C17-C18-C20
8	m	401	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	f	105	PTY	O30-C30-C31-C32
14	5	103	SPO	C10-C11-C12-C14
8	m	403	BCL	C13-C15-C16-C17
8	M	402	BCL	C3-C5-C6-C7
8	M	402	BCL	C1A-C2A-CAA-CBA
8	Q	103	BCL	C1A-C2A-CAA-CBA
8	Y	102	BCL	C1A-C2A-CAA-CBA
8	e	102	BCL	C1A-C2A-CAA-CBA
8	n	102	BCL	C1A-C2A-CAA-CBA
12	l	308	PGV	O12-C04-C05-C06
8	m	402	BCL	CAA-CBA-CGA-O1A
12	k	103	PGV	O04-C19-C20-C21
15	X	103	CDL	C11-C12-C13-C14
16	h	804	PTY	C17-C18-C19-C20
12	q	102	PGV	O04-C19-O03-C01
8	L	301	BCL	C2-C1-O2A-CGA
15	m	413	CDL	C31-CA7-OA8-CA6
12	l	305	PGV	O04-C19-C20-C21
12	h	801	PGV	O02-C1-C2-C3
11	L	305	LMT	C4B-C5B-C6B-O6B
11	h	803	LMT	C5-C6-C7-C8
12	H	804	PGV	C23-C24-C25-C26
12	q	102	PGV	C02-C03-O11-P
8	M	401	BCL	CAA-CBA-CGA-O1A
14	v	102	SPO	C27-C28-C30-C31
11	q	101	LMT	C2-C3-C4-C5
10	L	304	U10	C6-C7-C8-C9
12	L	310	PGV	C04-O12-P-O13
12	1	201	PGV	C03-O11-P-O13
12	1	201	PGV	C04-O12-P-O13
12	l	306	PGV	C03-O11-P-O13
12	m	412	PGV	C04-O12-P-O13
12	x	101	PGV	C03-O11-P-O13
15	Y	101	CDL	CB3-OB5-PB2-OB3
15	X	102	CDL	CB2-OB2-PB2-OB3
12	L	310	PGV	O02-C1-C2-C3
12	m	412	PGV	O02-C1-C2-C3
12	f	103	PGV	O02-C1-C2-C3
12	K	403	PGV	O01-C1-C2-C3
12	l	308	PGV	C01-C02-C03-O11
12	f	103	PGV	C01-C02-C03-O11
15	m	410	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
8	08	102	BCL	CAA-CBA-CGA-O2A
12	F	503	PGV	C5-C6-C7-C8
15	M	410	CDL	C71-C72-C73-C74
10	L	303	U10	C2-C3-O3-C3M
14	01	103	SPO	C35-C36-C37-C38
12	L	310	PGV	C7-C8-C9-C10
8	A	702	BCL	CAD-CBD-CGD-O1D
8	D	101	BCL	CAD-CBD-CGD-O1D
8	V	101	BCL	CAD-CBD-CGD-O1D
8	v	101	BCL	CAD-CBD-CGD-O1D
8	F	502	BCL	O1A-CGA-O2A-C1
8	Q	103	BCL	O1A-CGA-O2A-C1
8	E	101	BCL	C15-C16-C17-C18
8	G	102	BCL	C14-C13-C15-C16
8	1	202	BCL	C10-C11-C12-C13
15	h	805	CDL	CA7-C31-C32-C33
12	M	411	PGV	O03-C19-C20-C21
15	Y	101	CDL	C32-C31-CA7-OA8
14	01	102	SPO	C1-C4-C5-C6
15	M	410	CDL	C57-C58-C59-C60
15	K	401	CDL	CA2-C1-CB2-OB2
15	m	410	CDL	CA2-C1-CB2-OB2
11	s	101	LMT	C5-C6-C7-C8
11	U	102	LMT	O5B-C1B-O1B-C4'
14	g	102	SPO	C34-C33-C35-C36
8	M	402	BCL	C3A-C2A-CAA-CBA
8	M	402	BCL	C12-C13-C15-C16
8	Q	103	BCL	C3A-C2A-CAA-CBA
8	5	102	BCL	C3A-C2A-CAA-CBA
8	m	402	BCL	C11-C12-C13-C15
8	e	102	BCL	C3A-C2A-CAA-CBA
8	n	102	BCL	C11-C12-C13-C15
8	y	103	BCL	C11-C10-C8-C7
8	08	102	BCL	C6-C7-C8-C10
9	L	302	BPH	C11-C12-C13-C15
12	H	801	PGV	O01-C1-C2-C3
11	q	101	LMT	C4-C5-C6-C7
12	m	412	PGV	C23-C24-C25-C26
14	B	103	SPO	C11-C10-C9-C7
12	1	201	PGV	C22-C23-C24-C25
12	L	307	PGV	O03-C19-C20-C21
12	l	306	PGV	O01-C1-C2-C3

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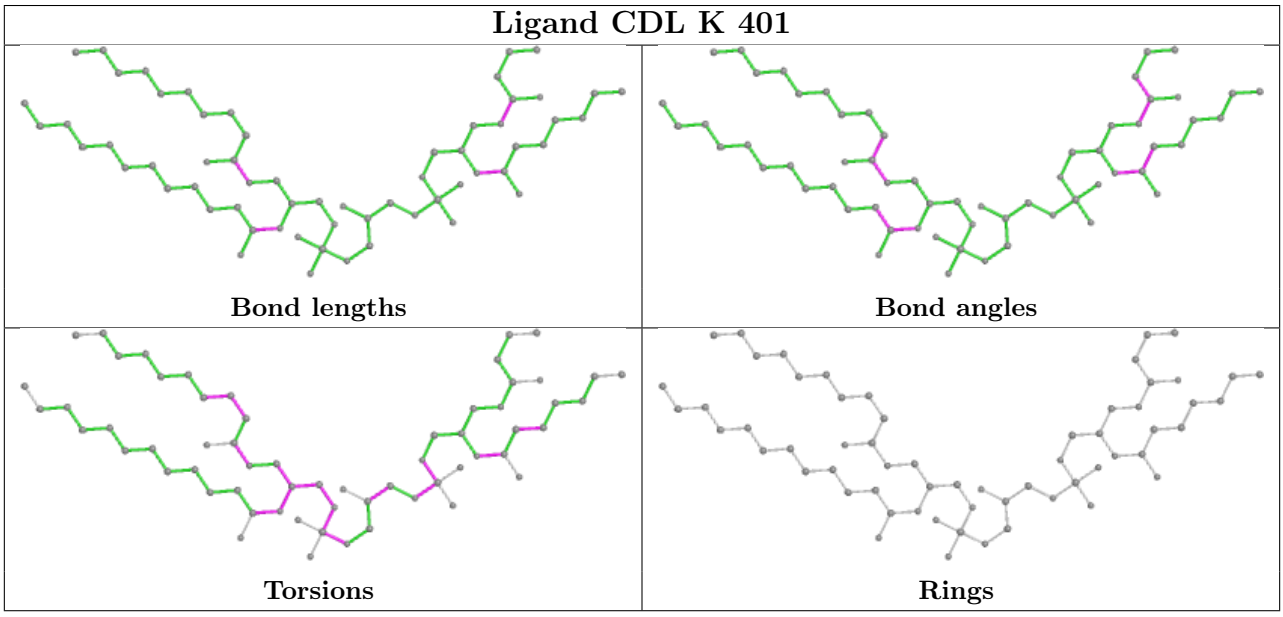
Mol	Chain	Res	Type	Atoms
8	n	102	BCL	C8-C10-C11-C12
10	l	303	U10	C3-C4-O4-C4M
15	m	410	CDL	C13-C14-C15-C16
8	1	202	BCL	C13-C15-C16-C17
11	m	409	LMT	C2B-C1B-O1B-C4'
12	K	403	PGV	O02-C1-C2-C3
8	o	101	BCL	C2A-CAA-CBA-CGA
11	U	101	LMT	O5B-C5B-C6B-O6B
15	X	103	CDL	C72-C71-CB7-OB9
14	B	101	SPO	C34-C33-C35-C36

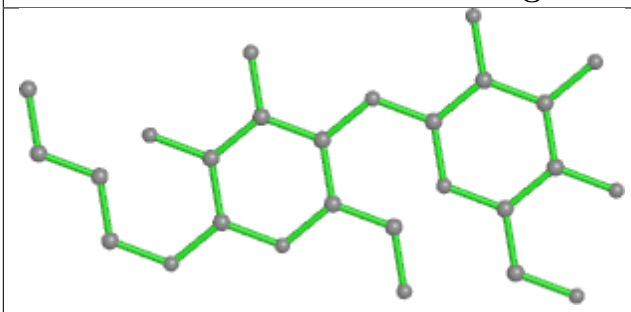
There are no ring outliers.

No monomer is involved in short contacts.

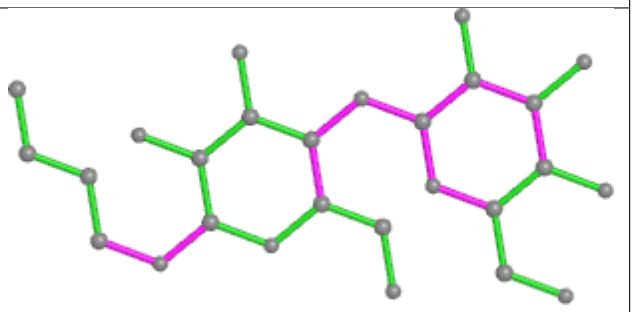
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



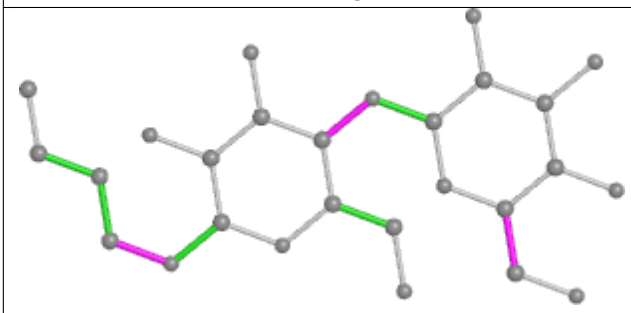
Ligand LMT L 305



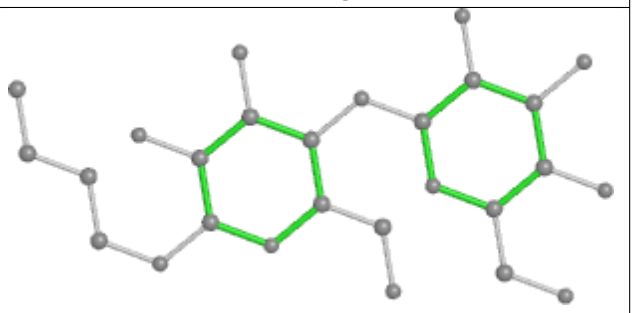
Bond lengths



Bond angles

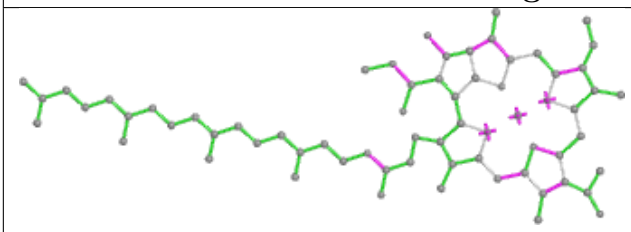


Torsions

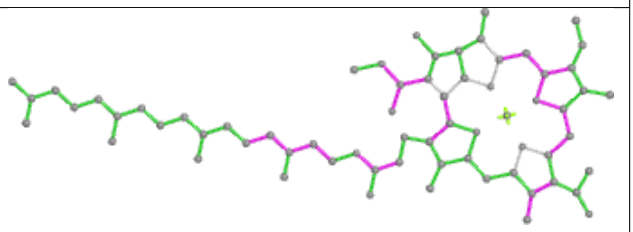


Rings

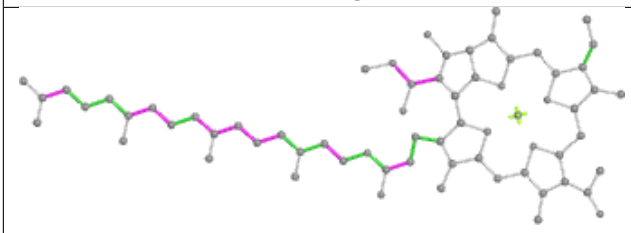
Ligand BCL m 402



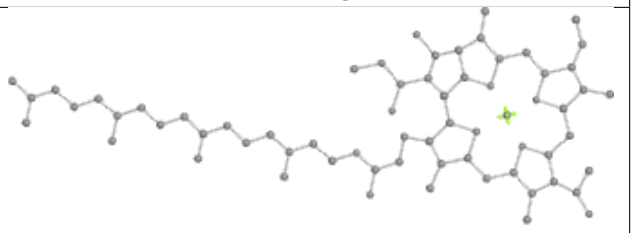
Bond lengths



Bond angles

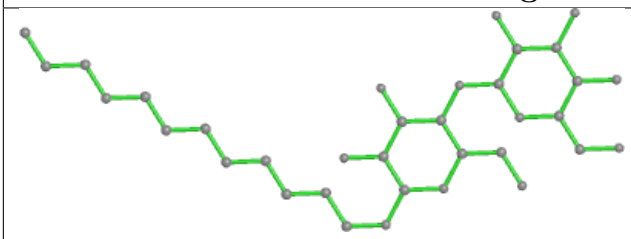


Torsions

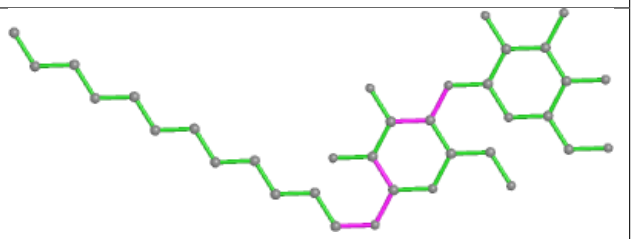


Rings

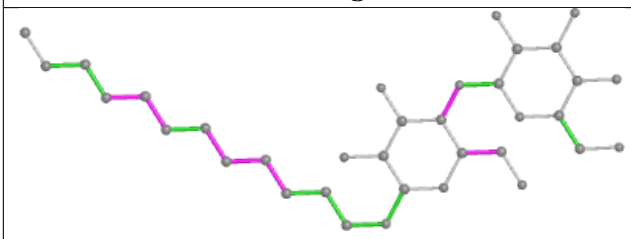
Ligand LMT H 802



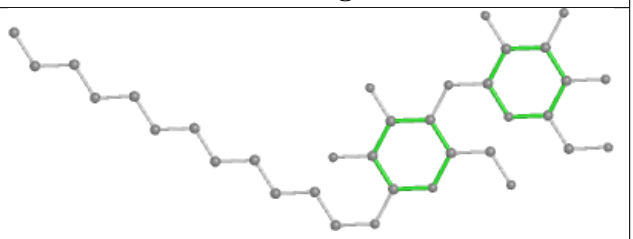
Bond lengths



Bond angles

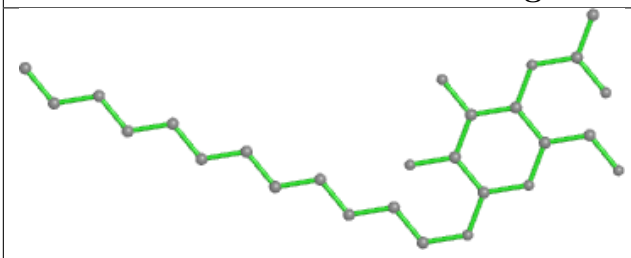


Torsions

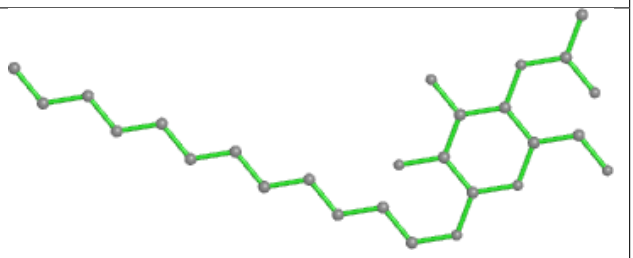


Rings

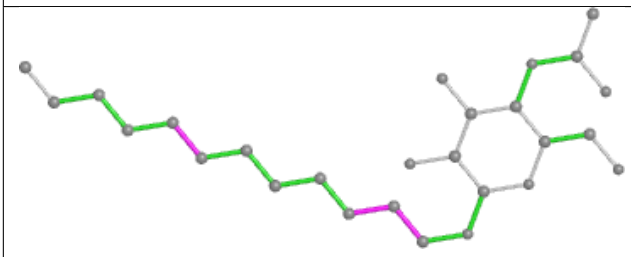
Ligand LMT h 802



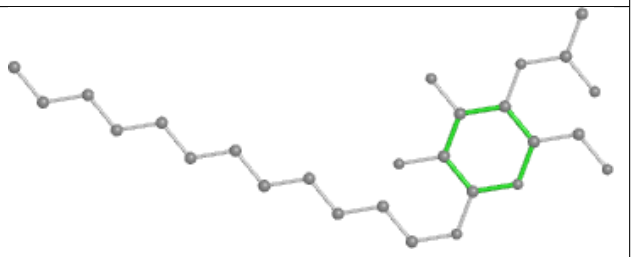
Bond lengths



Bond angles

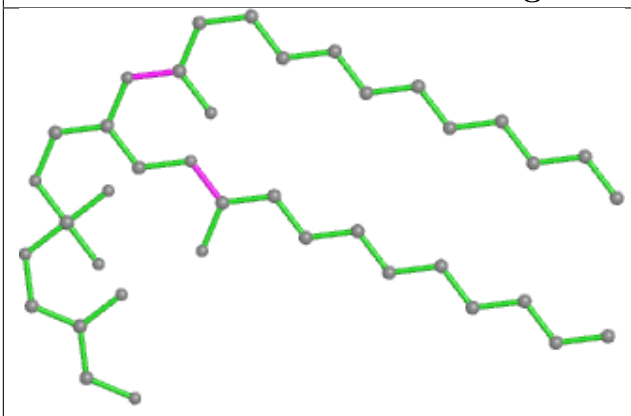


Torsions

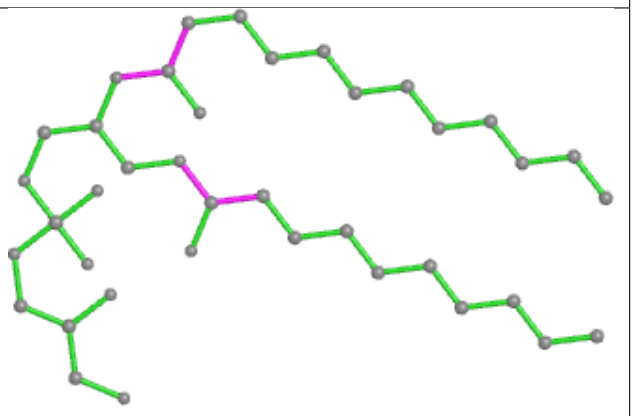


Rings

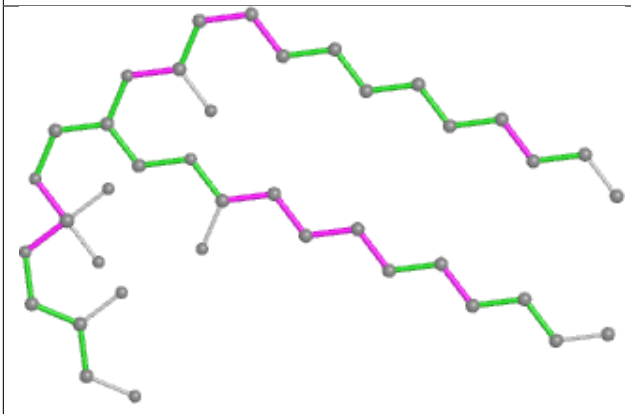
Ligand PGV L 307



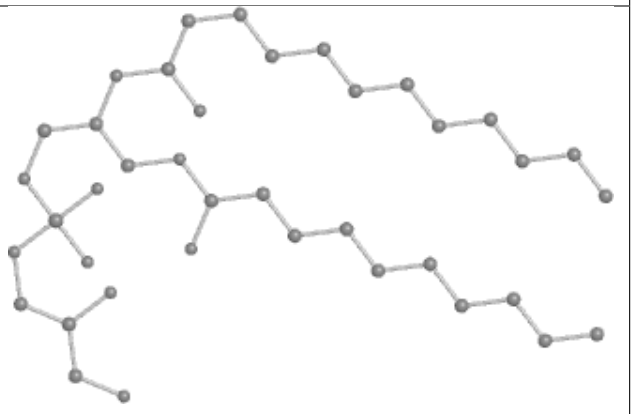
Bond lengths



Bond angles

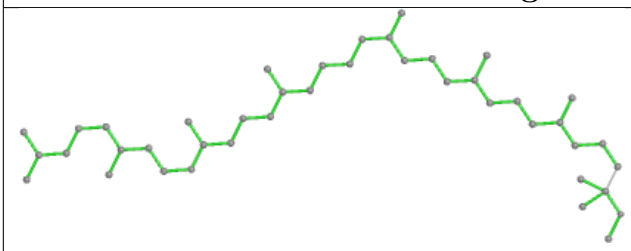


Torsions

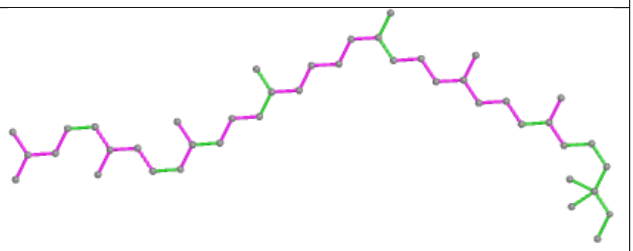


Rings

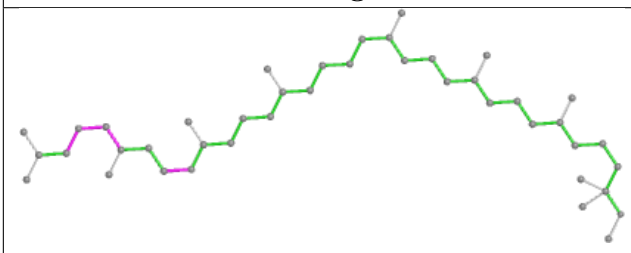
Ligand SPO 01 103



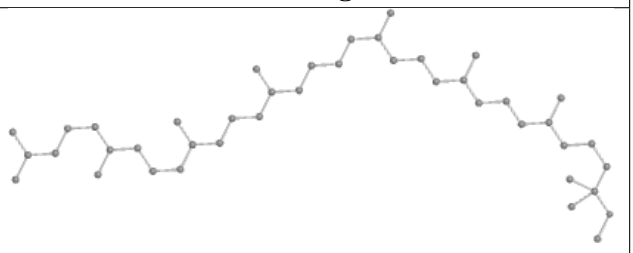
Bond lengths



Bond angles

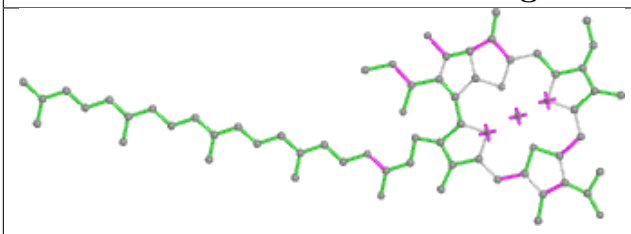


Torsions

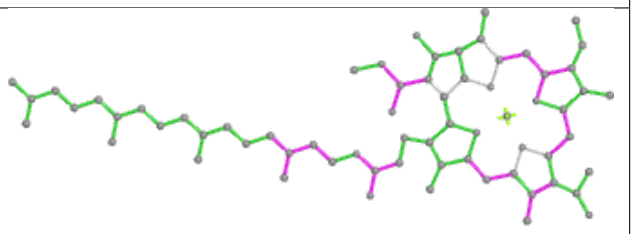


Rings

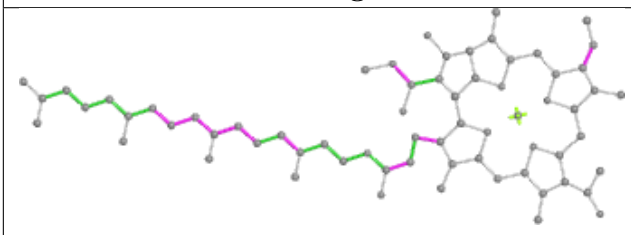
Ligand BCL 02 101



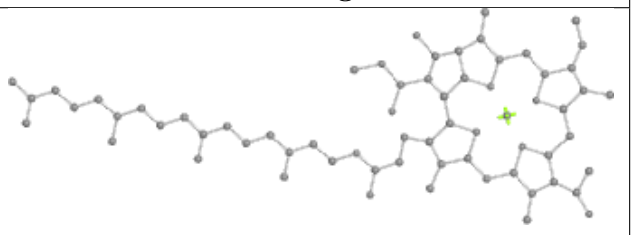
Bond lengths



Bond angles

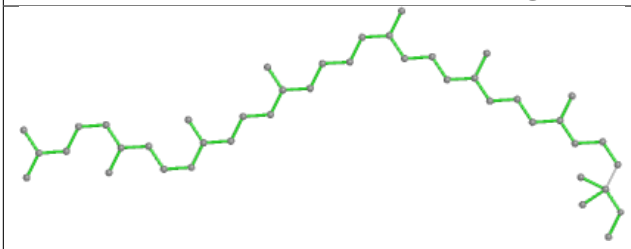


Torsions

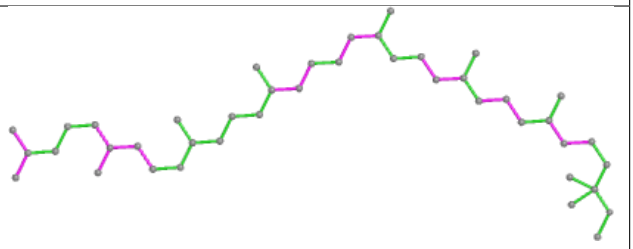


Rings

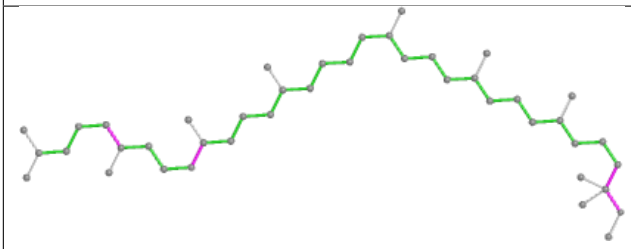
Ligand SPO m 407



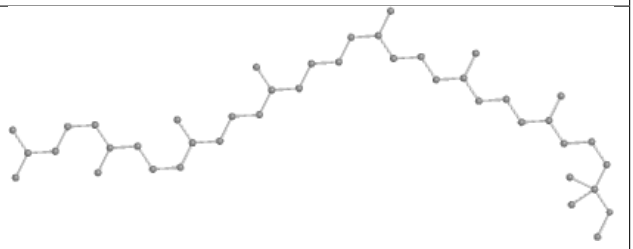
Bond lengths



Bond angles

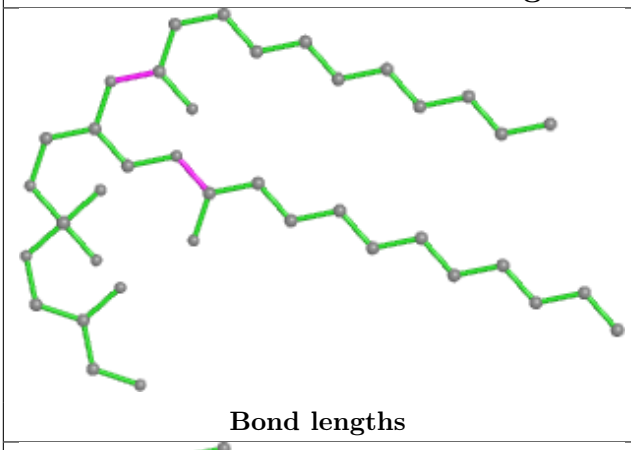


Torsions

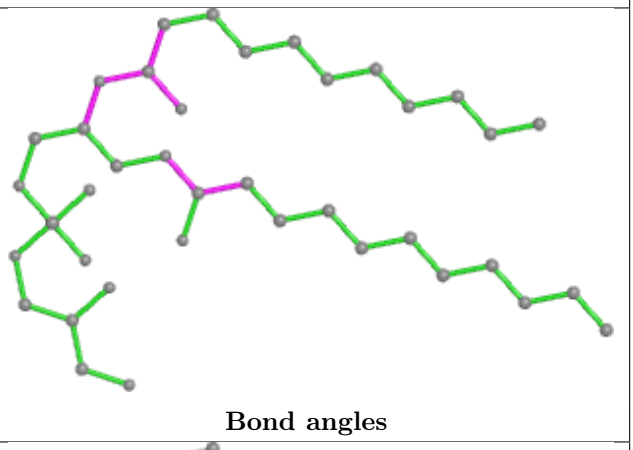


Rings

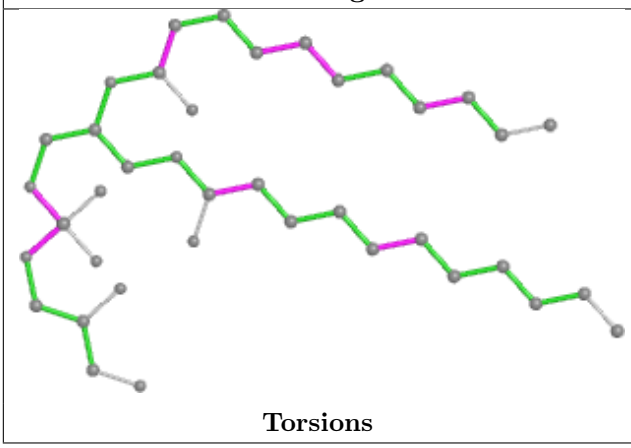
Ligand PGV L 310



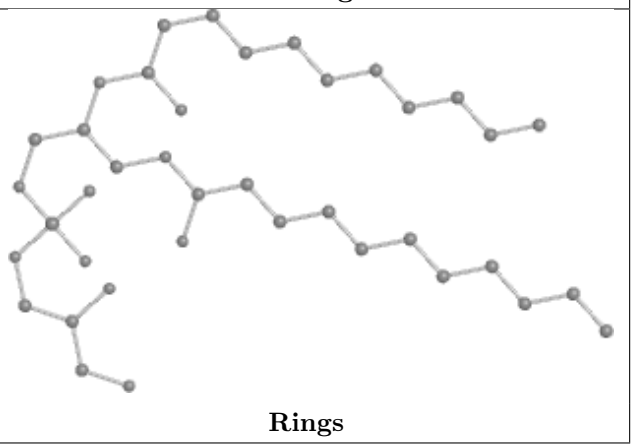
Bond lengths



Bond angles

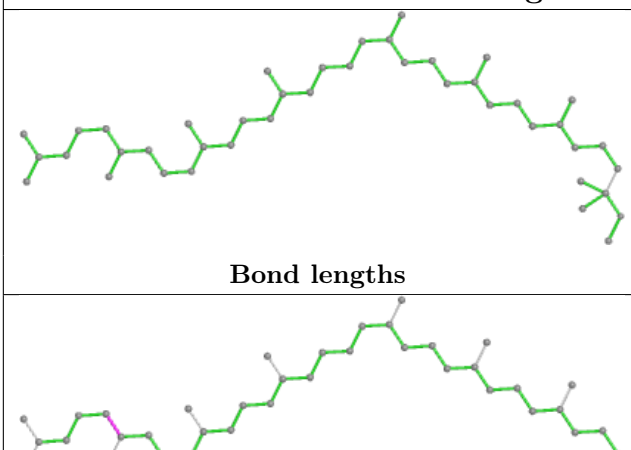


Torsions

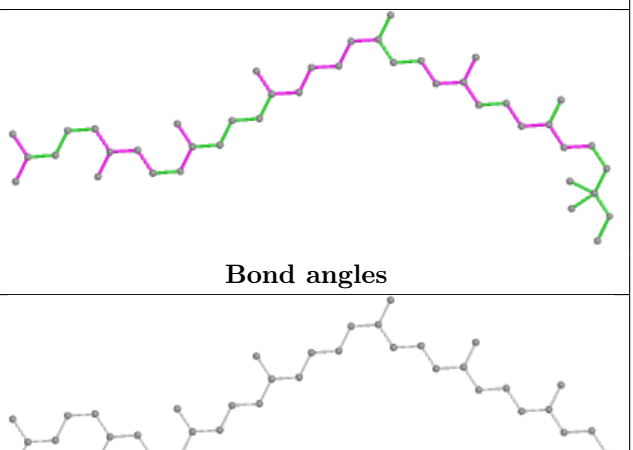


Rings

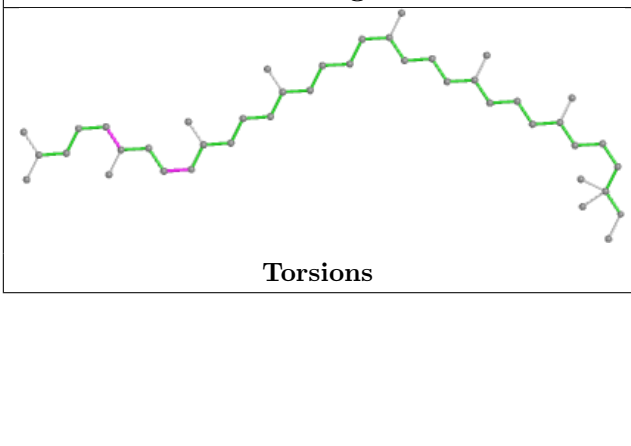
Ligand SPO R 101



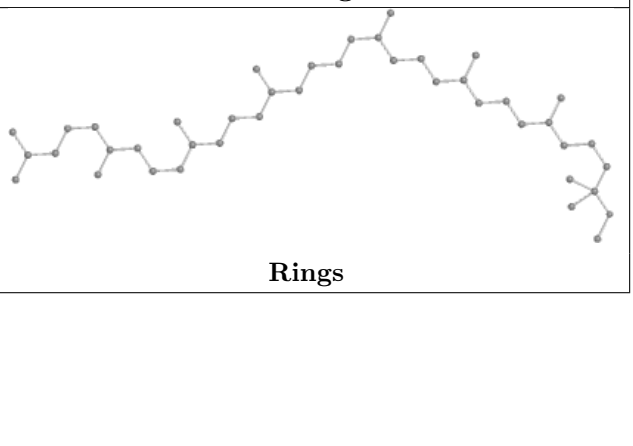
Bond lengths



Bond angles

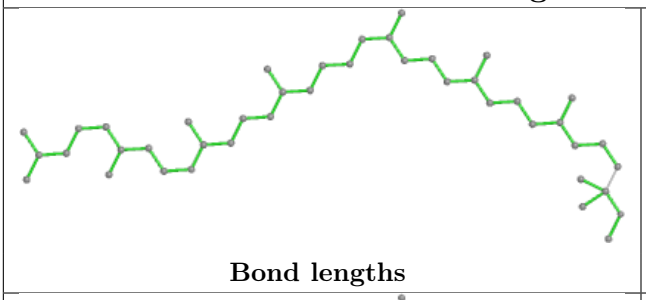


Torsions

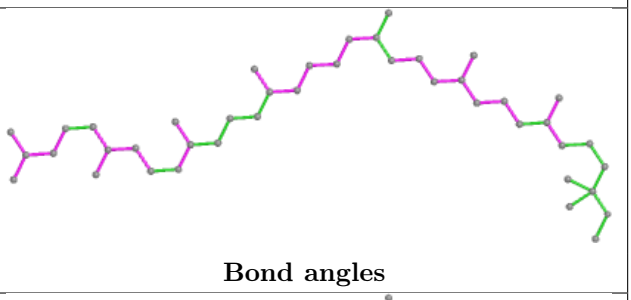


Rings

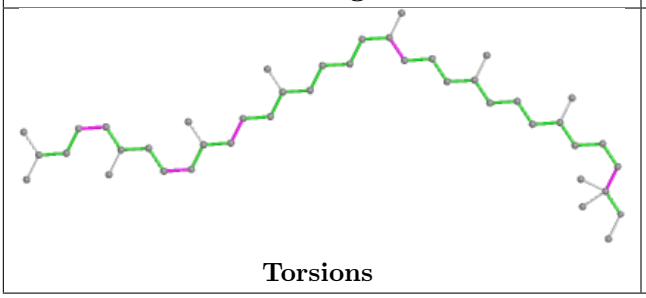
Ligand SPO 3 103



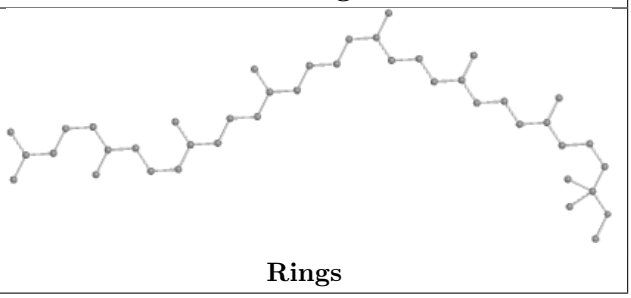
Bond lengths



Bond angles

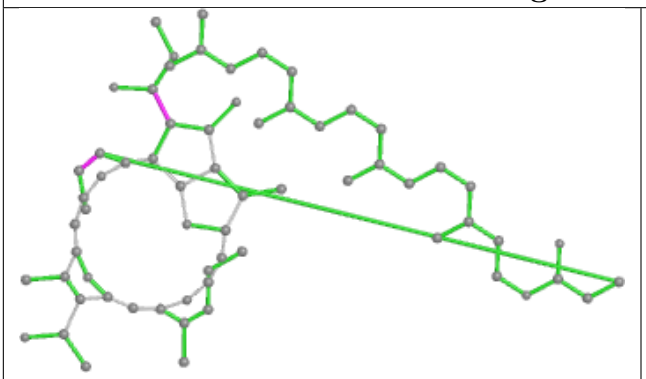


Torsions

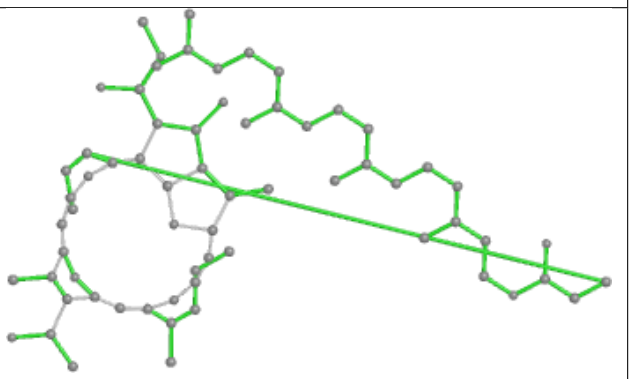


Rings

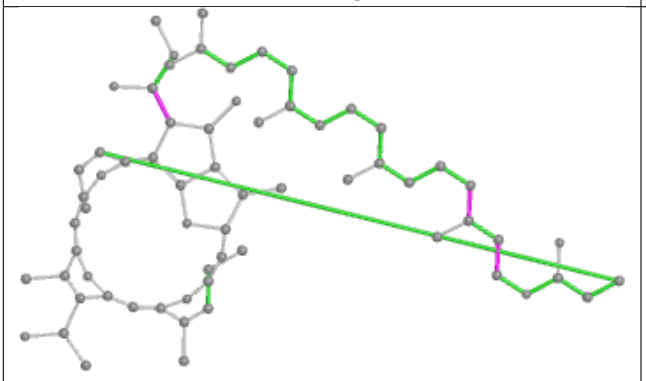
Ligand BPH l 302



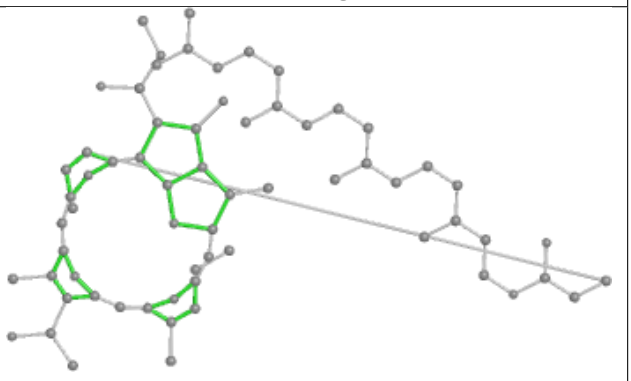
Bond lengths



Bond angles

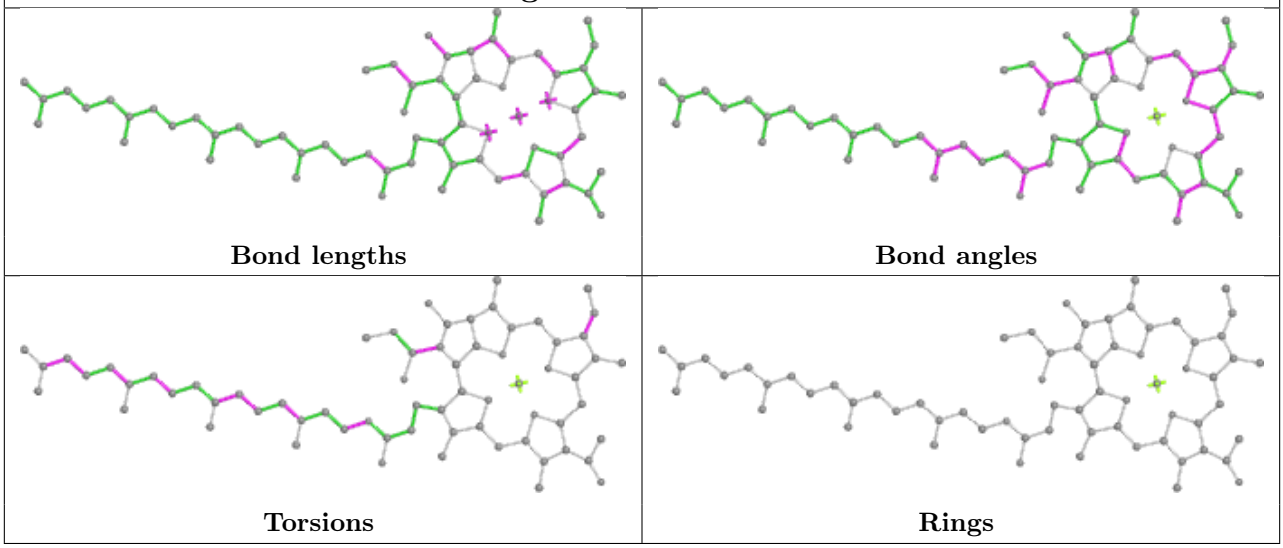


Torsions

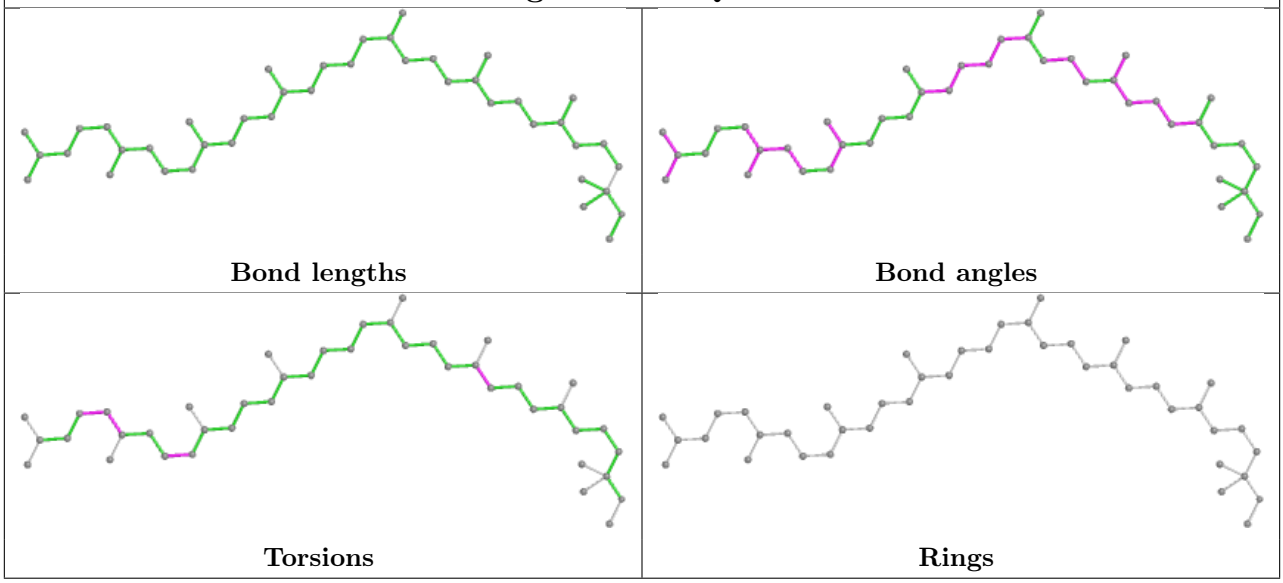


Rings

Ligand BCL 05 101



Ligand SPO Q 104



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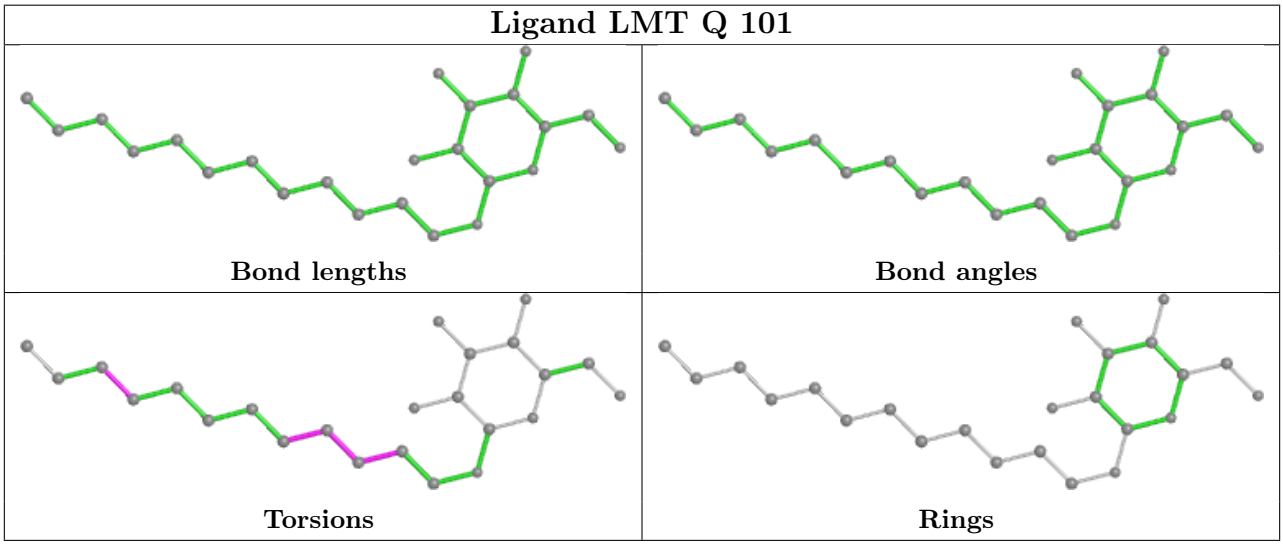
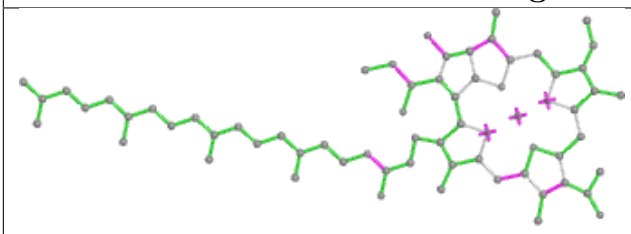
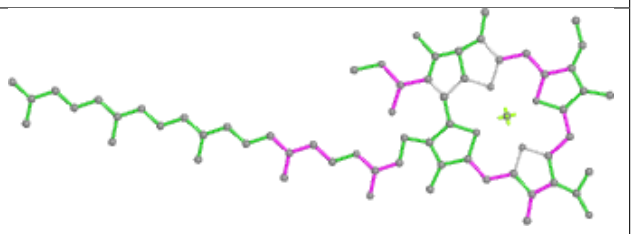


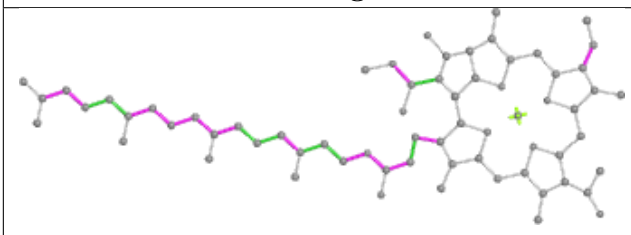
Ligand BCL 2 103



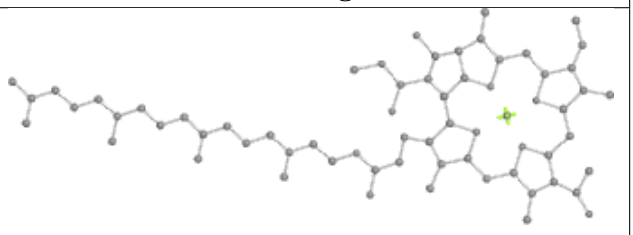
Bond lengths



Bond angles

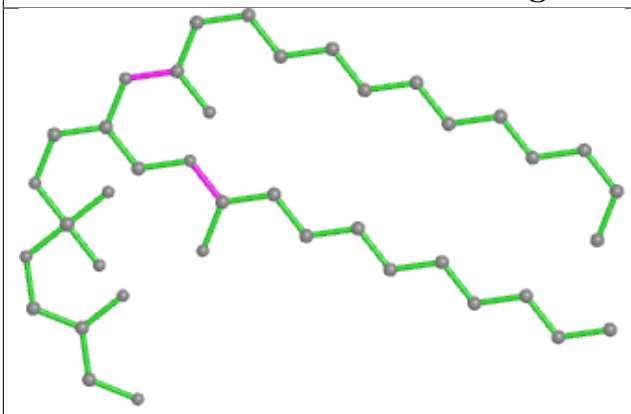


Torsions

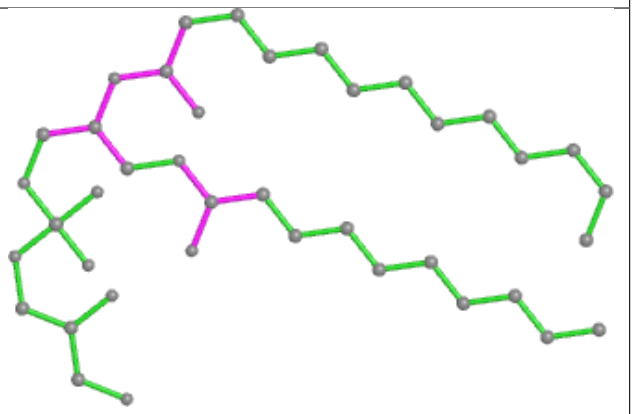


Rings

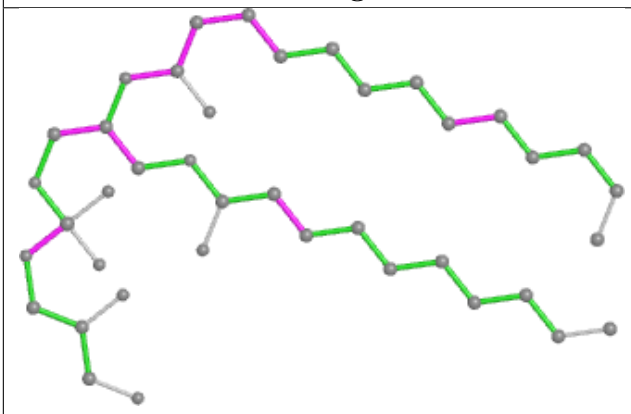
Ligand PGV f 103



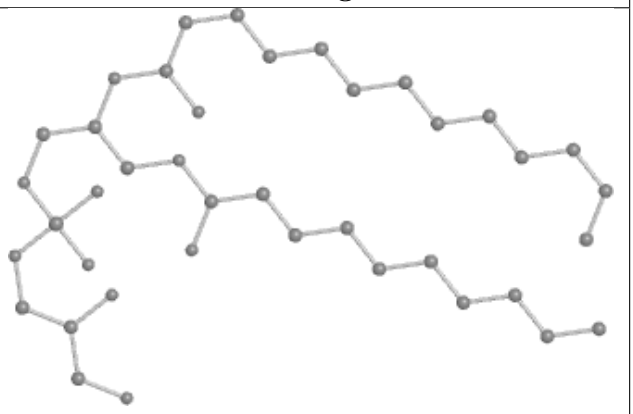
Bond lengths



Bond angles

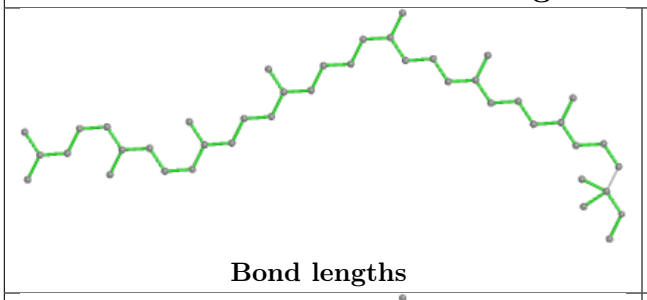


Torsions

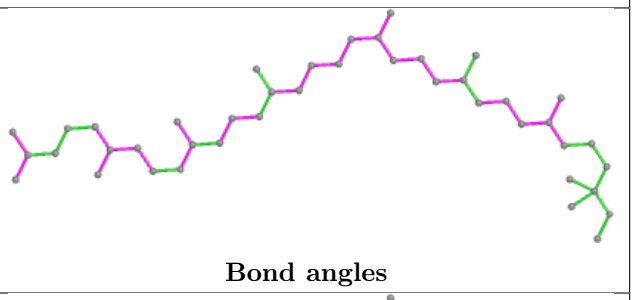


Rings

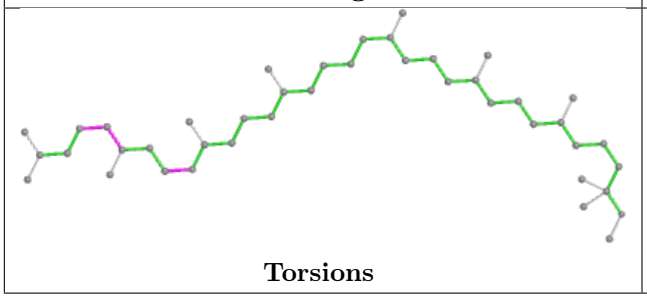
Ligand SPO I 103



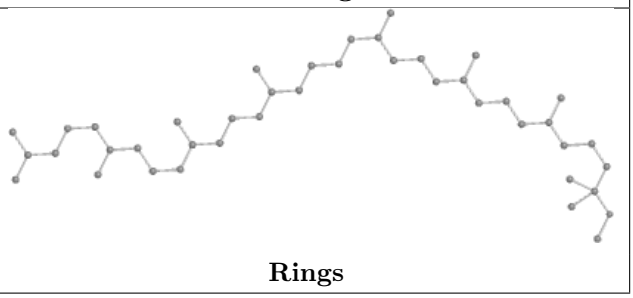
Bond lengths



Bond angles

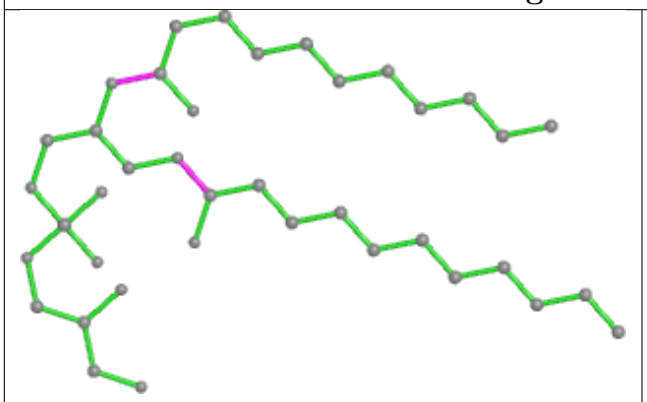


Torsions

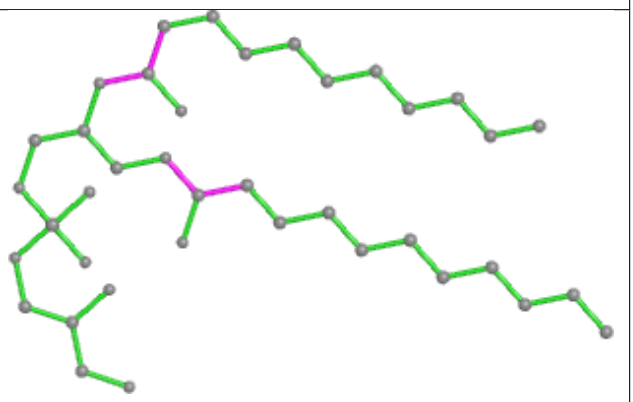


Rings

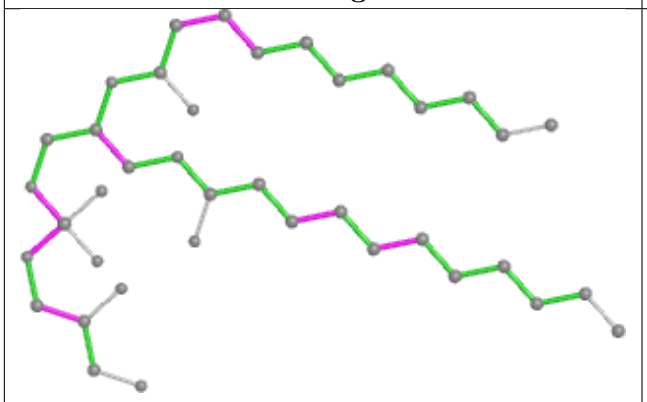
Ligand PGV x 101



Bond lengths



Bond angles



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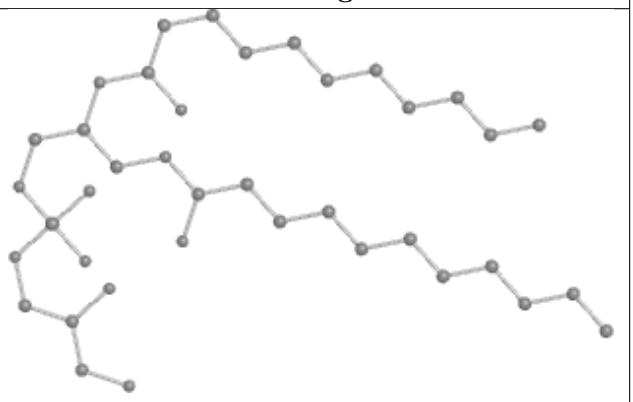
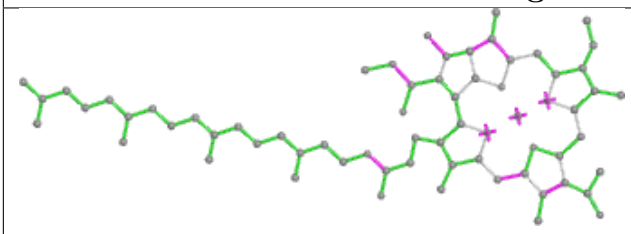
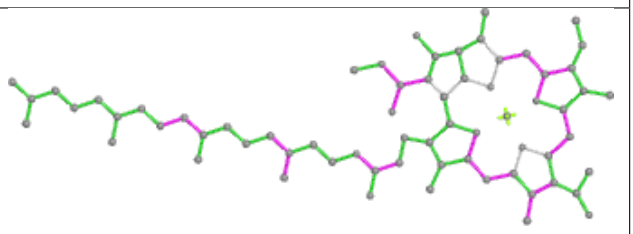


Rings

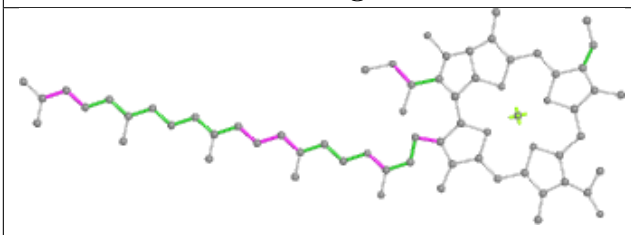
Ligand BCL Z 101



Bond lengths



Bond angles



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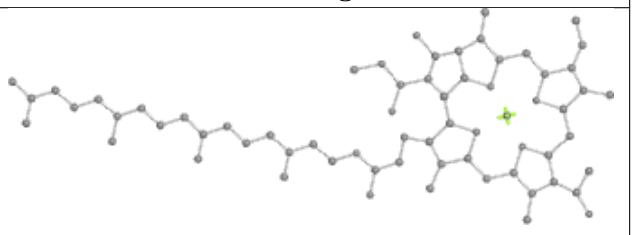
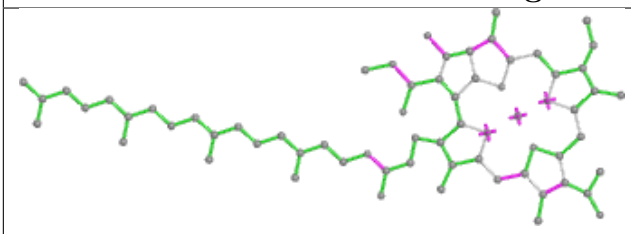
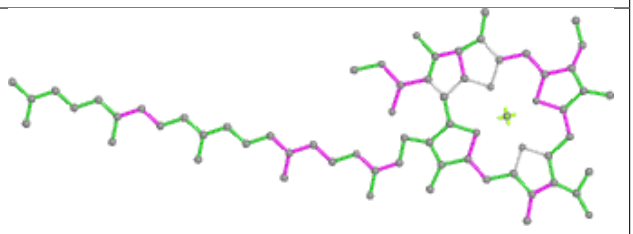


Rings

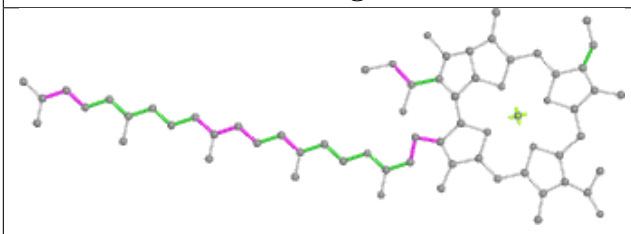
Ligand BCL O 101



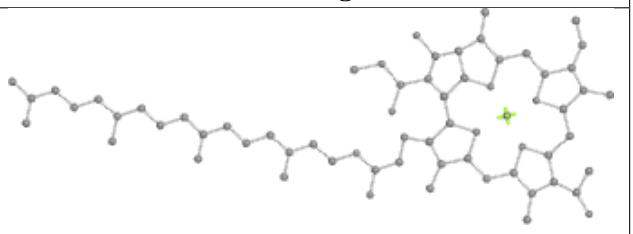
Bond lengths



Bond angles

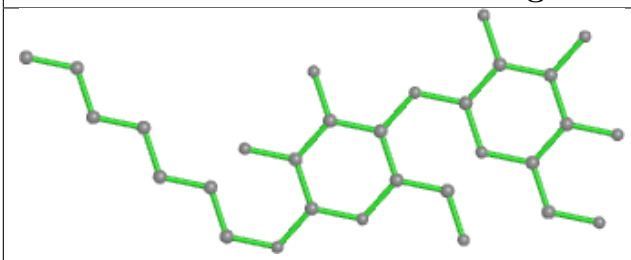


Torsions

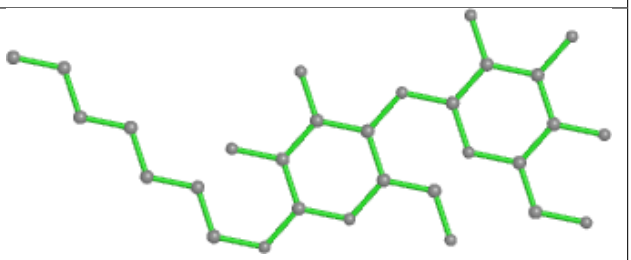


Rings

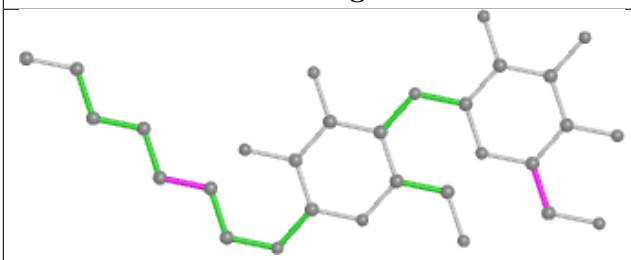
Ligand LMT s 104



Bond lengths



Bond angles



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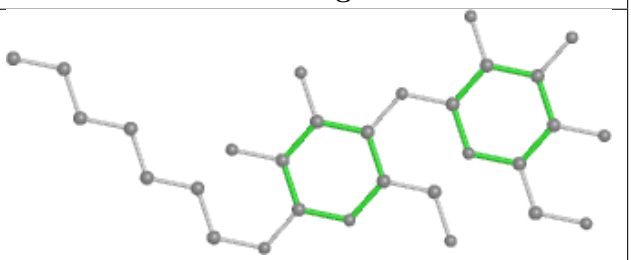
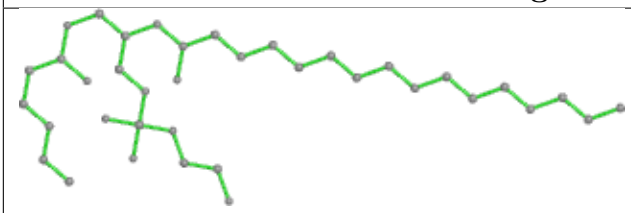
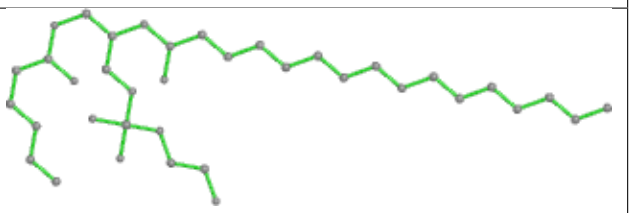


Rings

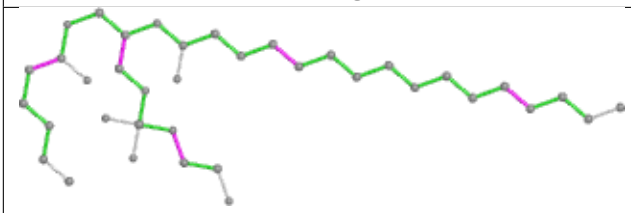
Ligand PTY f 105



Bond lengths



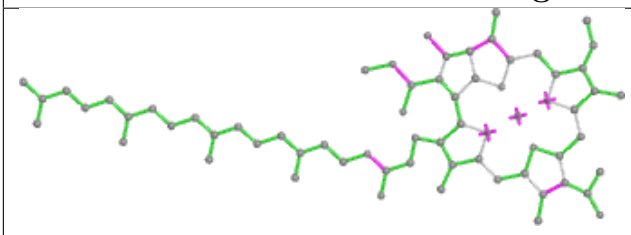
Bond angles



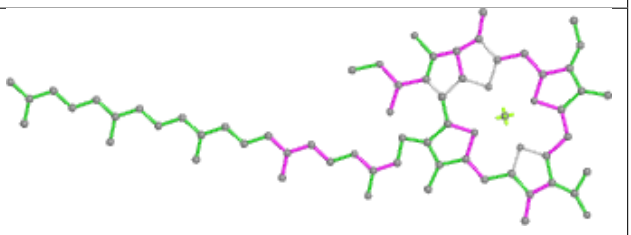
Torsions

Rings

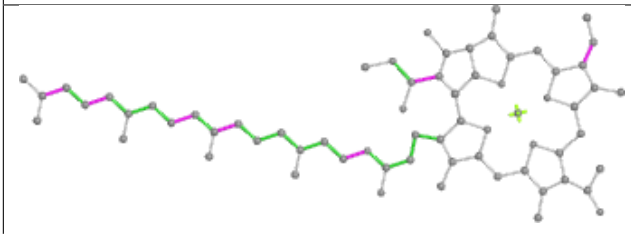
Ligand BCL f 102



Bond lengths



Bond angles



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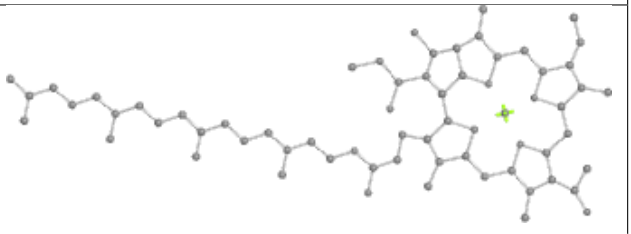
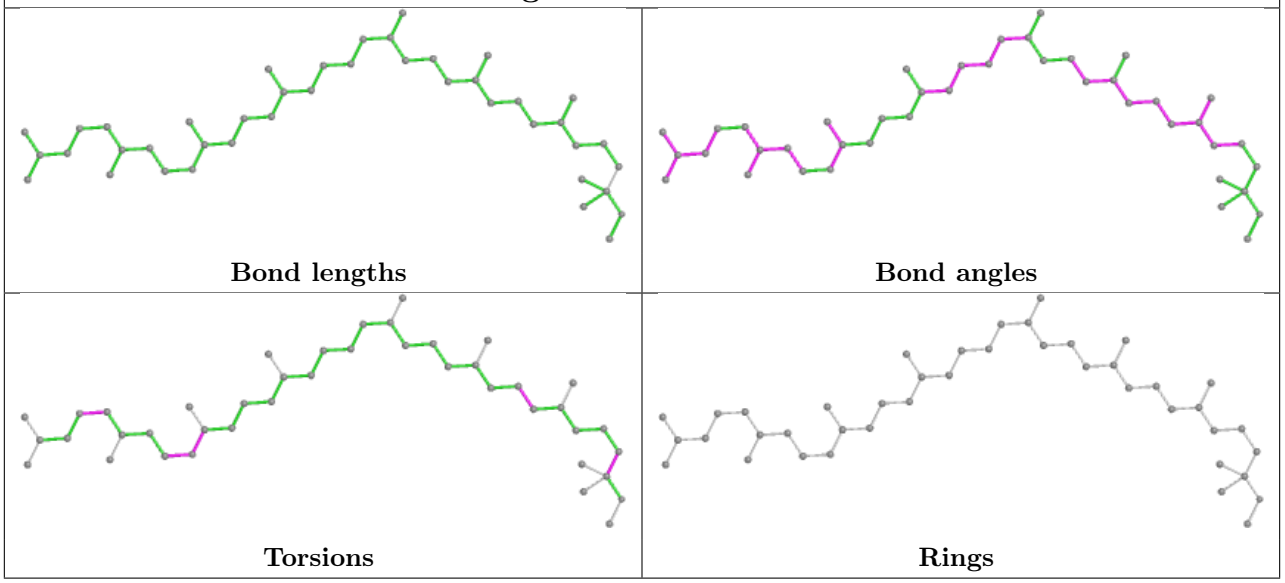
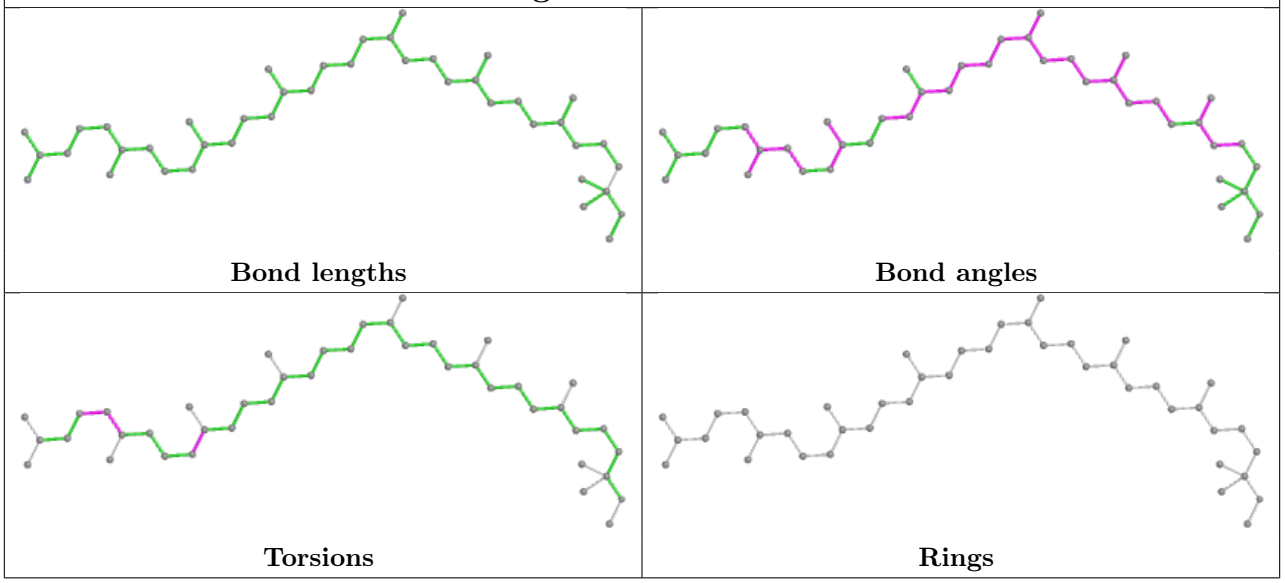


Rings

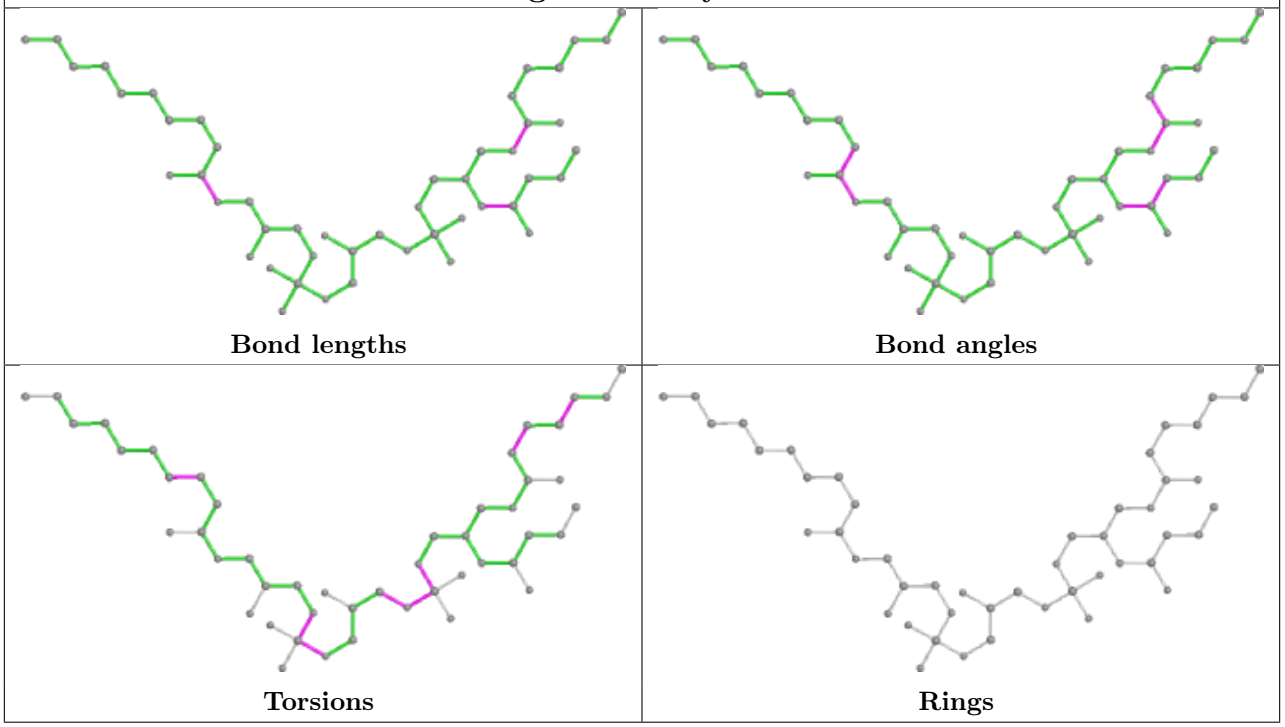
Ligand SPO 05 103



Ligand SPO s 105



Ligand CDL y 102



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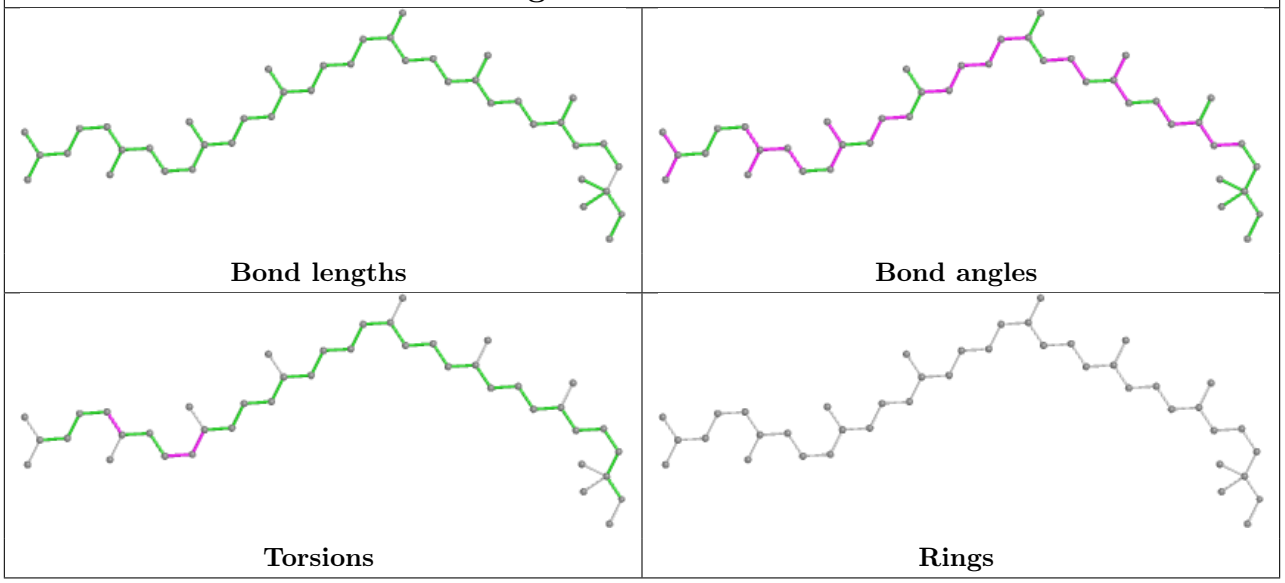
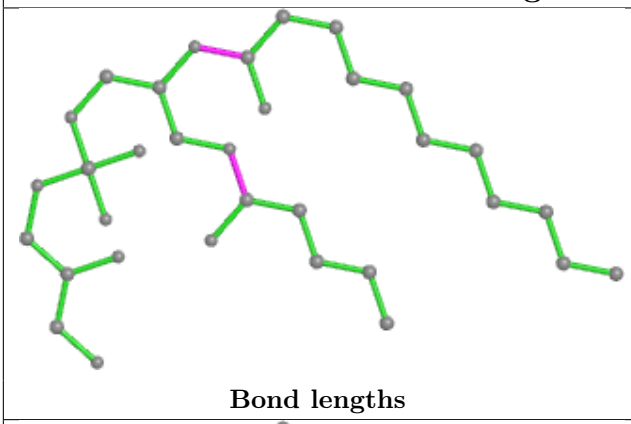
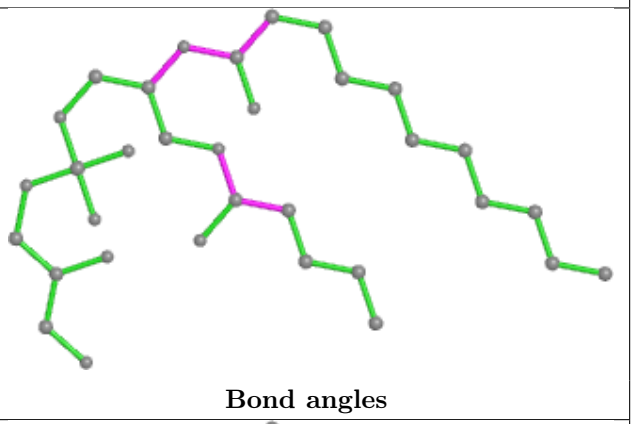


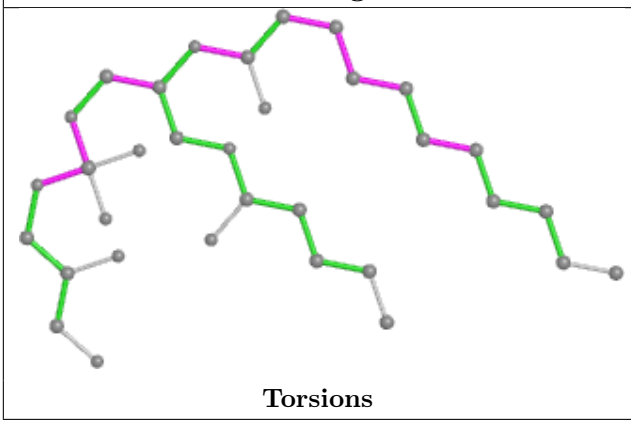
Ligand PGV L 309



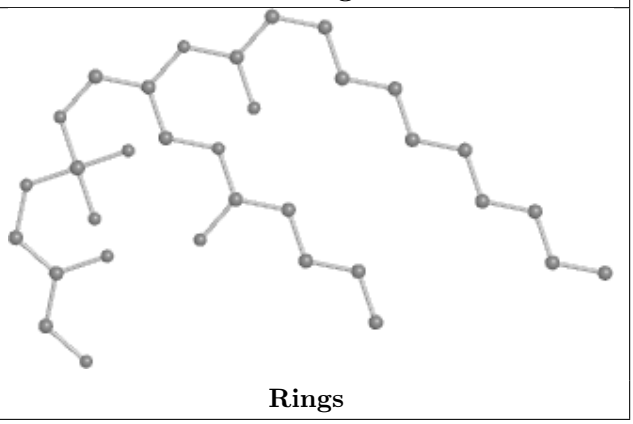
Bond lengths



Bond angles

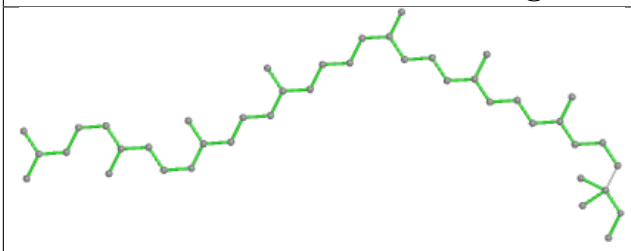


Torsions

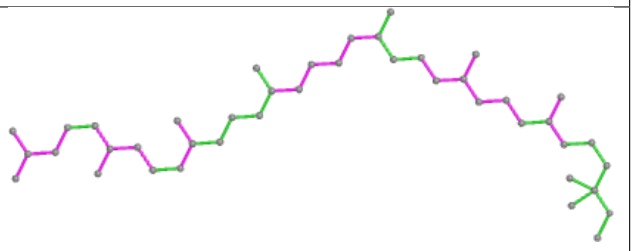


Rings

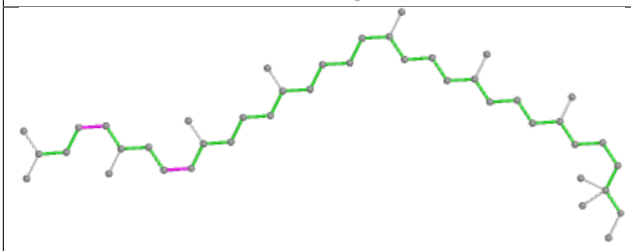
Ligand SPO O 102



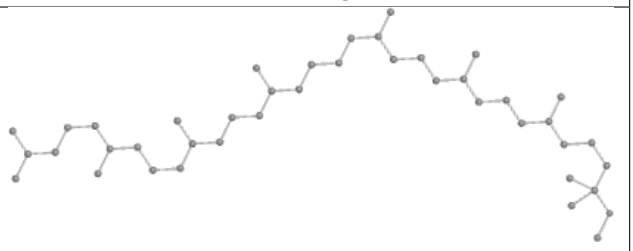
Bond lengths



Bond angles

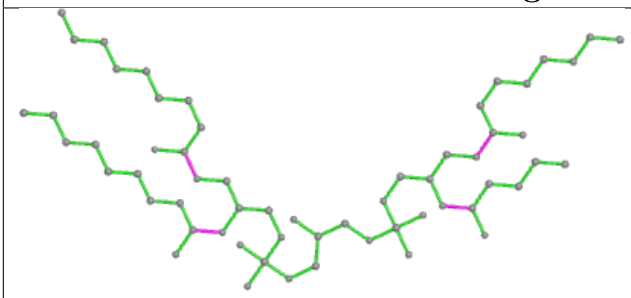


Torsions



Rings

Ligand CDL X 101



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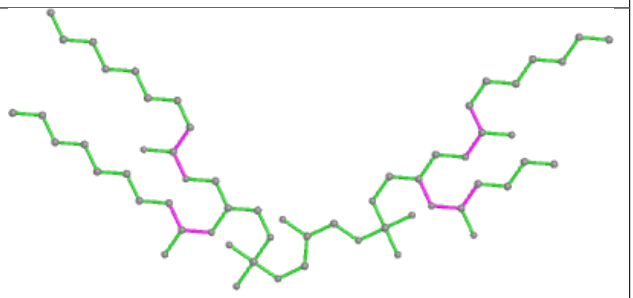
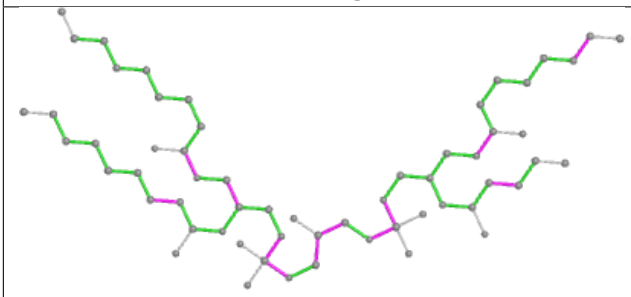


Bond angles



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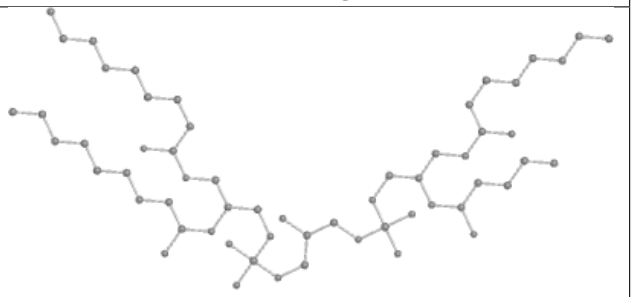
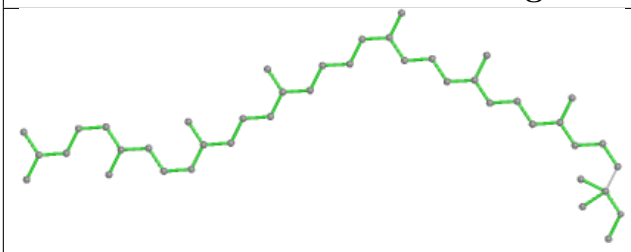
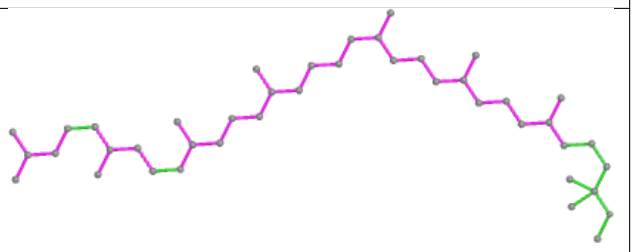


Rings

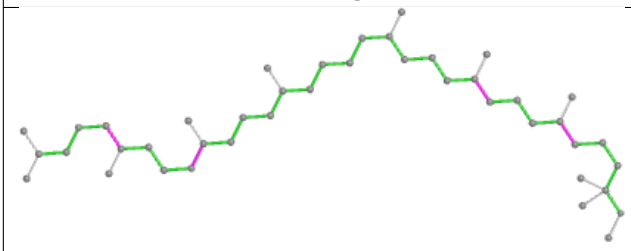
Ligand SPO A 703



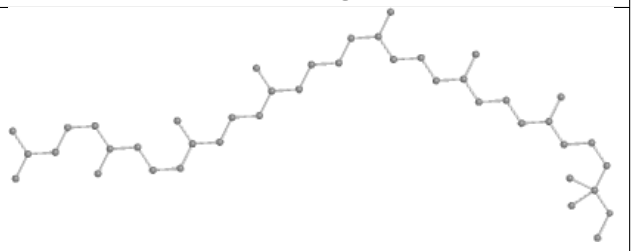
Bond lengths



Bond angles

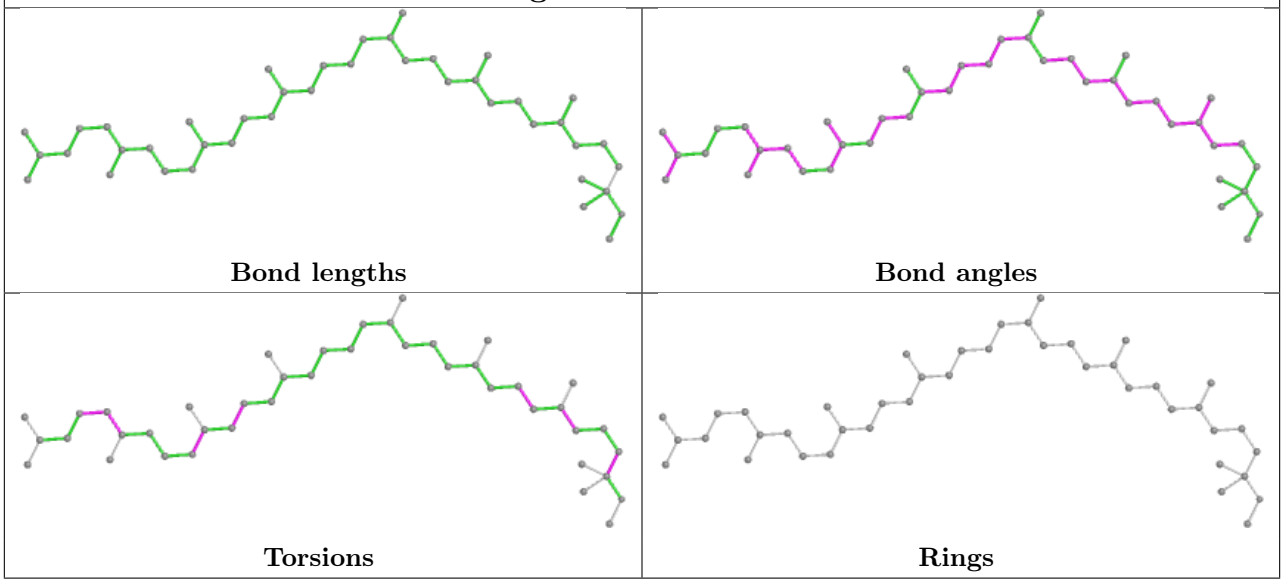


Torsions

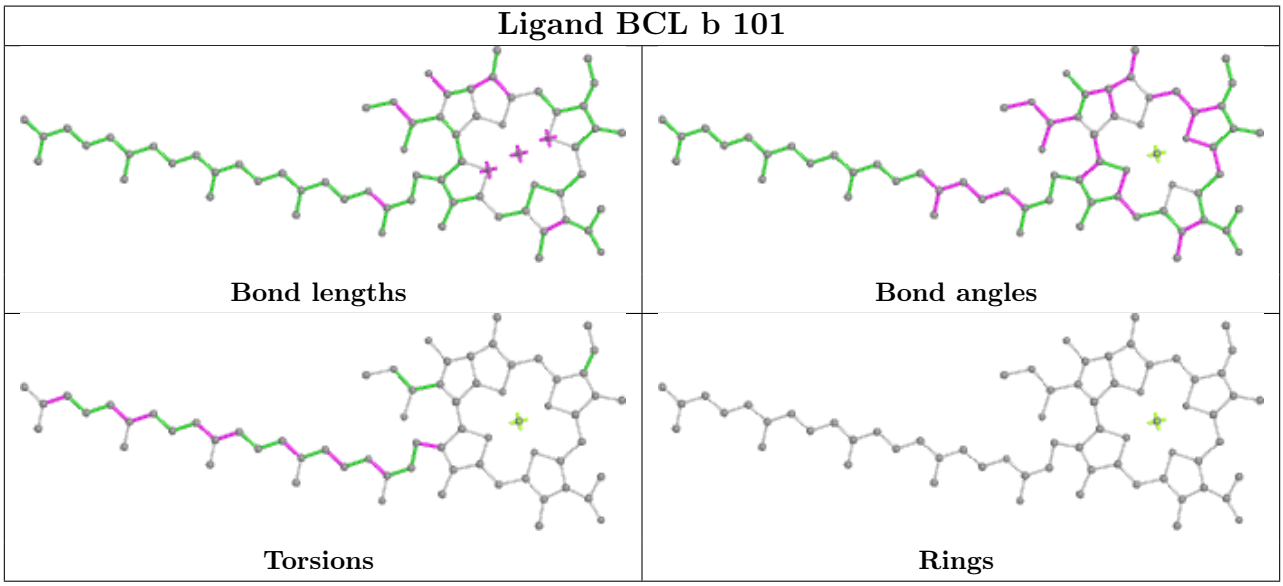


Rings

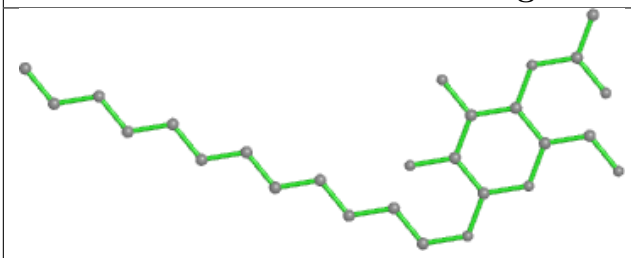
Ligand SPO n 101



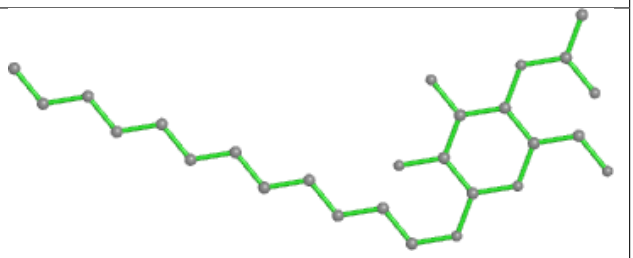
Ligand BCL b 101



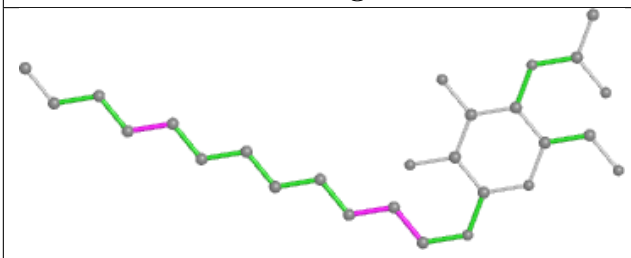
Ligand LMT M 407



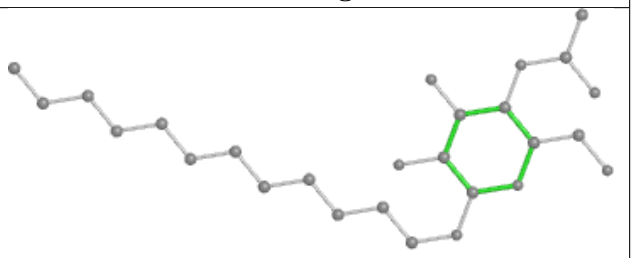
Bond lengths



Bond angles

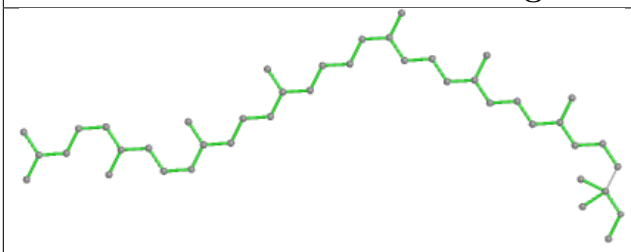


Torsions

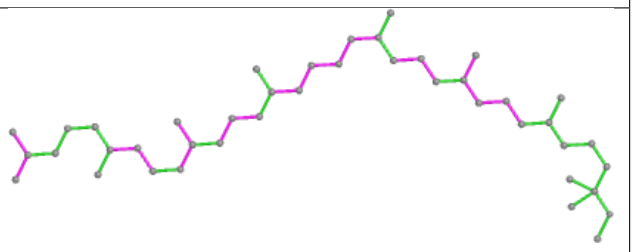


Rings

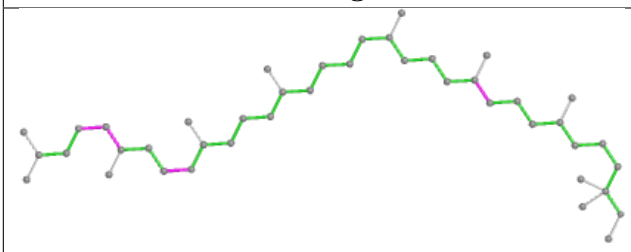
Ligand SPO G 101



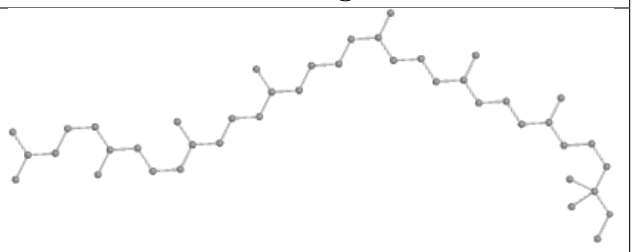
Bond lengths



Bond angles

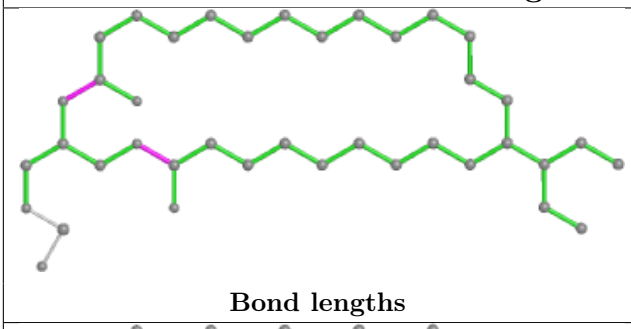


Torsions

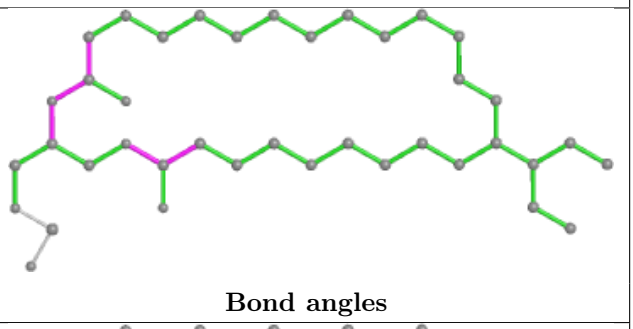


Rings

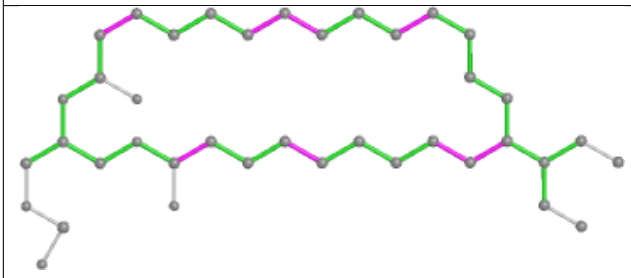
Ligand PGV k 103



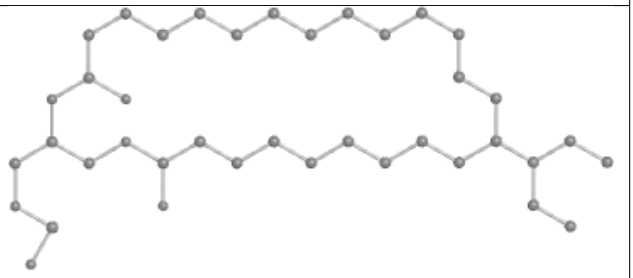
Bond lengths



Bond angles

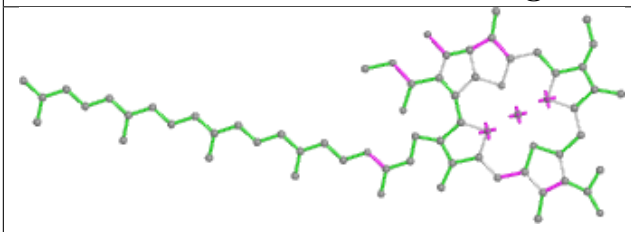


Torsions



Rings

Ligand BCL w 102



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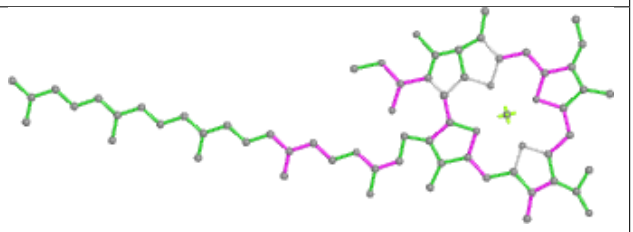
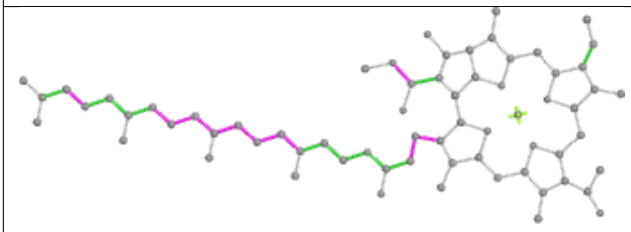


Bond angles



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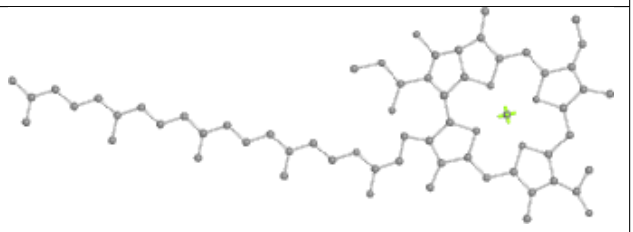
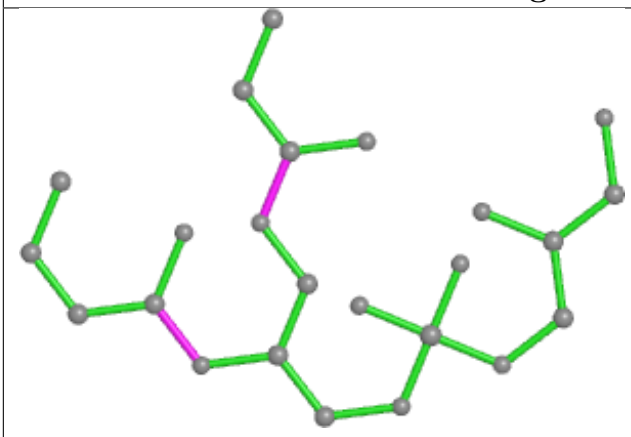
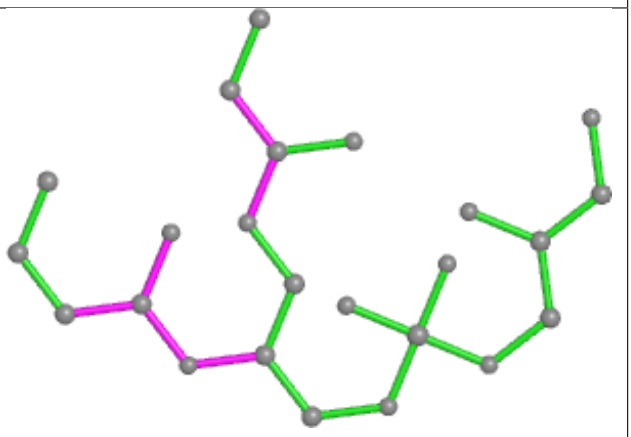


Rings

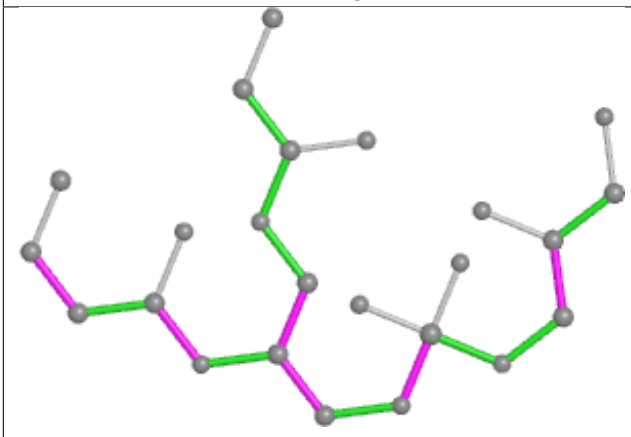
Ligand PGV l 308



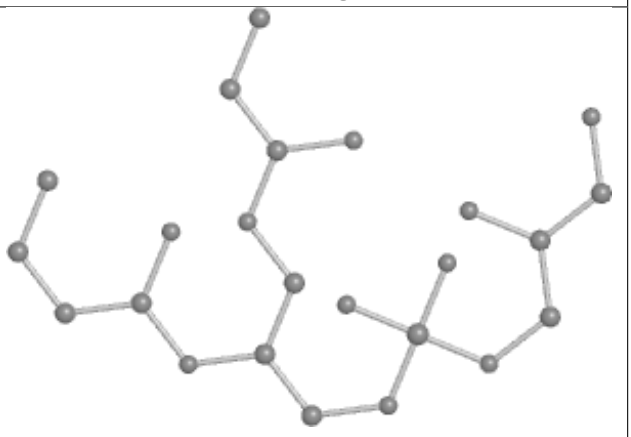
Bond lengths



Bond angles

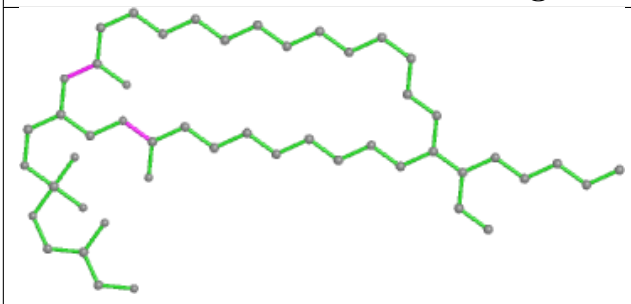


Torsions

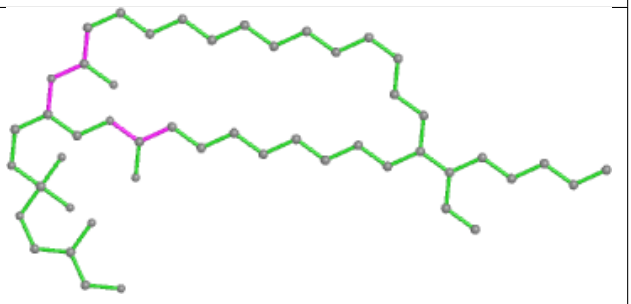


Rings

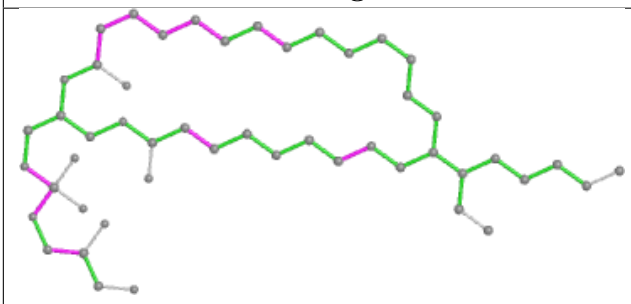
Ligand PGV l 306



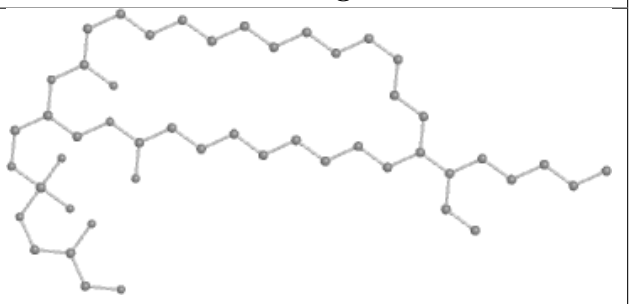
Bond lengths



Bond angles

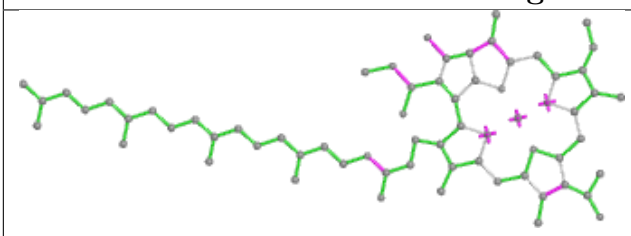


Torsions

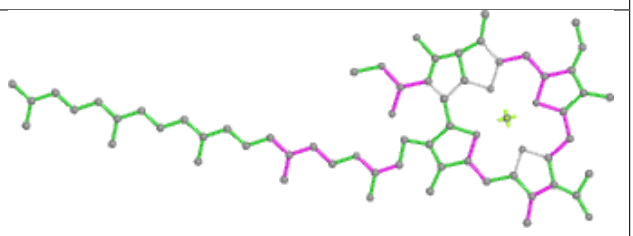


Rings

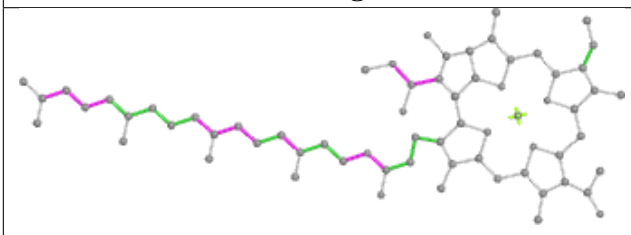
Ligand BCL F 502



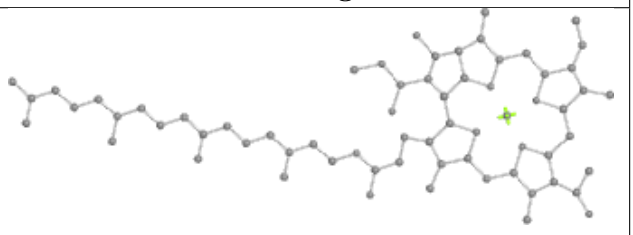
Bond lengths



Bond angles

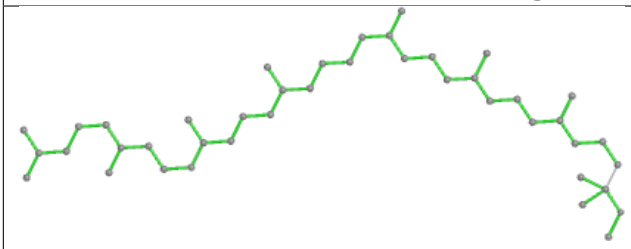


Torsions

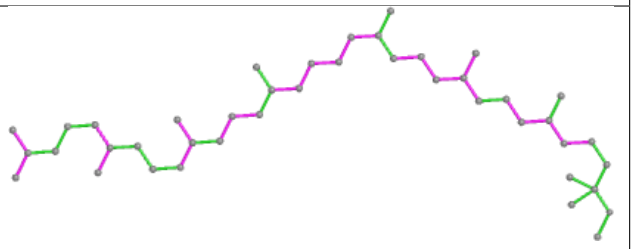


Rings

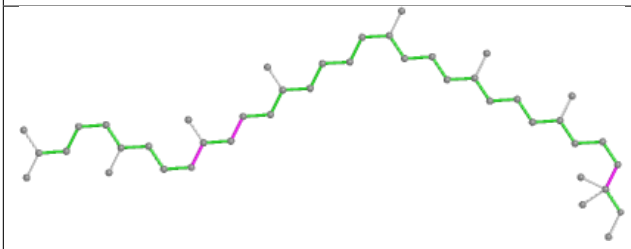
Ligand SPO n 103



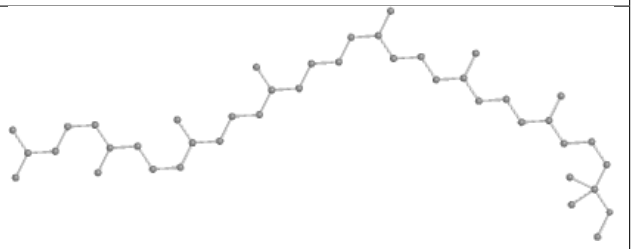
Bond lengths



Bond angles

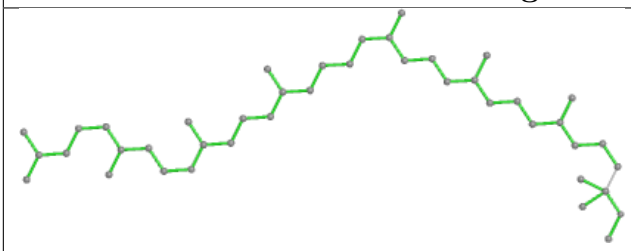


Torsions

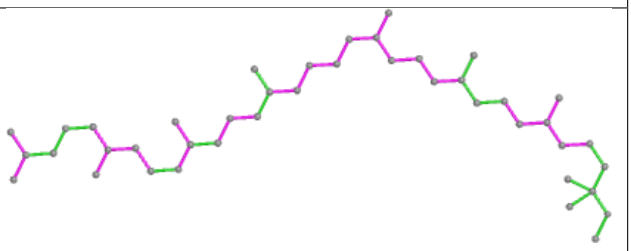


Rings

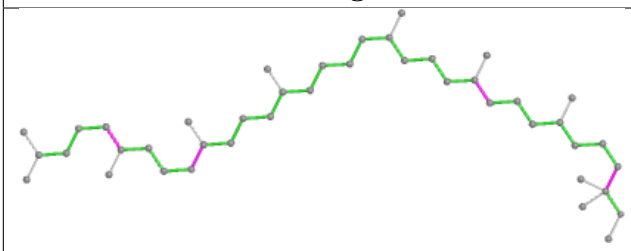
Ligand SPO 08 101



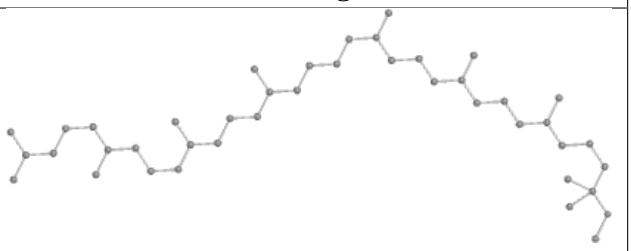
Bond lengths



Bond angles

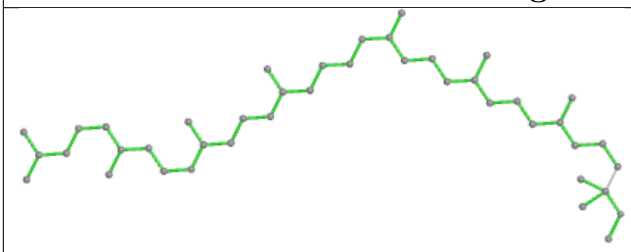


Torsions

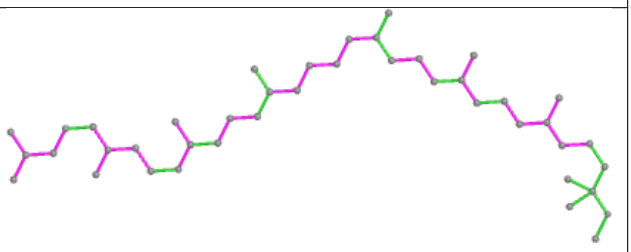


Rings

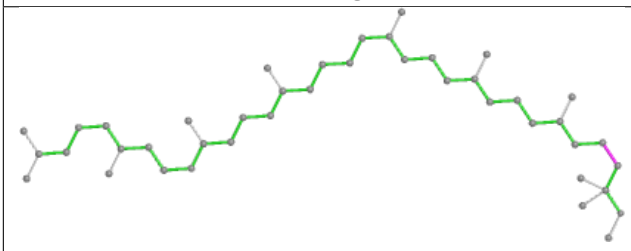
Ligand SPO 2 104



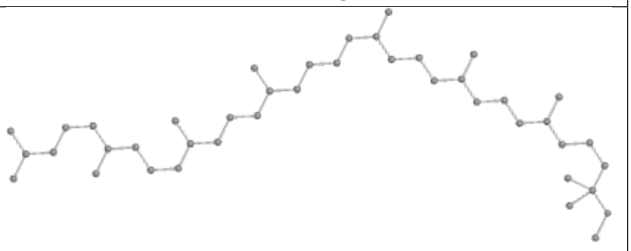
Bond lengths



Bond angles

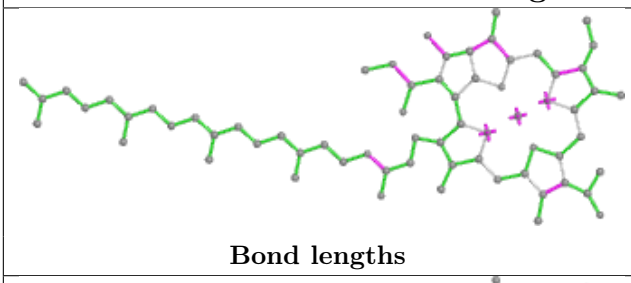


Torsions

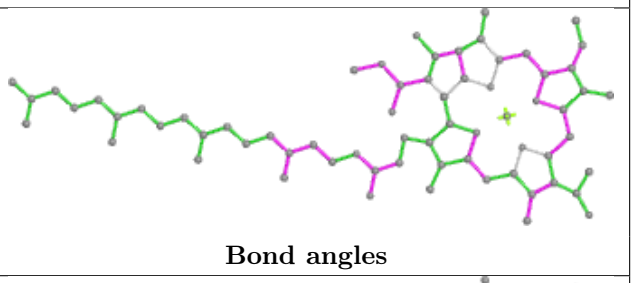


Rings

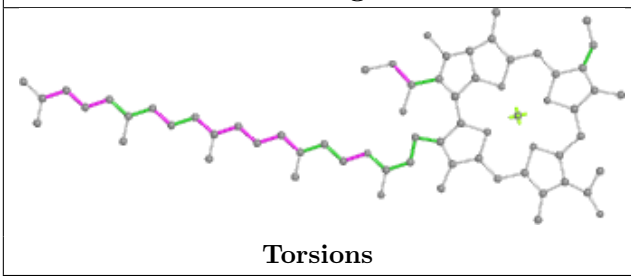
Ligand BCL 1 202



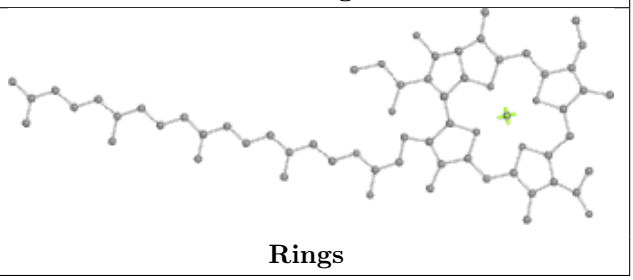
Bond lengths



Bond angles

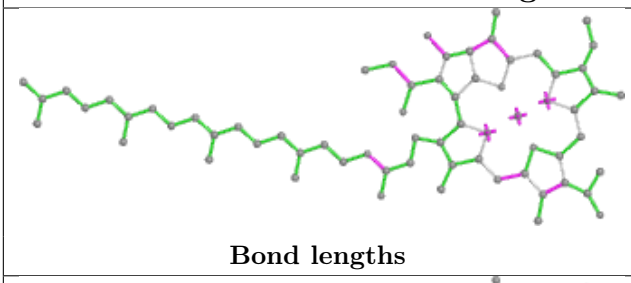


Torsions

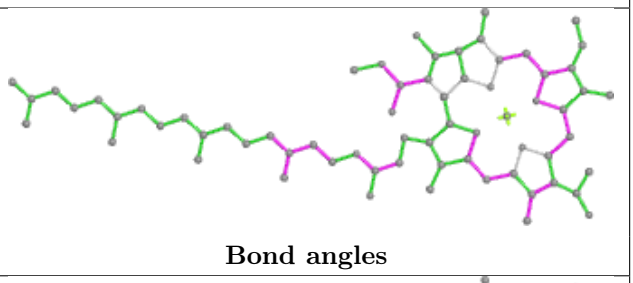


Rings

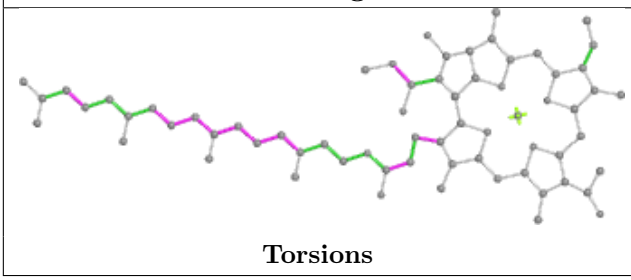
Ligand BCL W 101



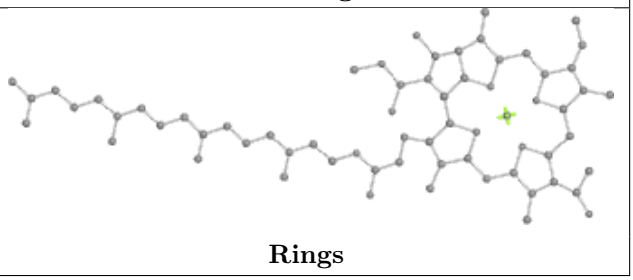
Bond lengths



Bond angles

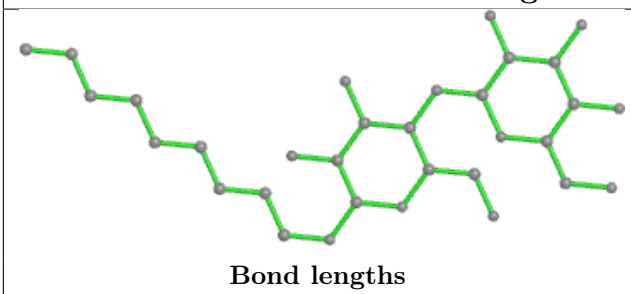


Torsions

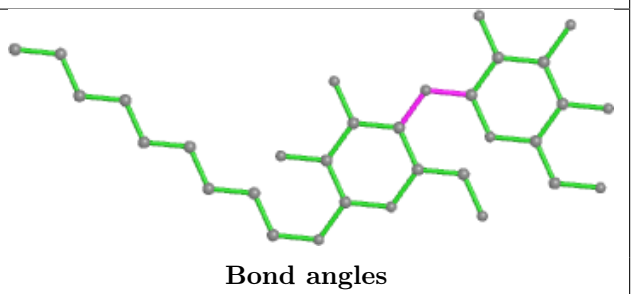


Rings

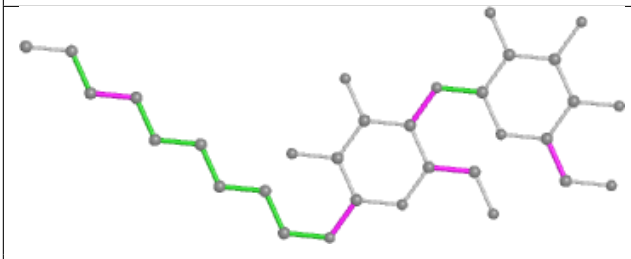
Ligand LMT U 101



Bond lengths



Bond angles



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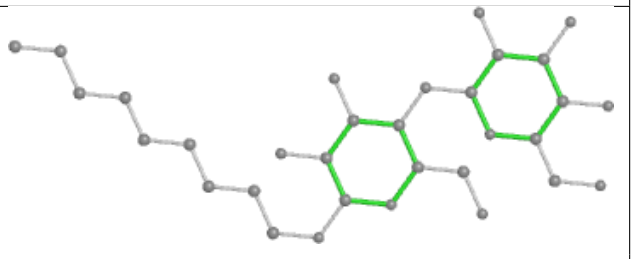
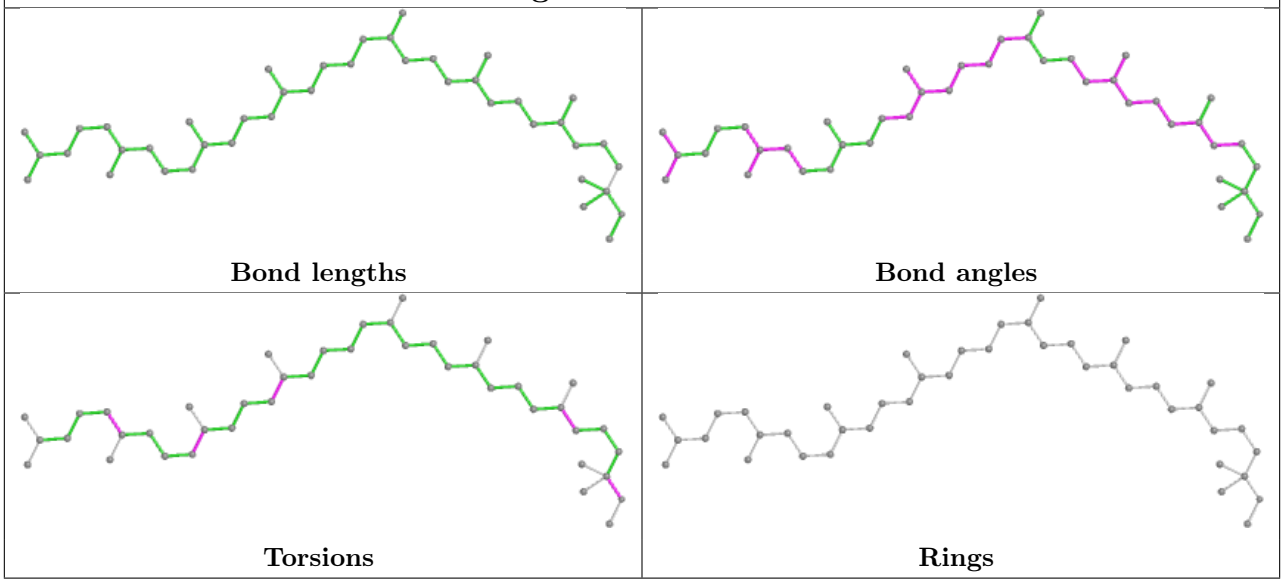
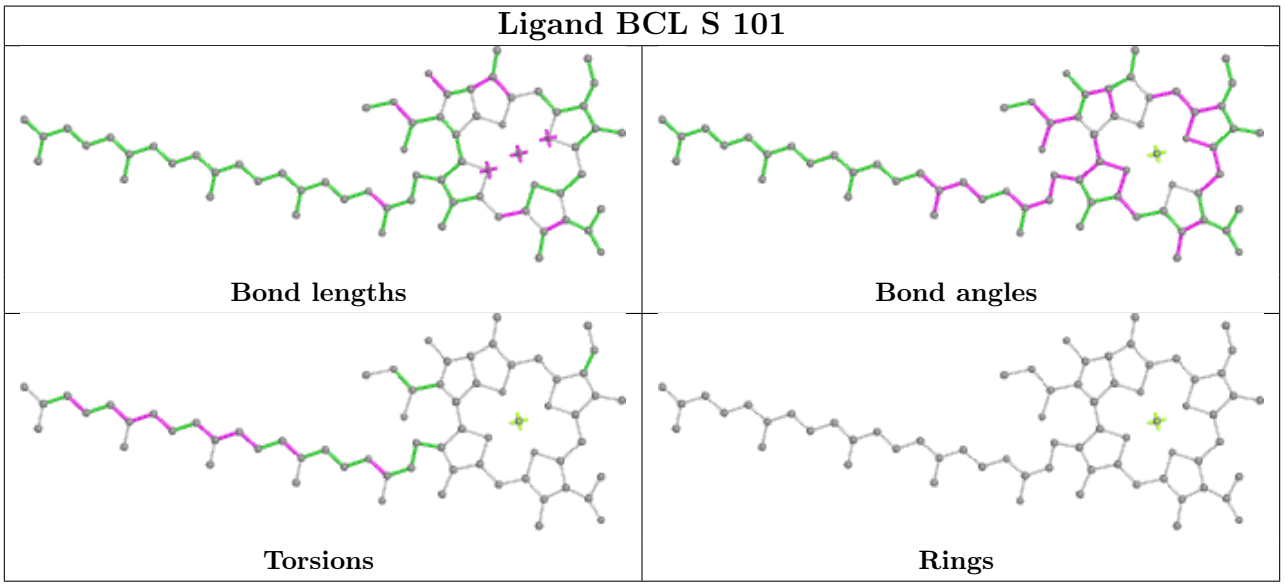


Rings

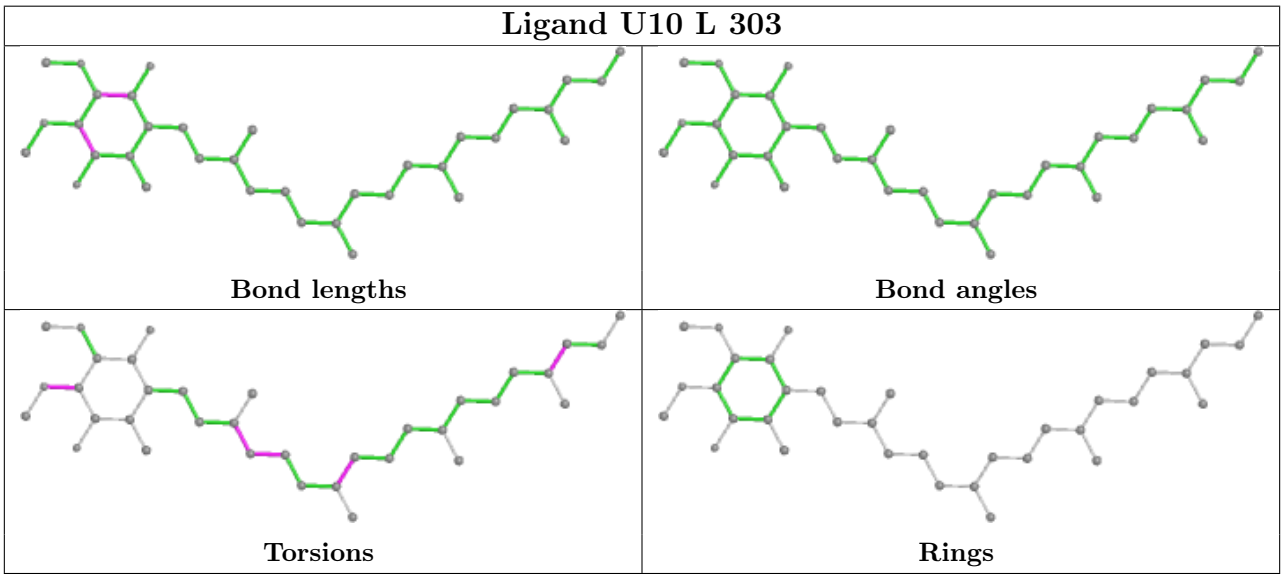
Ligand SPO z 101



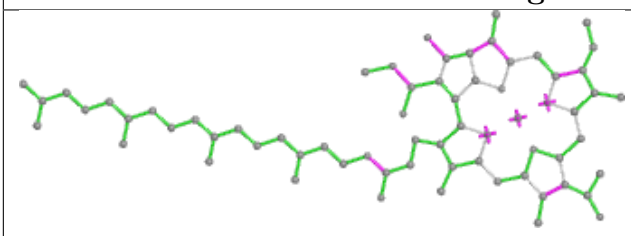
Ligand BCL S 101



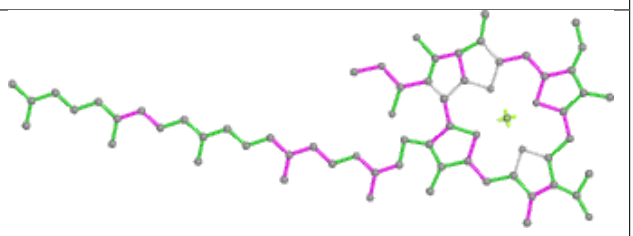
Ligand U10 L 303



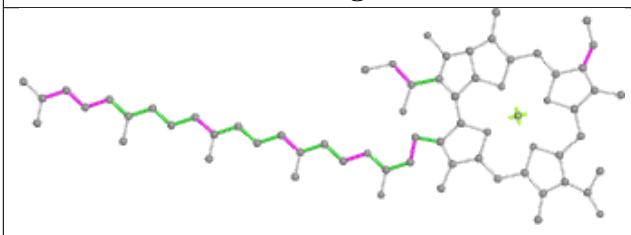
Ligand BCL L 301



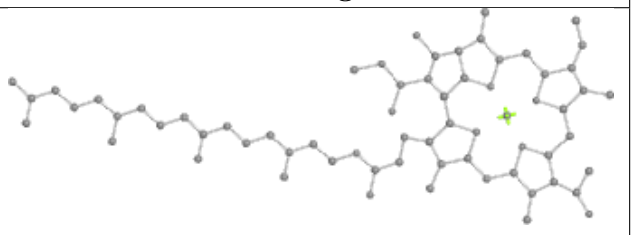
Bond lengths



Bond angles

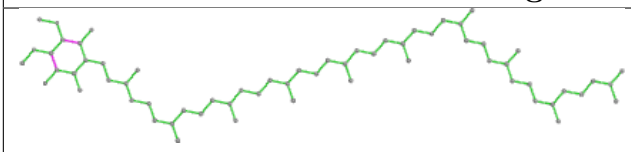


Torsions



Rings

Ligand U10 M 405



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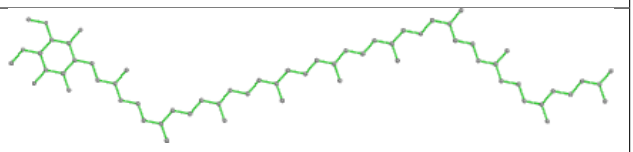
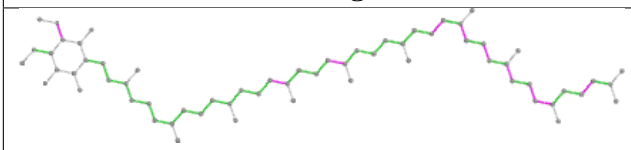
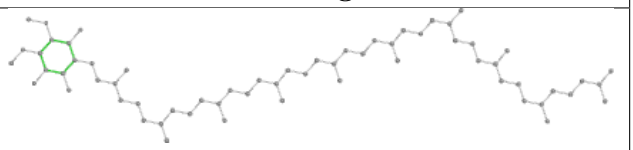


Bond angles

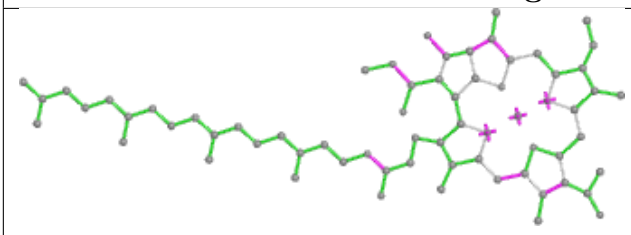


Torsions

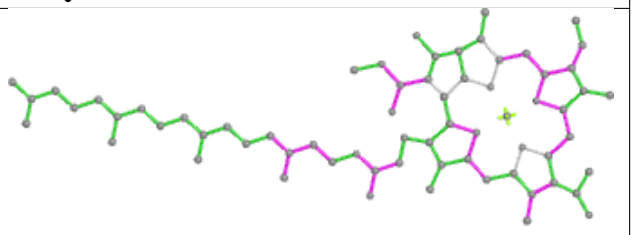


Rings

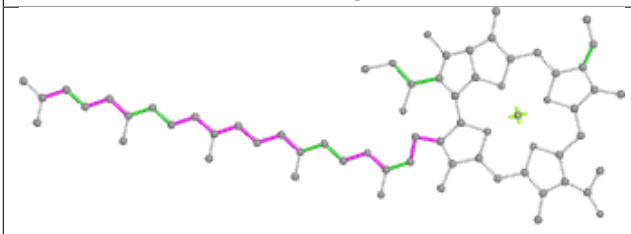
Ligand BCL Q 103



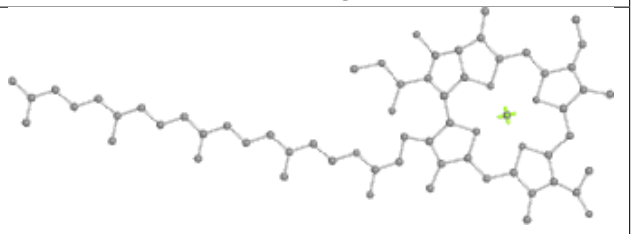
Bond lengths



Bond angles

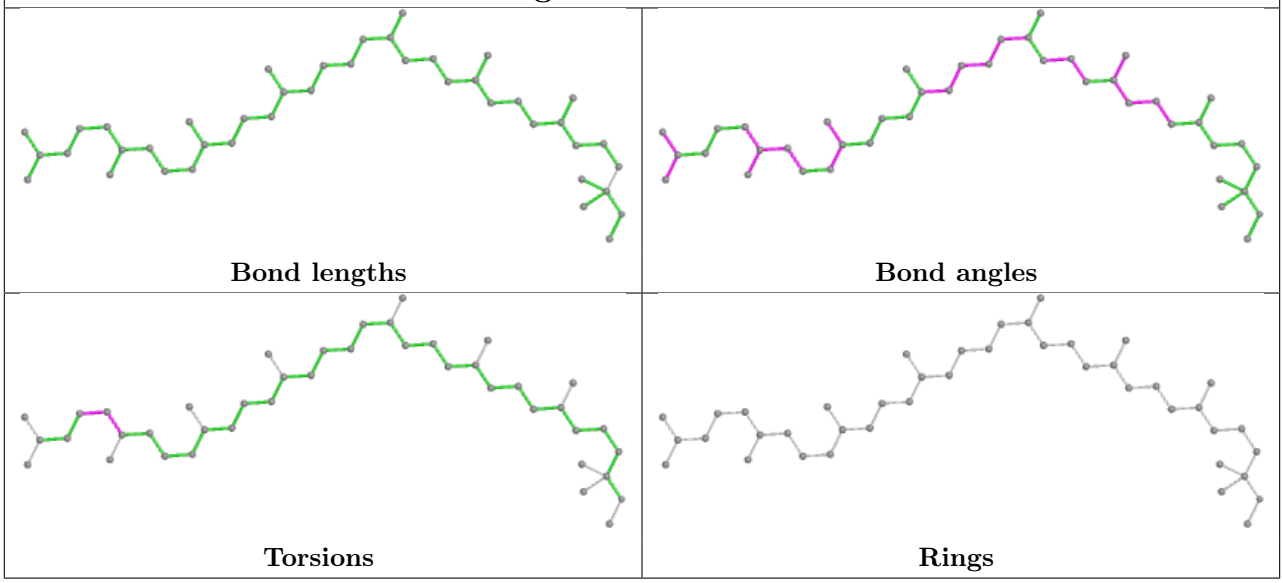


Torsions

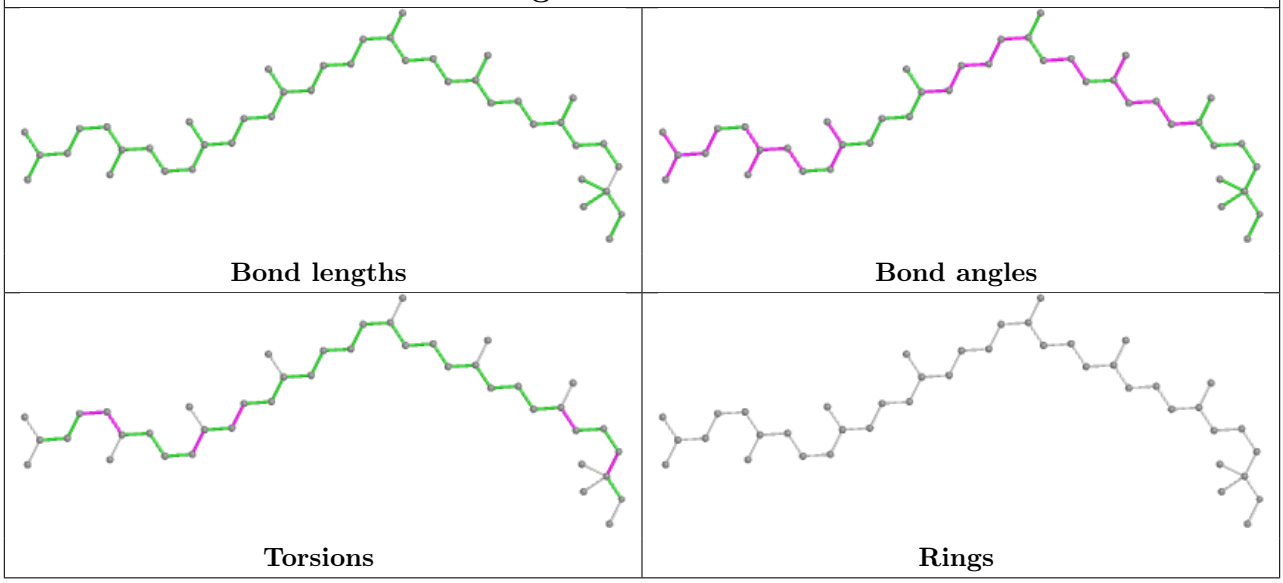


Rings

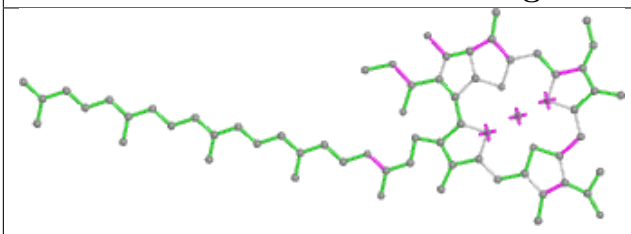
Ligand SPO f 106



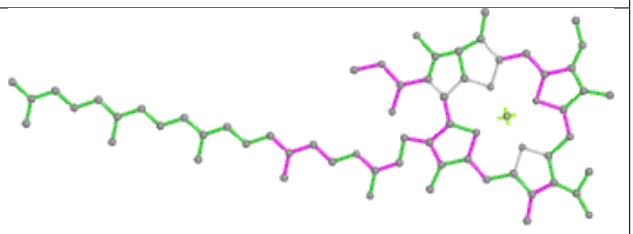
Ligand SPO r 103



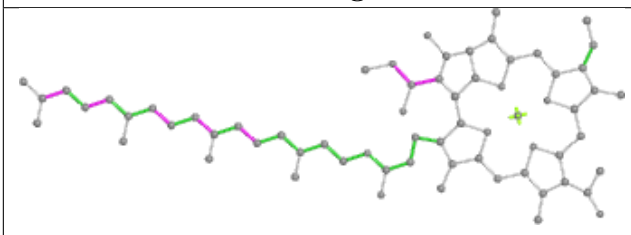
Ligand BCL m 403



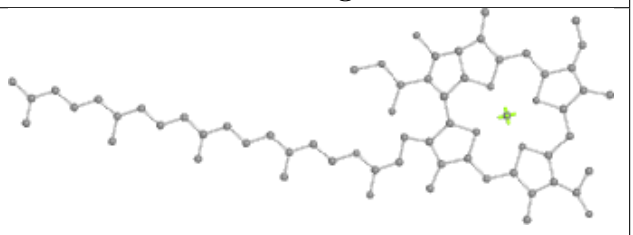
Bond lengths



Bond angles

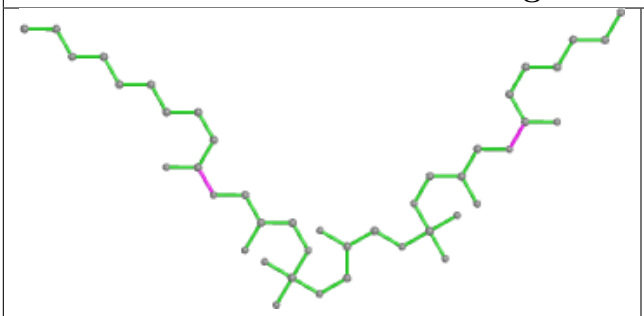


Torsions

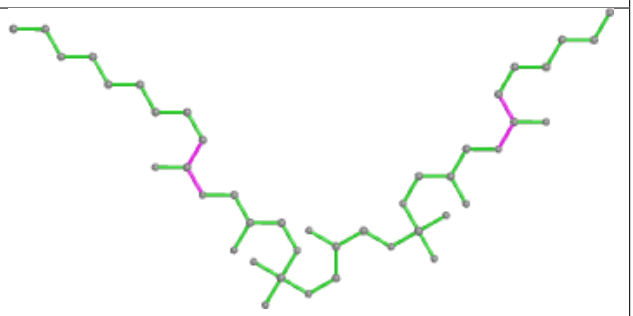


Rings

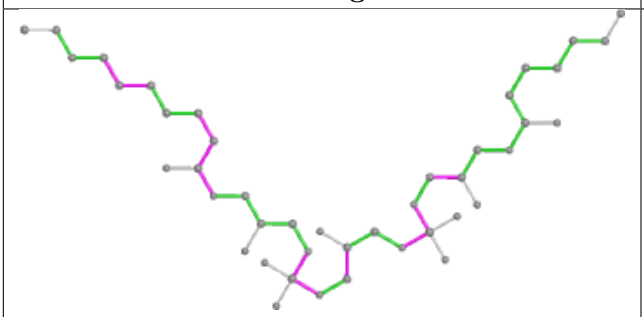
Ligand CDL Y 101



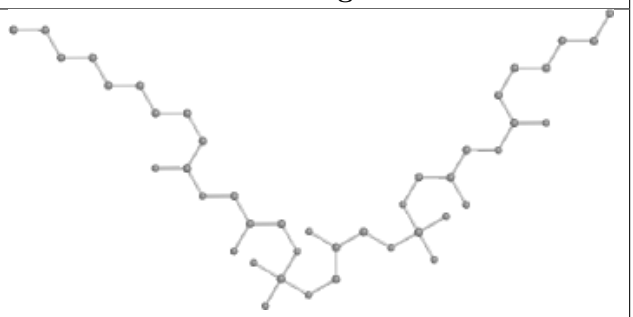
Bond lengths



Bond angles

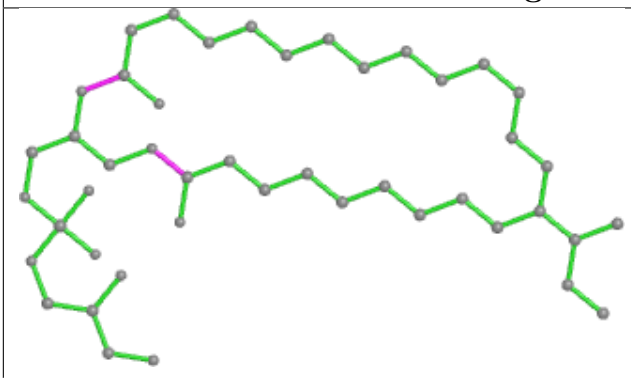


Torsions

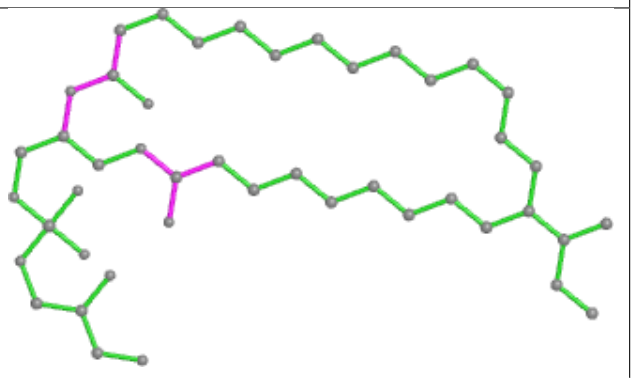


Rings

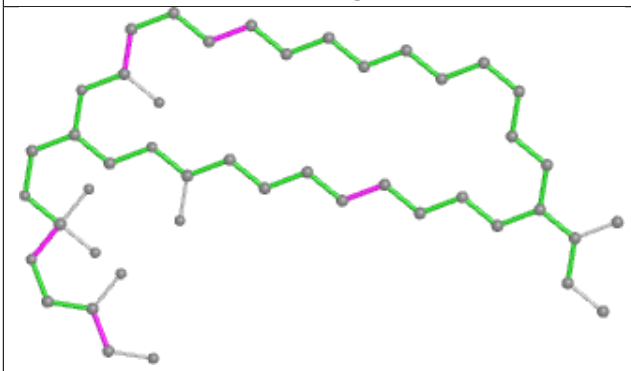
Ligand PGV h 801



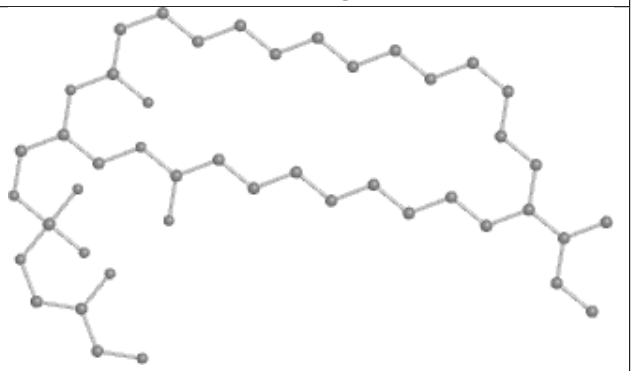
Bond lengths



Bond angles

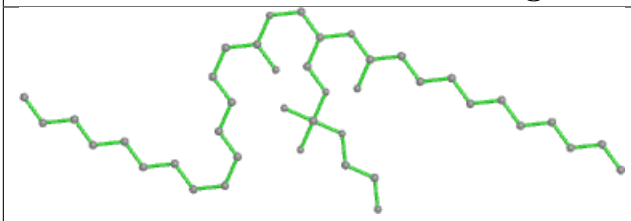


Torsions

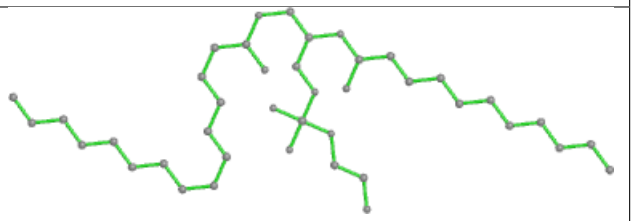


Rings

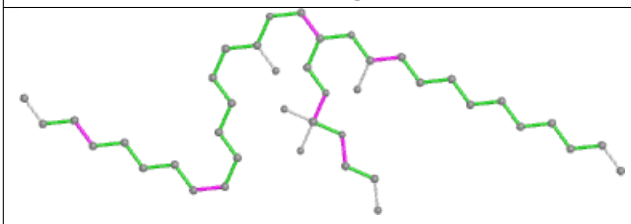
Ligand PTY F 501



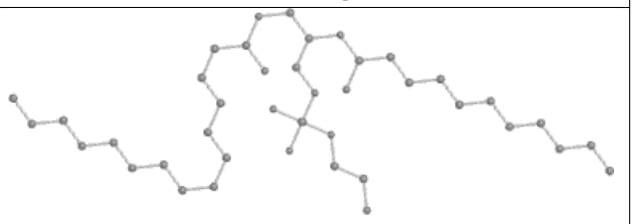
Bond lengths



Bond angles

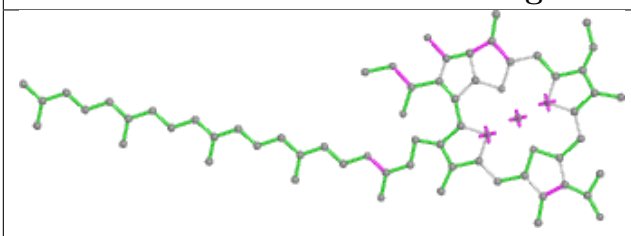


Torsions

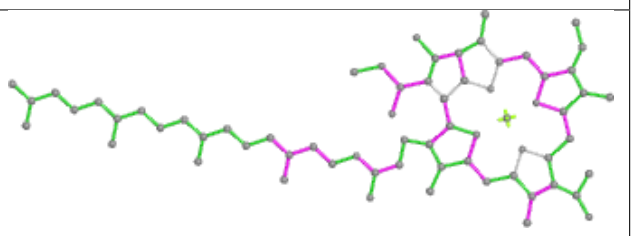


Rings

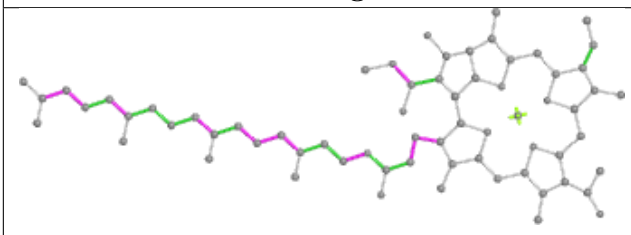
Ligand BCL B 102



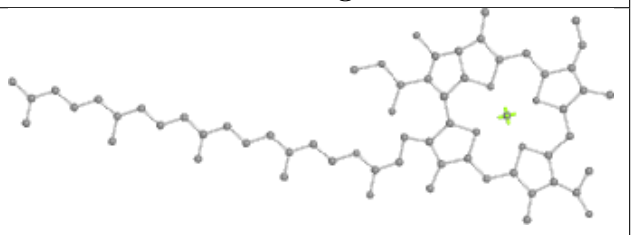
Bond lengths



Bond angles

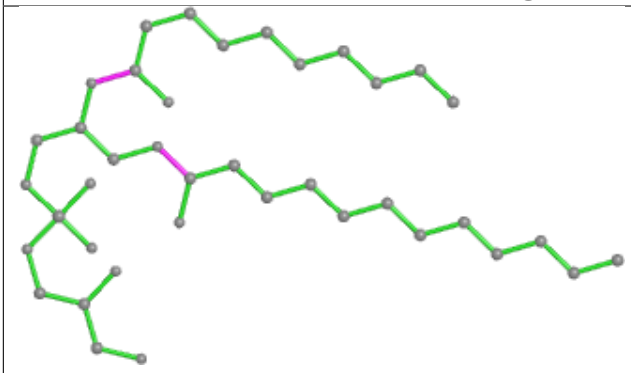


Torsions

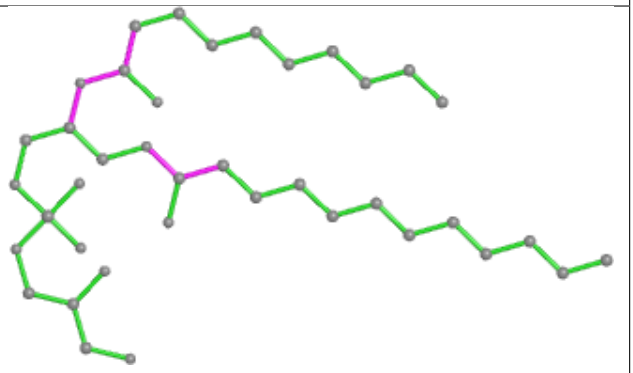


Rings

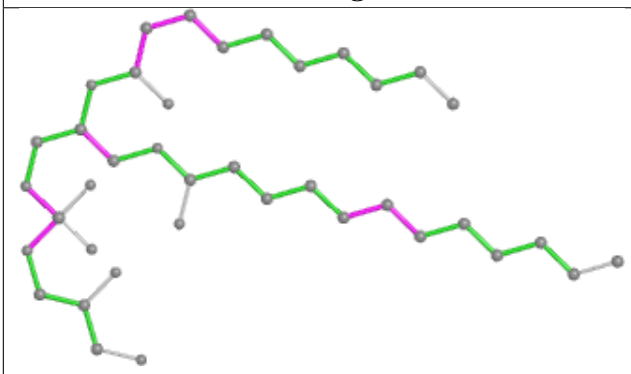
Ligand PGV m 412



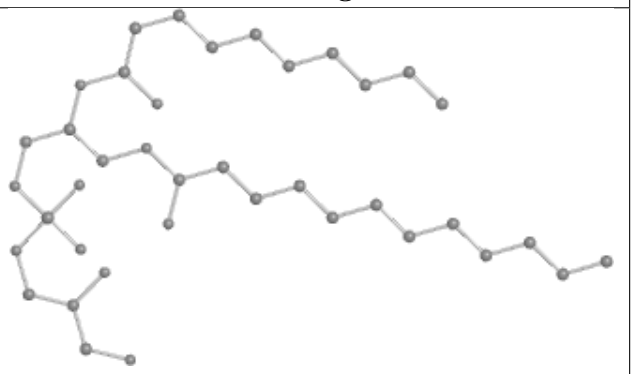
Bond lengths



Bond angles

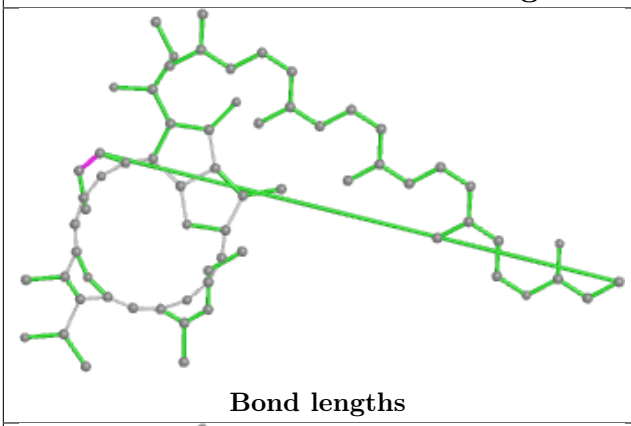


Torsions

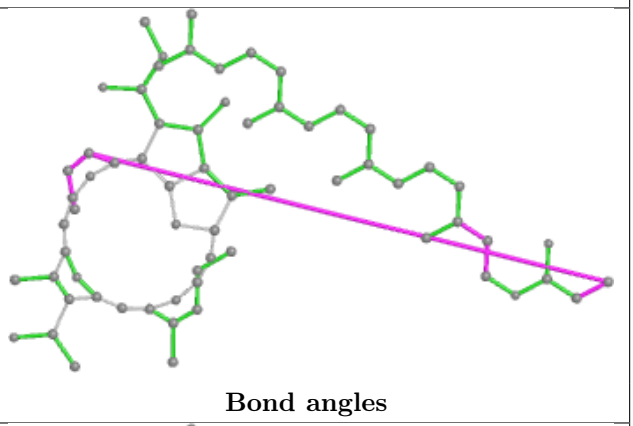


Rings

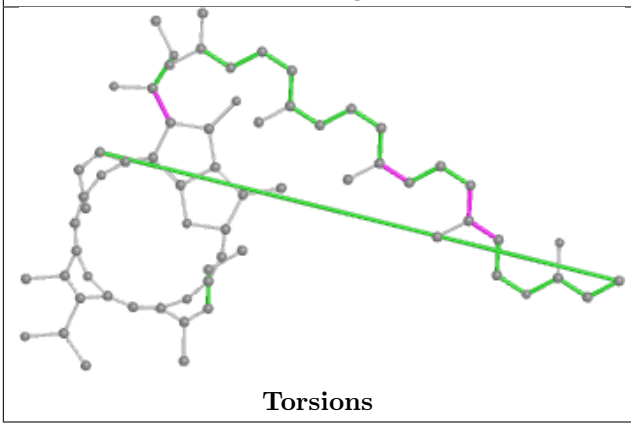
Ligand BPH m 404



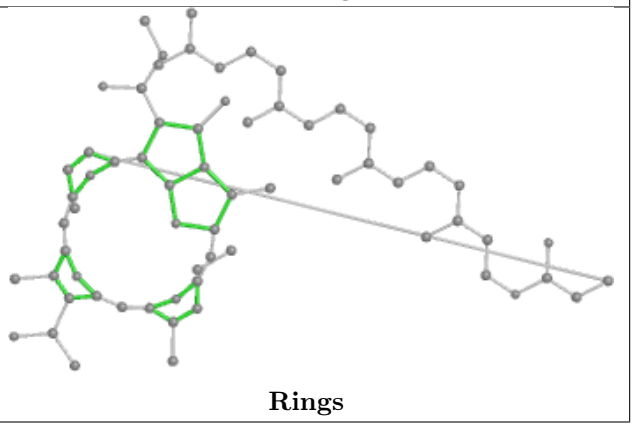
Bond lengths



Bond angles

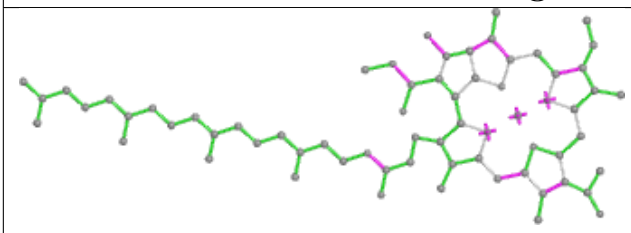


Torsions

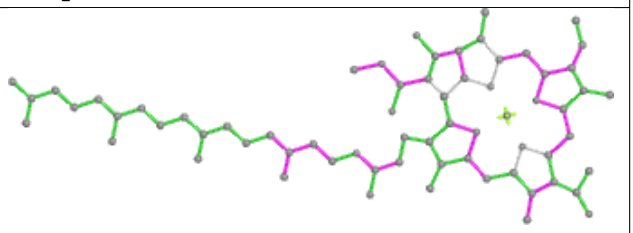


Rings

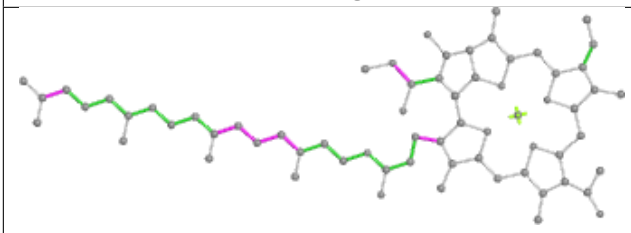
Ligand BCL q 103



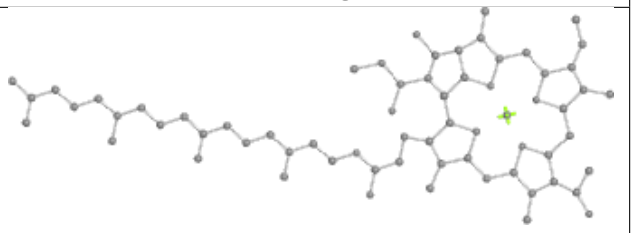
Bond lengths



Bond angles

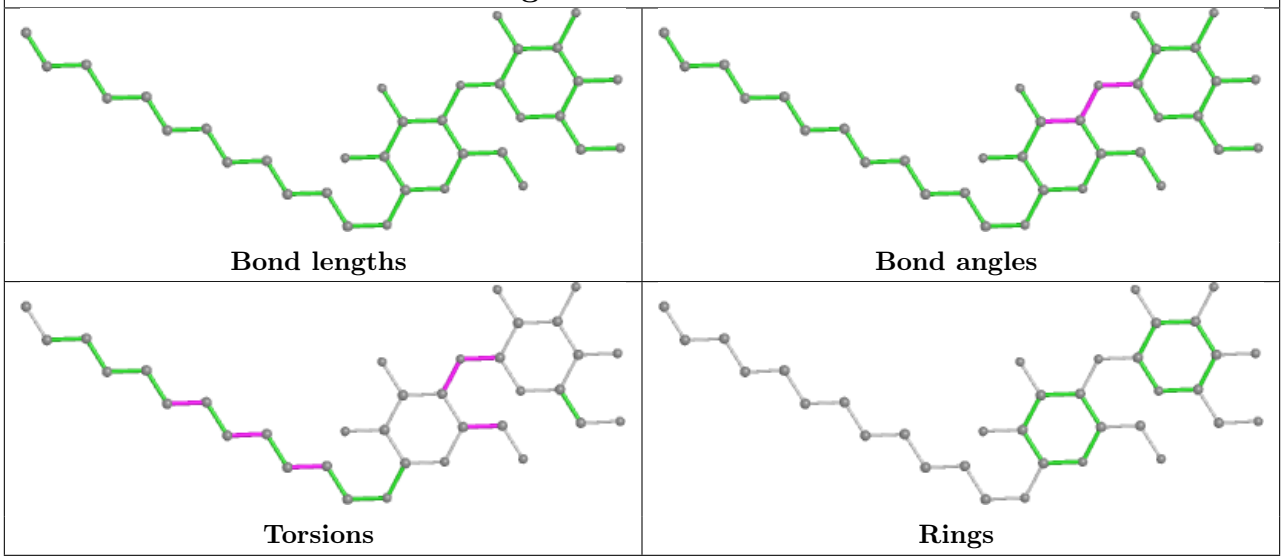


Torsions

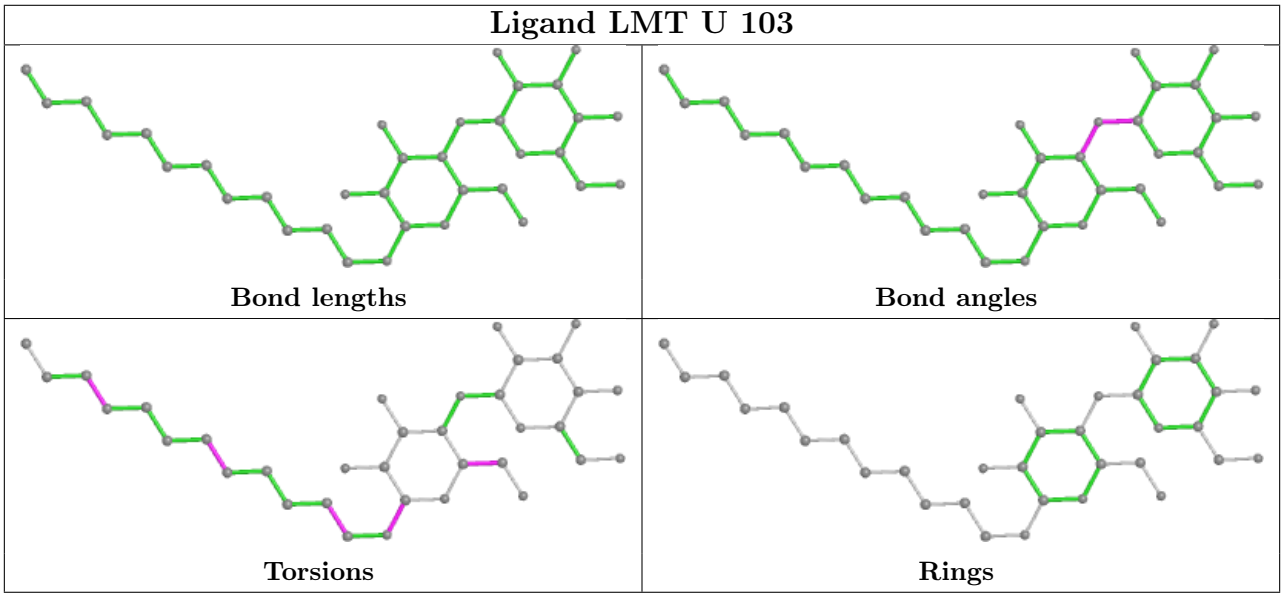


Rings

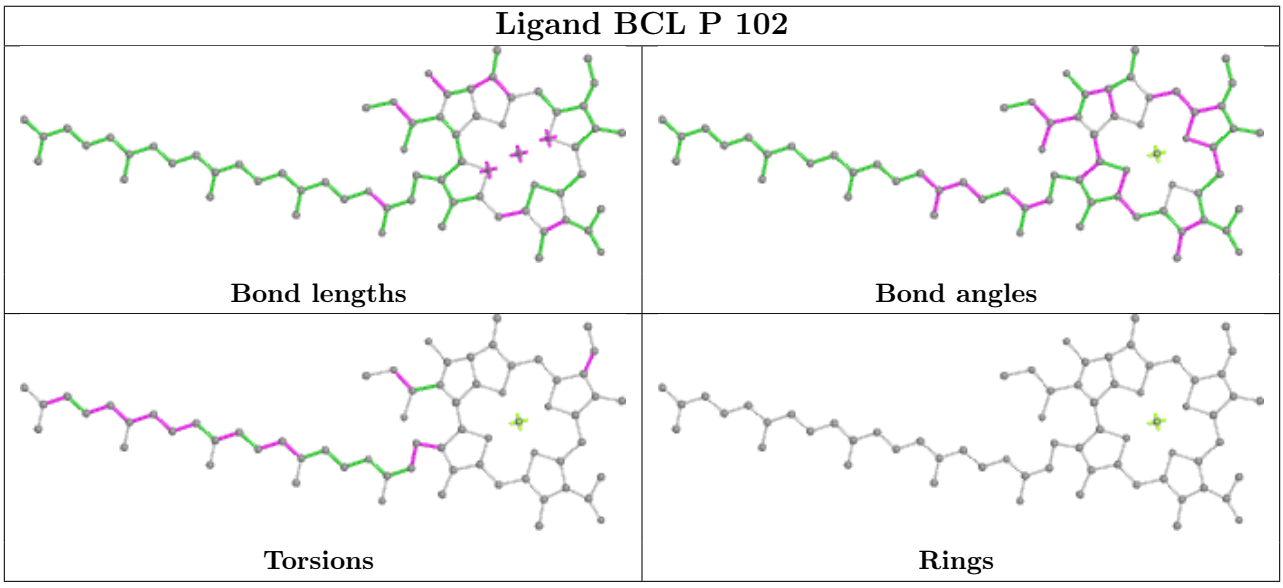
Ligand LMT U 102



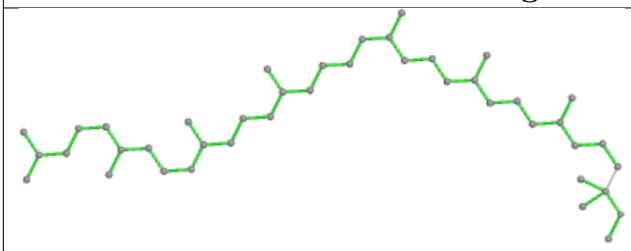
Ligand LMT U 103



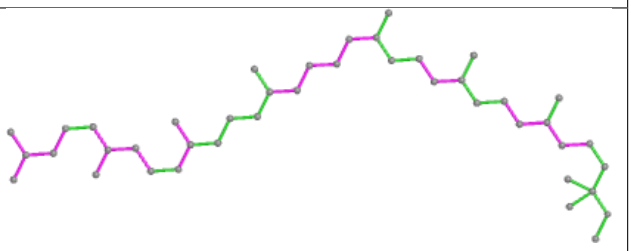
Ligand BCL P 102



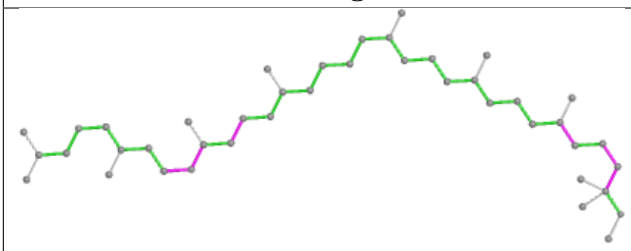
Ligand SPO 01 102



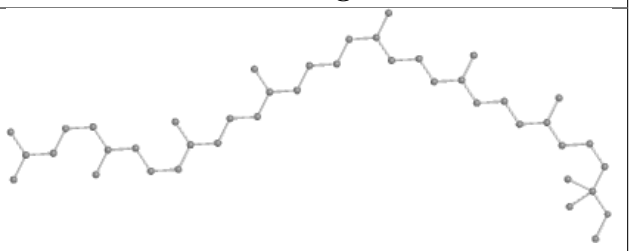
Bond lengths



Bond angles

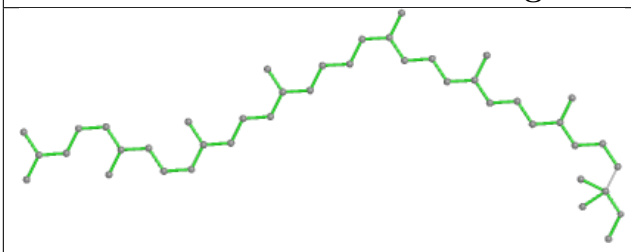


Torsions

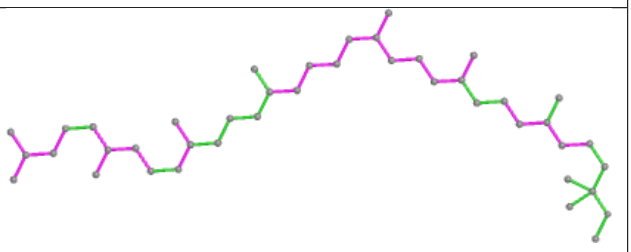


Rings

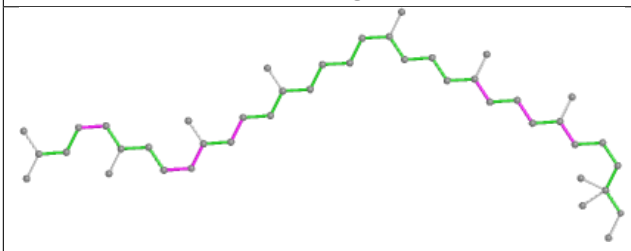
Ligand SPO G 103



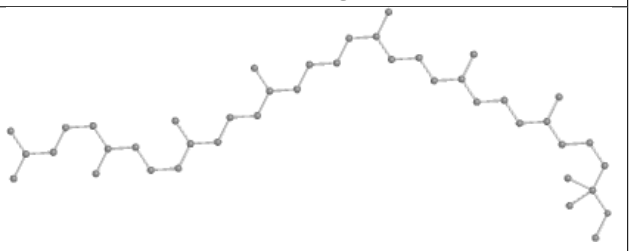
Bond lengths



Bond angles

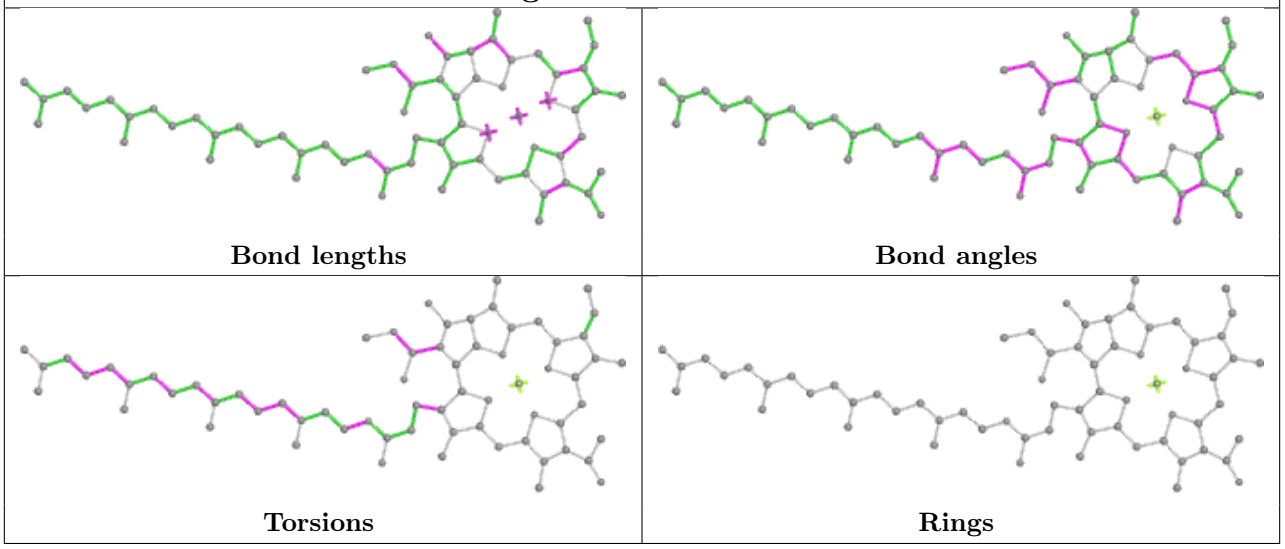


Torsions

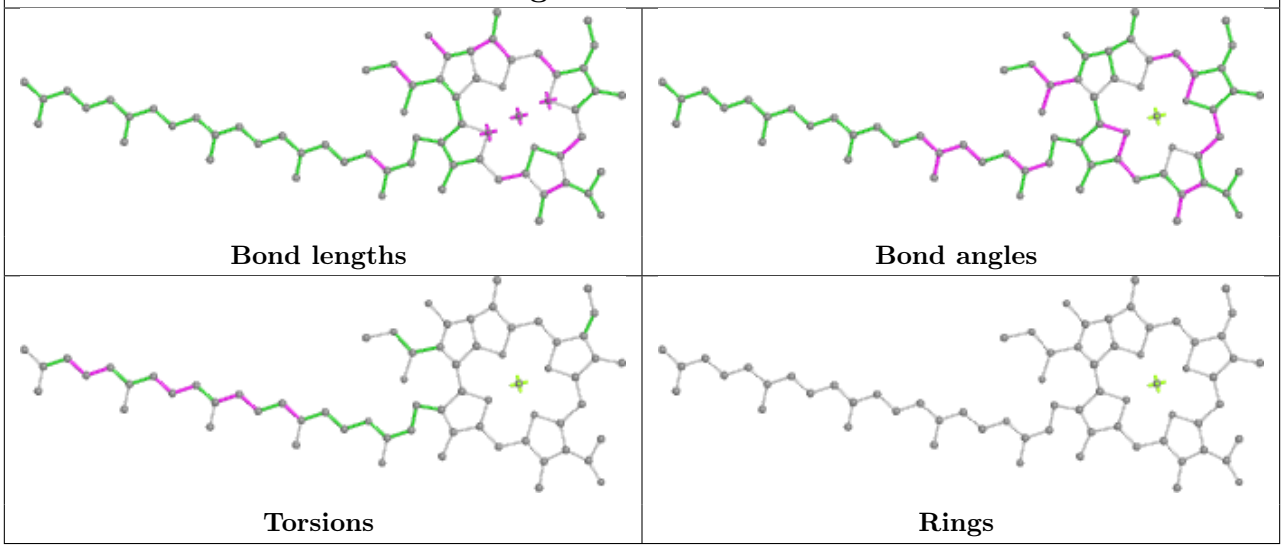


Rings

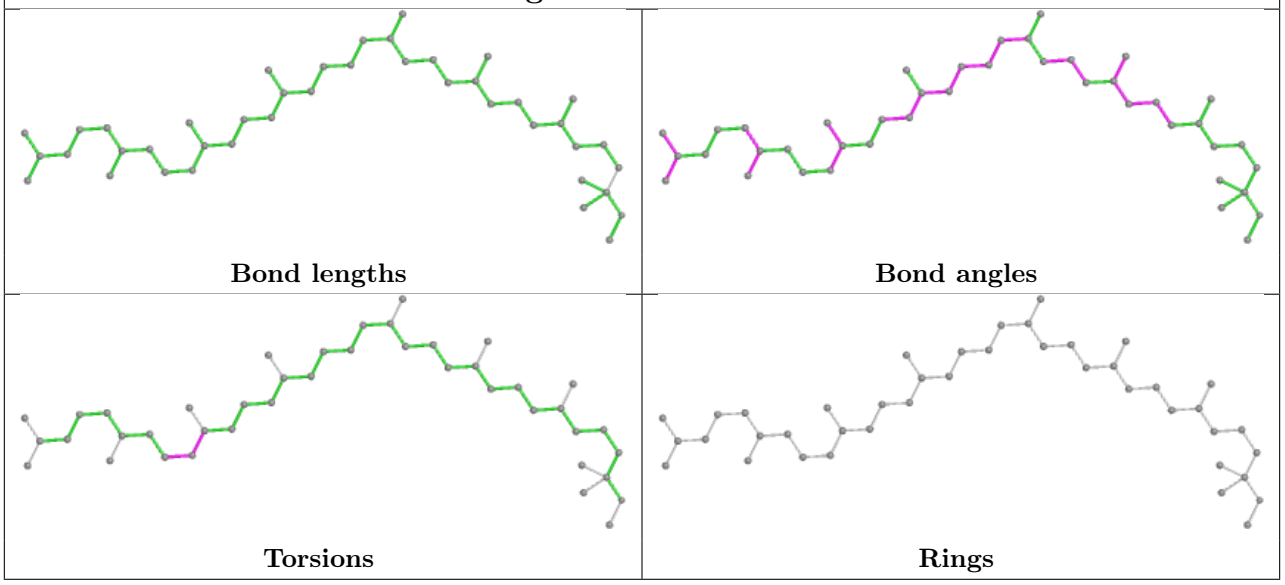
Ligand BCL M 402



Ligand BCL 7 101



Ligand SPO K 404



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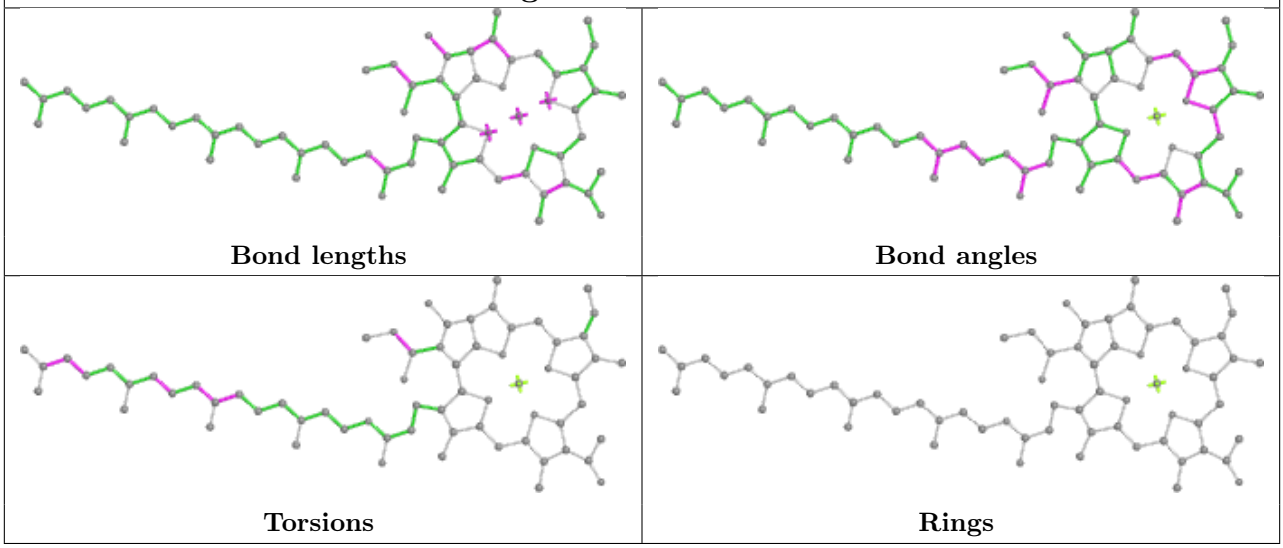
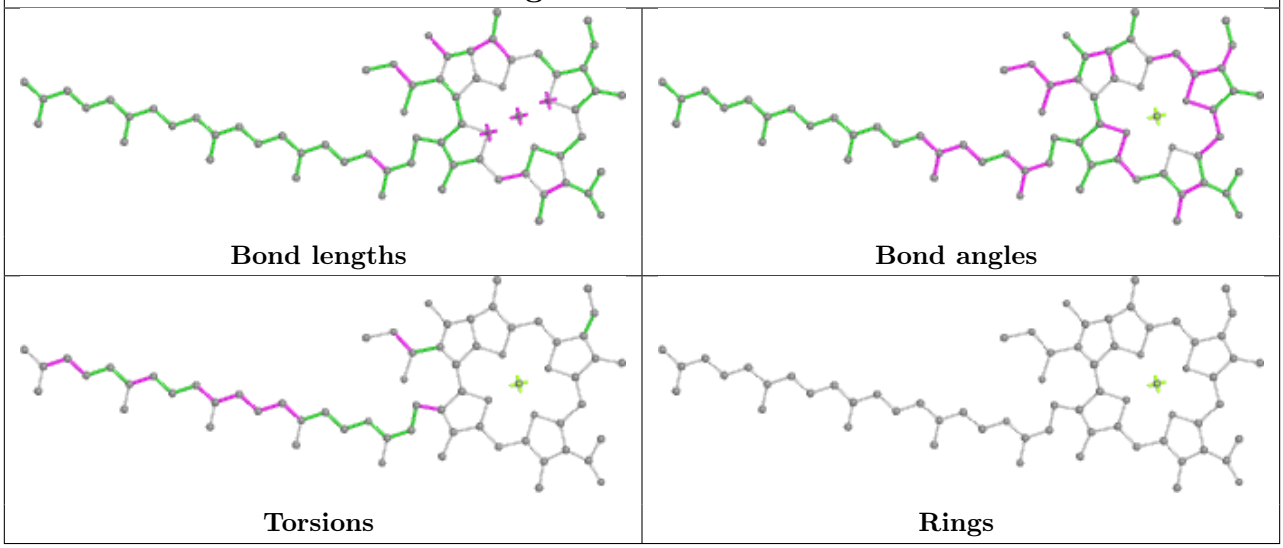


Ligand BCL Y 102



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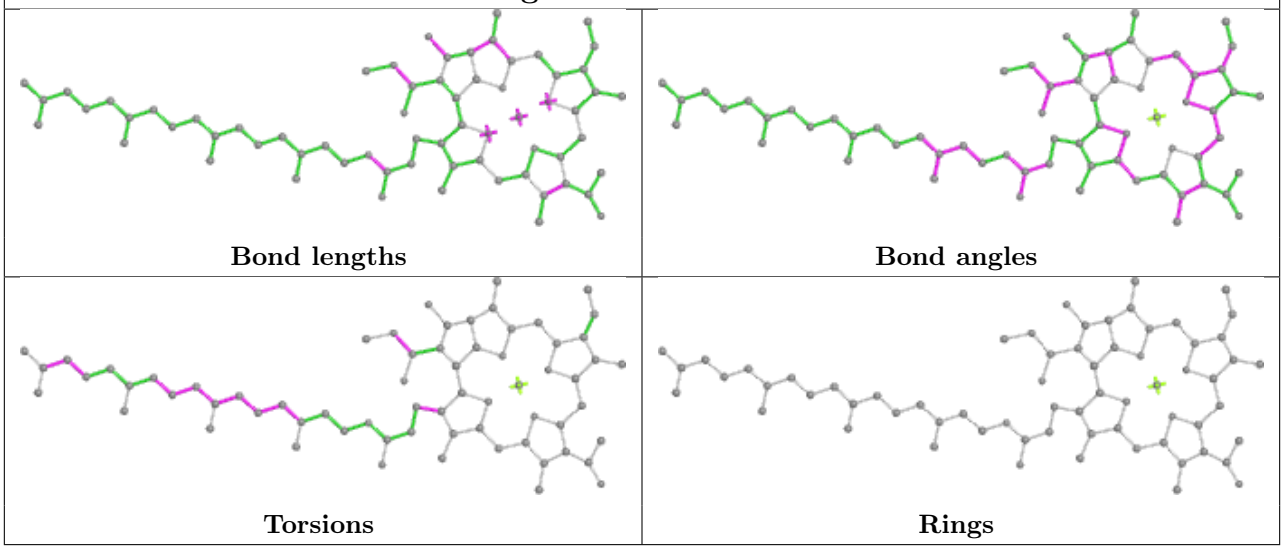
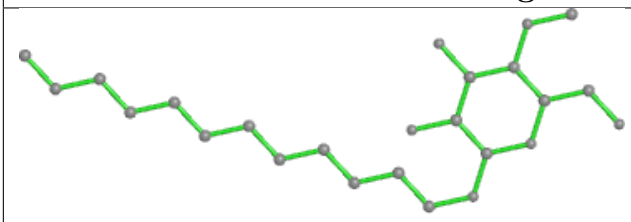
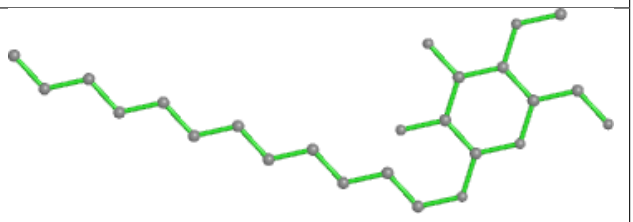


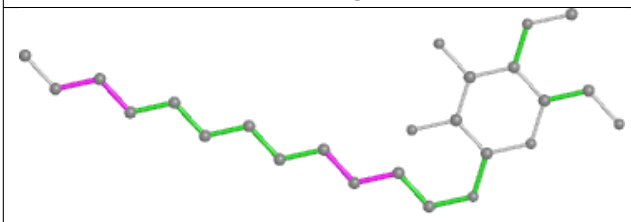
Ligand LMT M 408



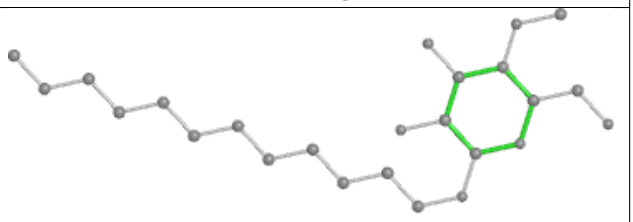
Bond lengths



Bond angles

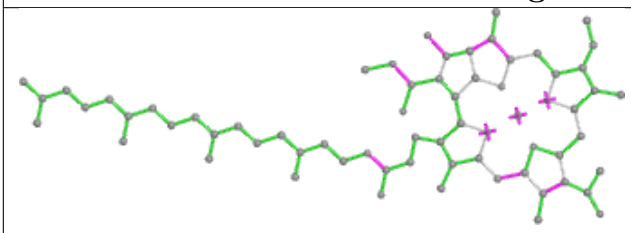


Torsions

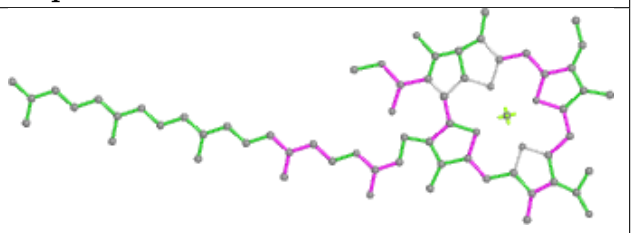


Rings

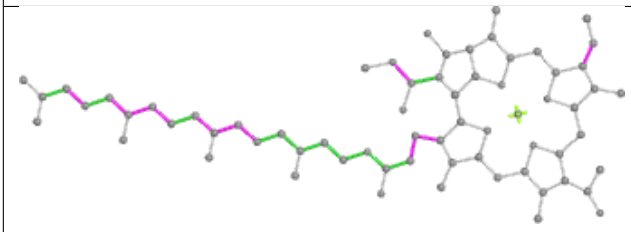
Ligand BCL p 102



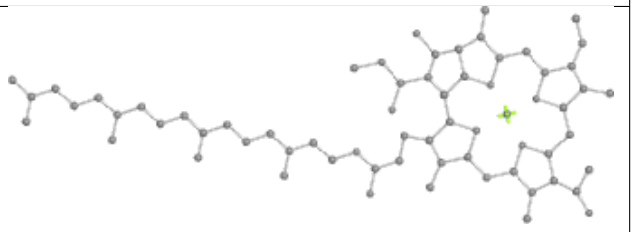
Bond lengths



Bond angles

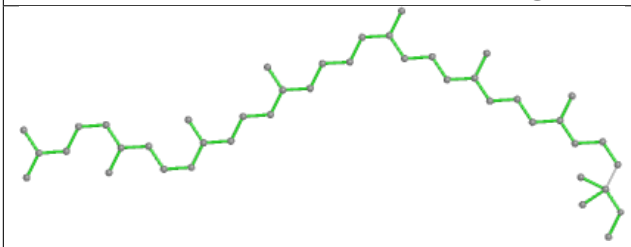


Torsions

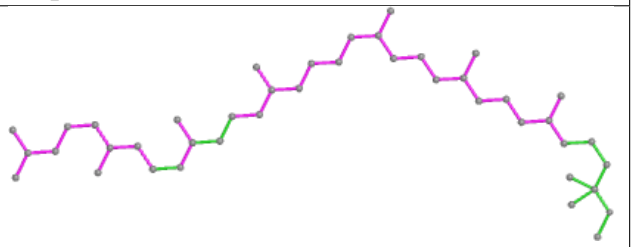


Rings

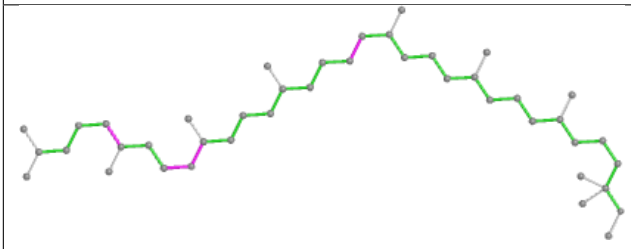
Ligand SPO p 101



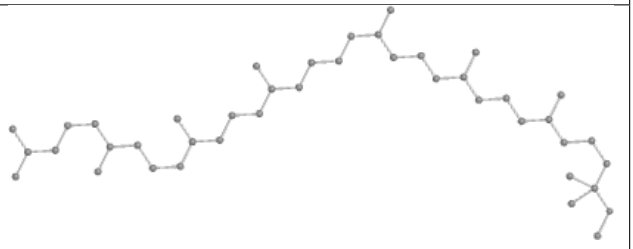
Bond lengths



Bond angles

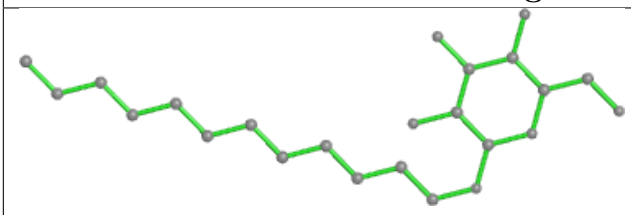


Torsions

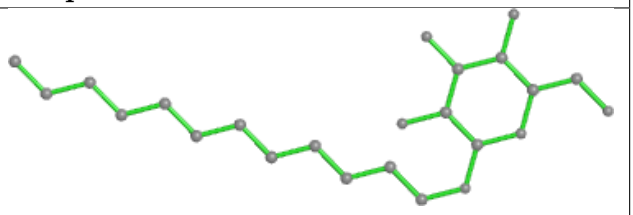


Rings

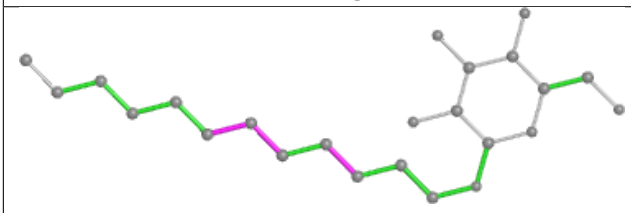
Ligand LMT q 101



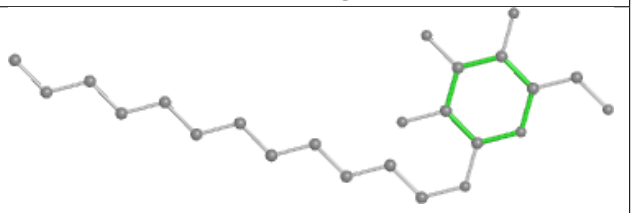
Bond lengths



Bond angles

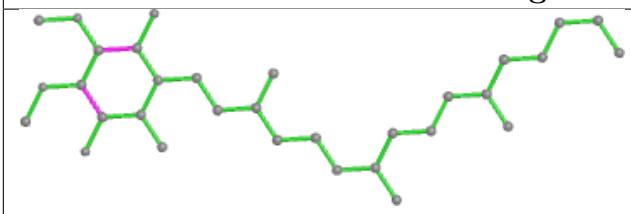


Torsions

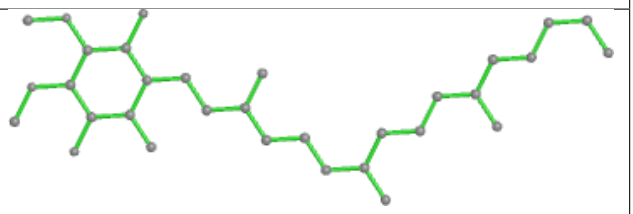


Rings

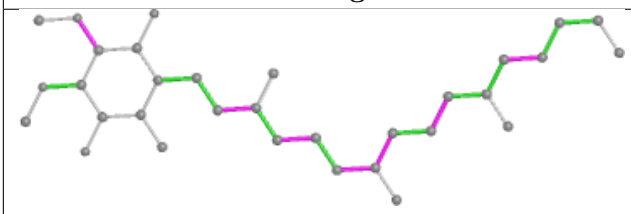
Ligand U10 D 102



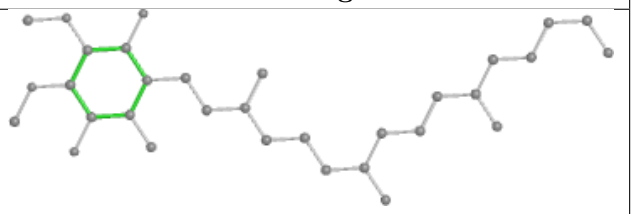
Bond lengths



Bond angles

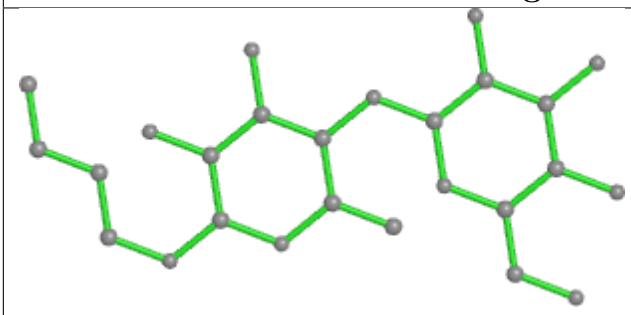


Torsions

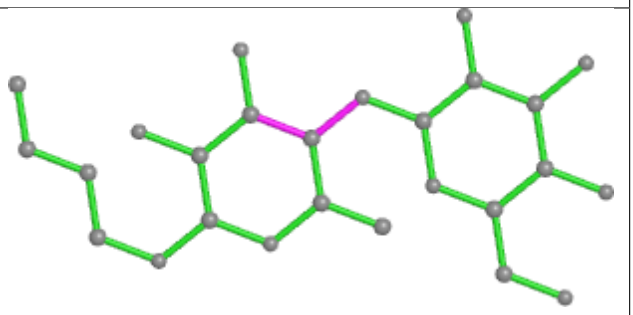


Rings

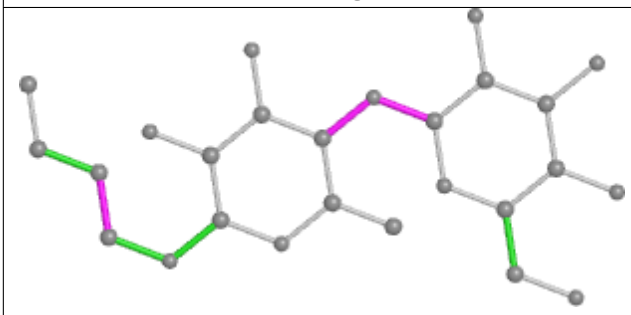
Ligand LMT L 306



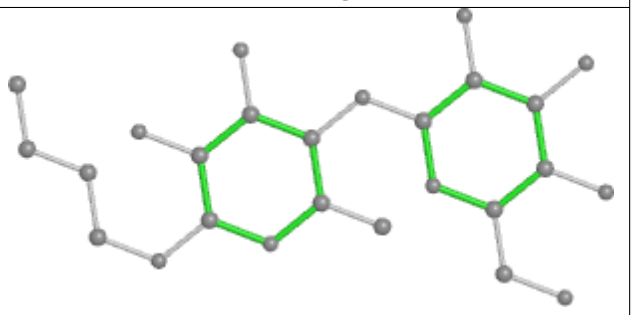
Bond lengths



Bond angles

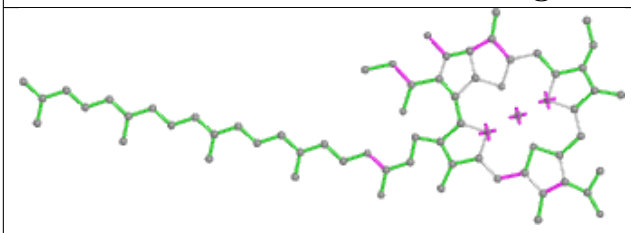


Torsions

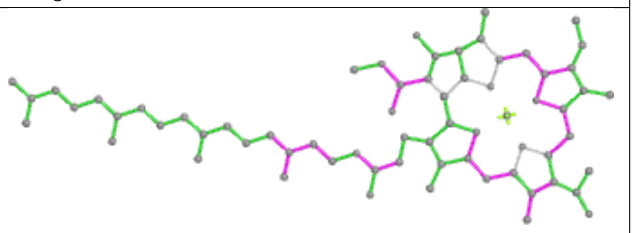


Rings

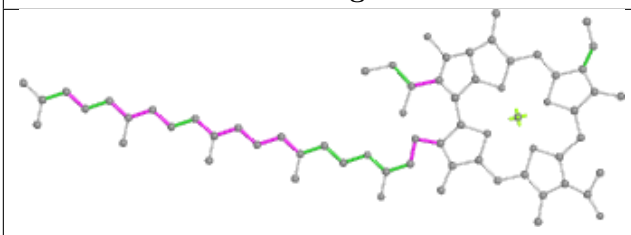
Ligand BCL j 102



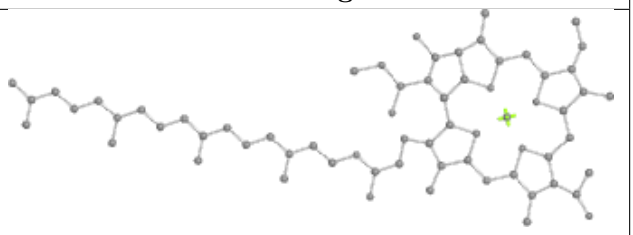
Bond lengths



Bond angles

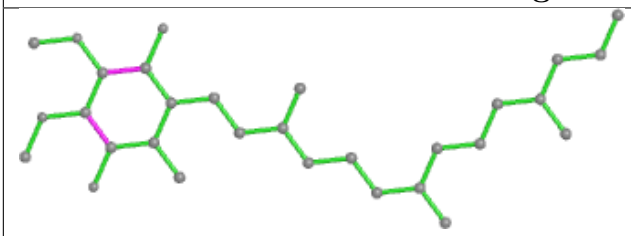


Torsions

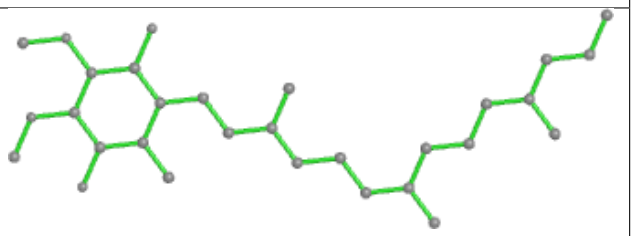


Rings

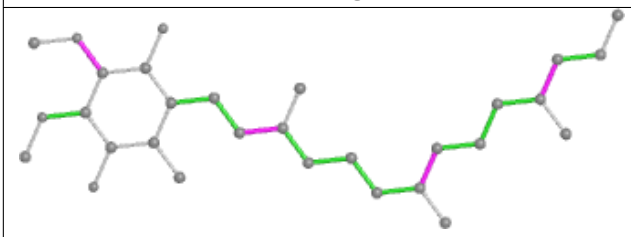
Ligand U10 d 102



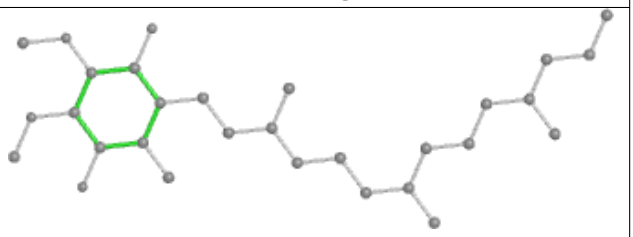
Bond lengths



Bond angles

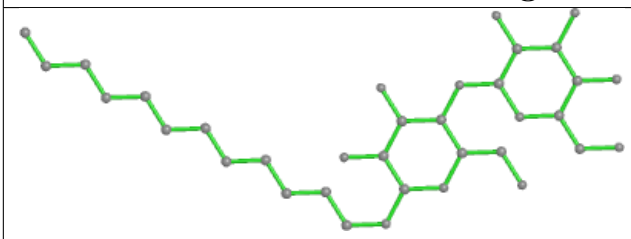


Torsions

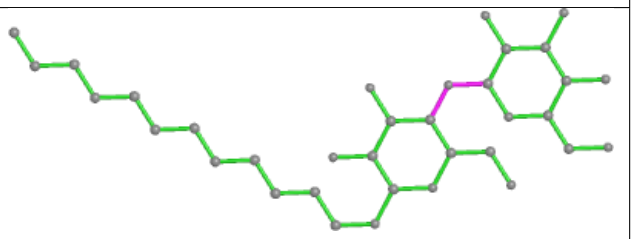


Rings

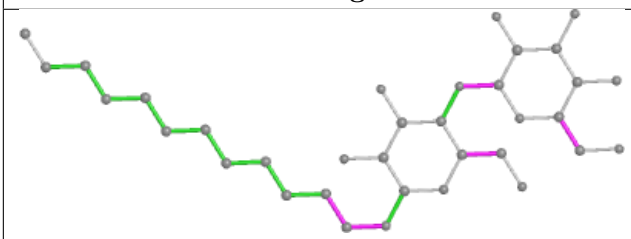
Ligand LMT m 408



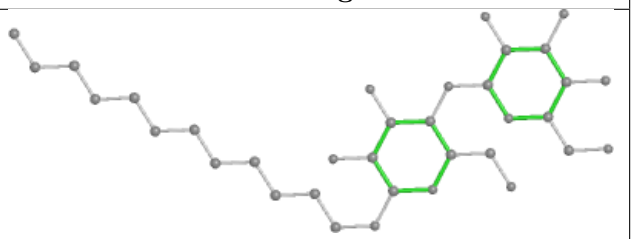
Bond lengths



Bond angles

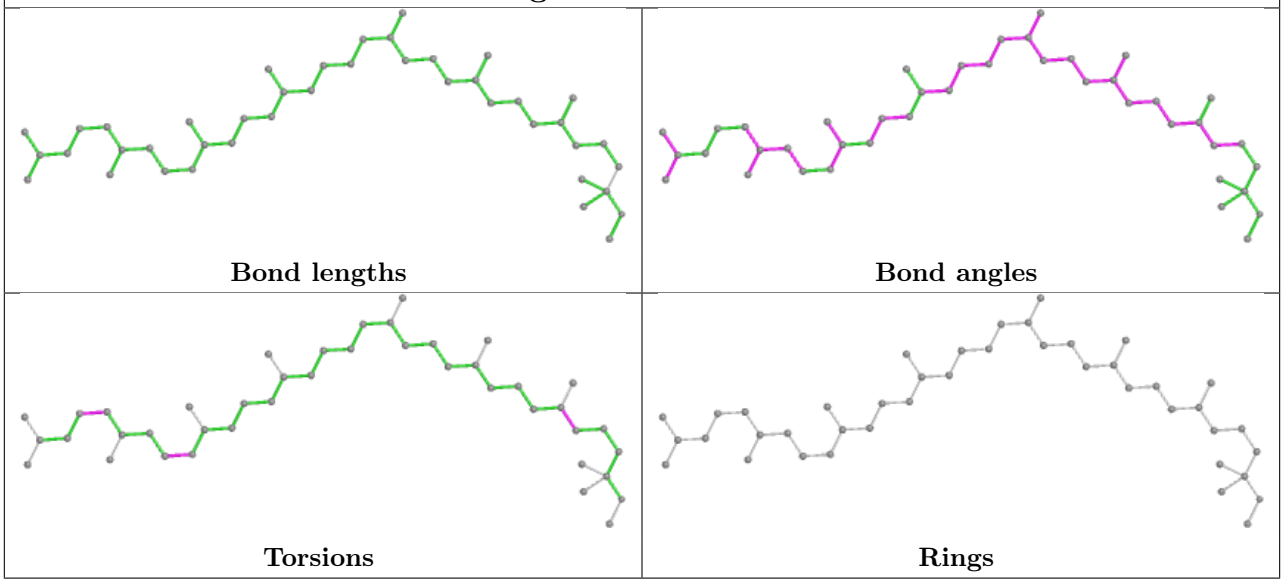


Torsions

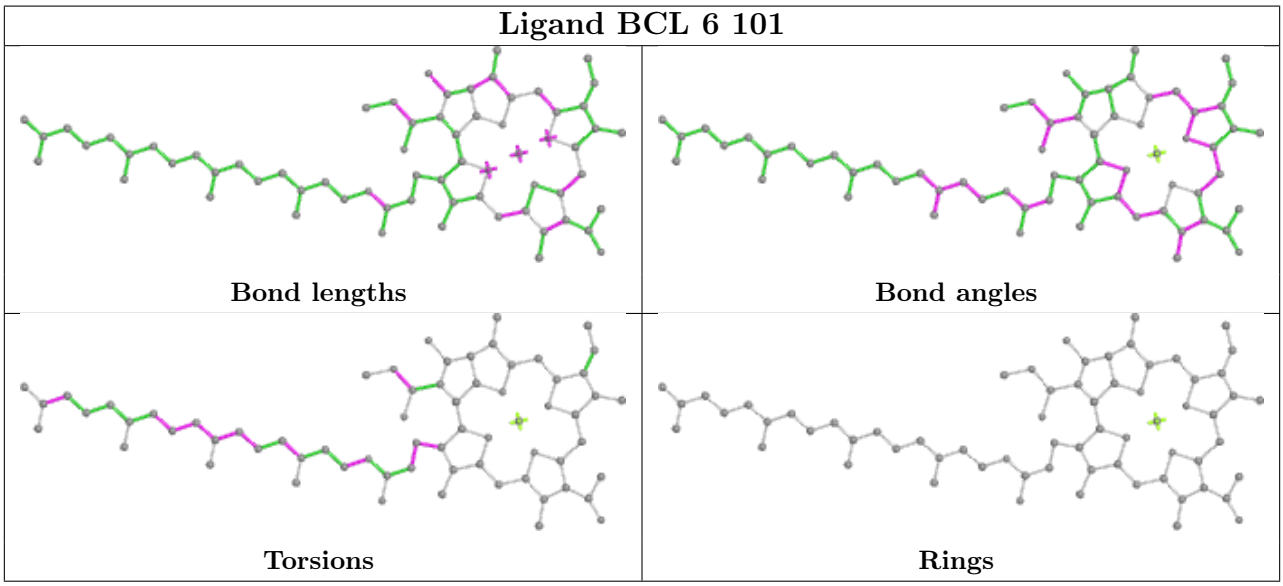


Rings

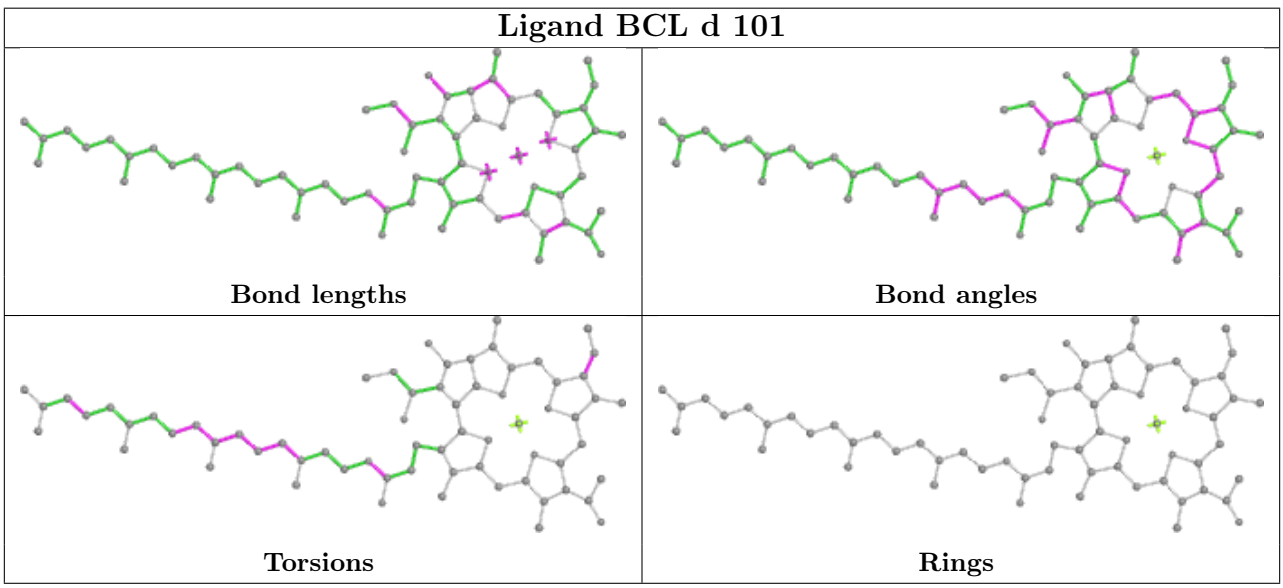
Ligand SPO S 102



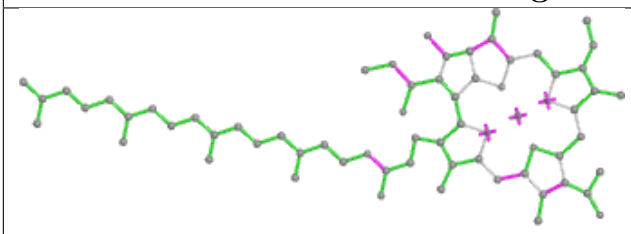
Ligand BCL 6 101



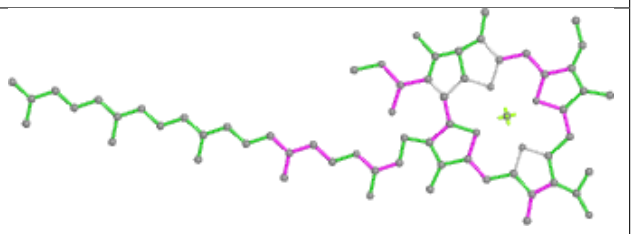
Ligand BCL d 101



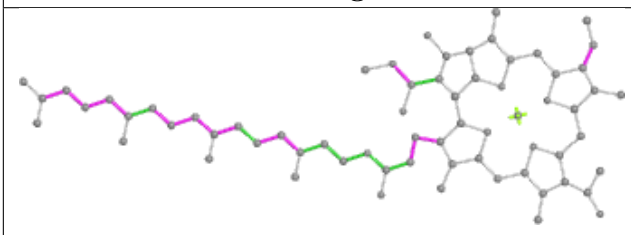
Ligand BCL t 101



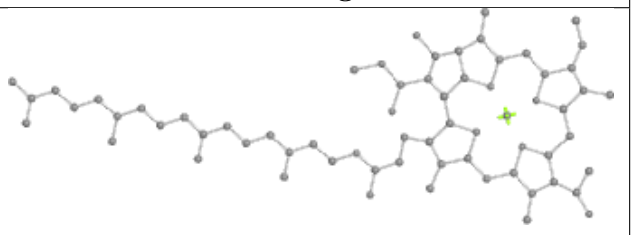
Bond lengths



Bond angles

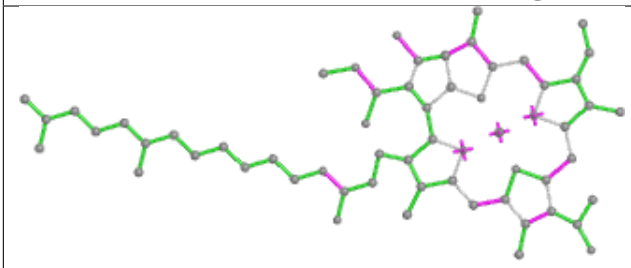


Torsions

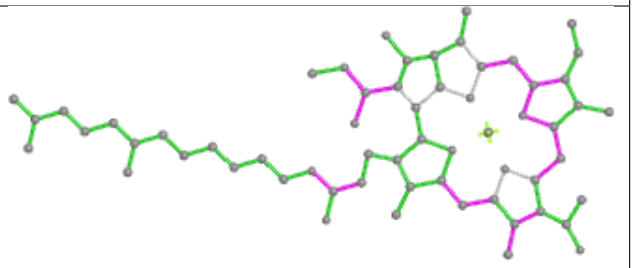


Rings

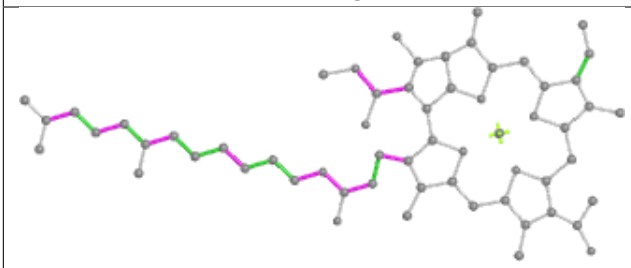
Ligand BCL 8 101



Bond lengths



Bond angles



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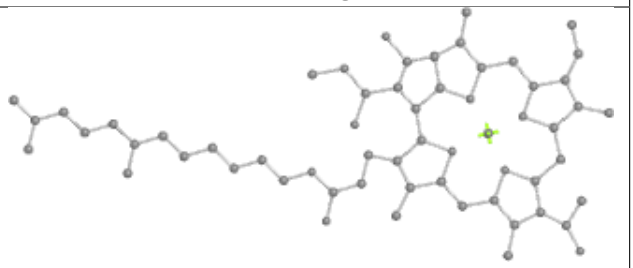
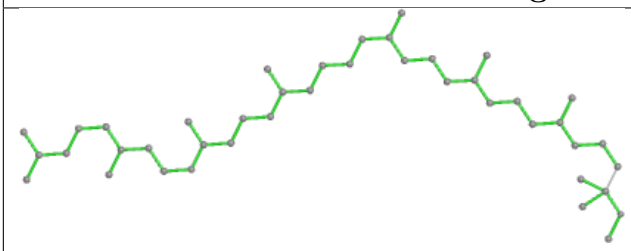
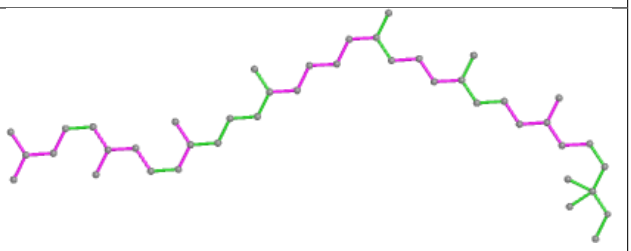


Rings

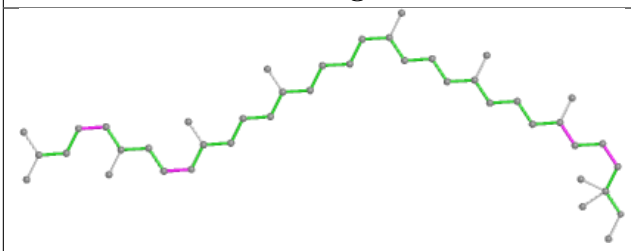
Ligand SPO 4 102



Bond lengths



Bond angles



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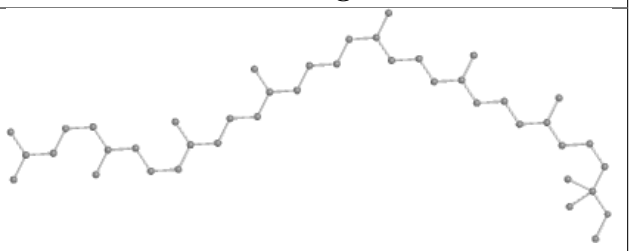
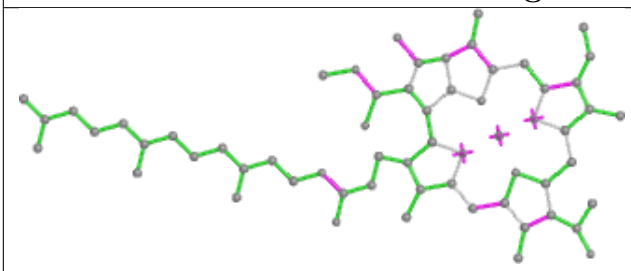
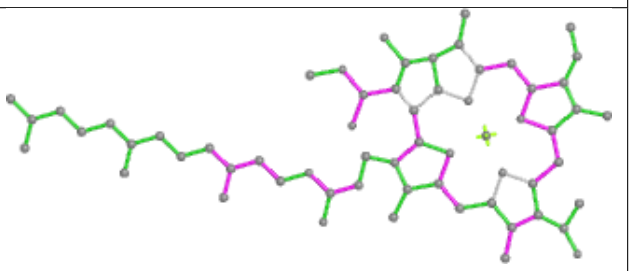


Rings

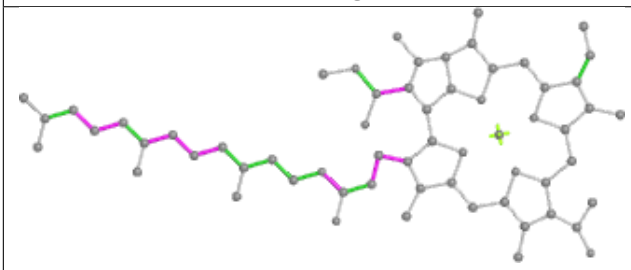
Ligand BCL A 702



Bond lengths



Bond angles



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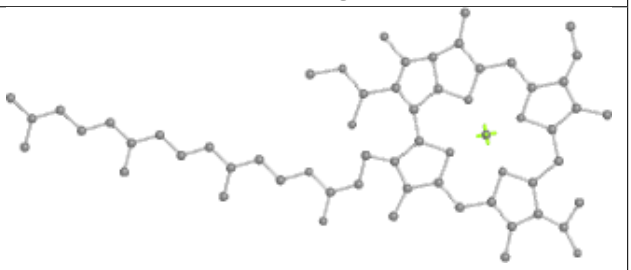
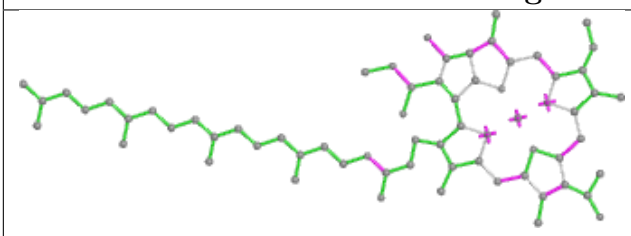
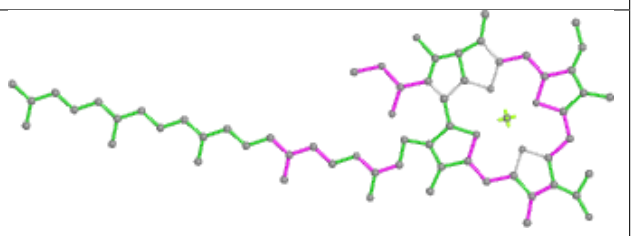


Rings

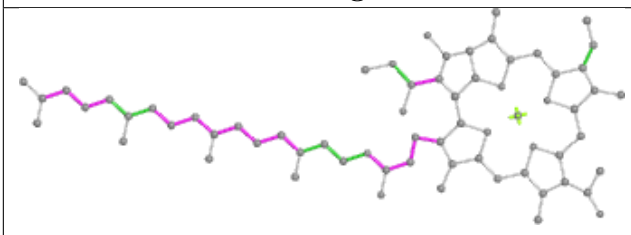
Ligand BCL R 102



Bond lengths



Bond angles



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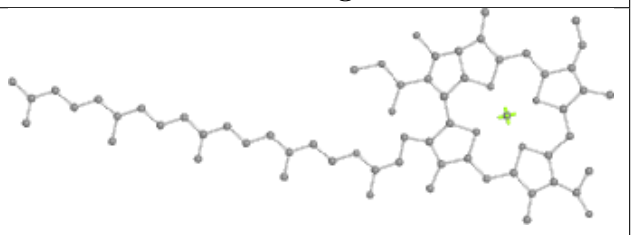
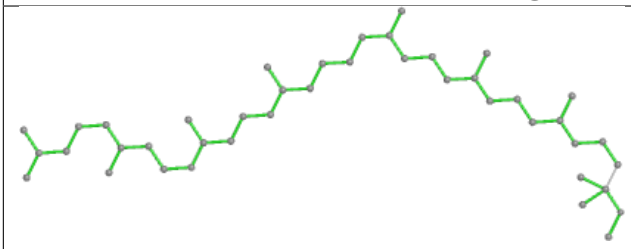


Rings

Ligand SPO B 103



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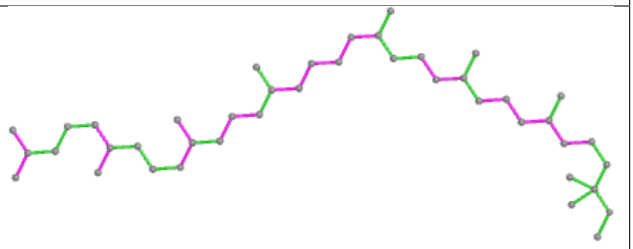
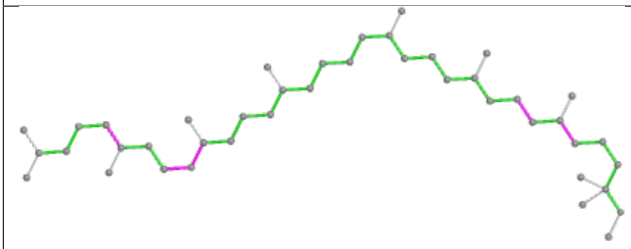


Bond angles



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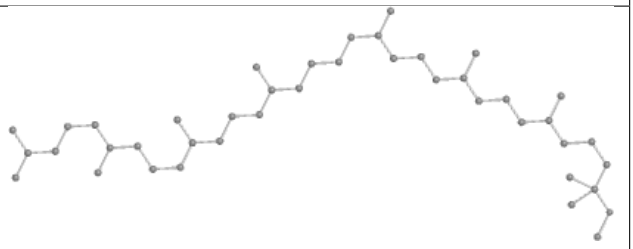
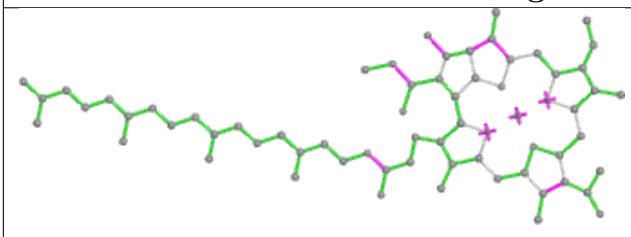
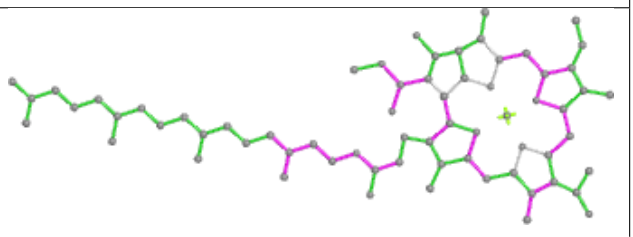


Rings

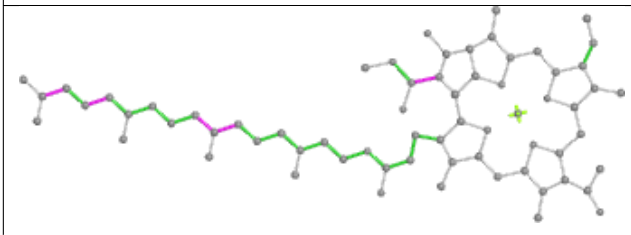
Ligand BCL L 311



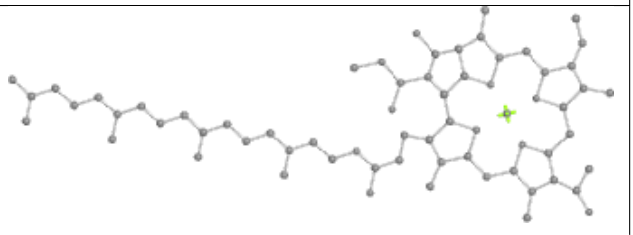
Bond lengths



Bond angles

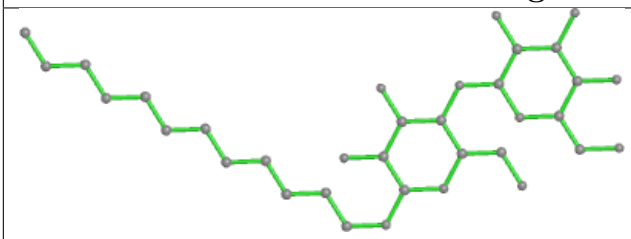


Torsions

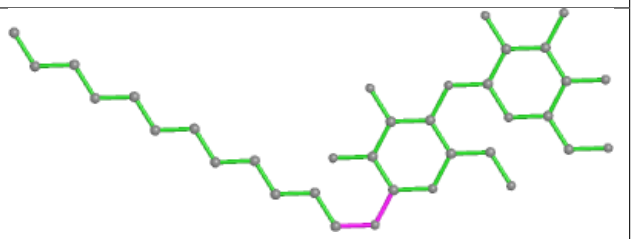


Rings

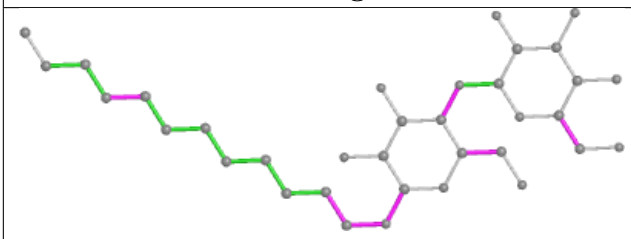
Ligand LMT I 101



Bond lengths



Bond angles



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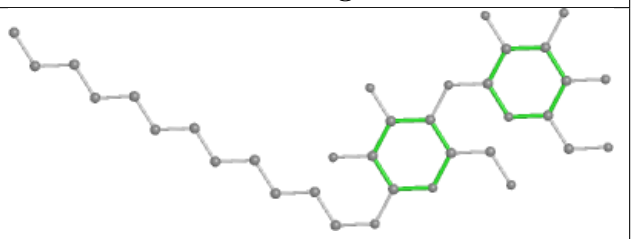
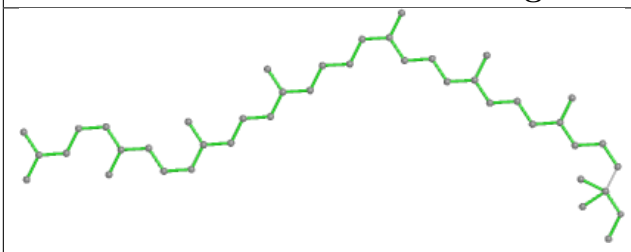


Rings

Ligand SPO N 101



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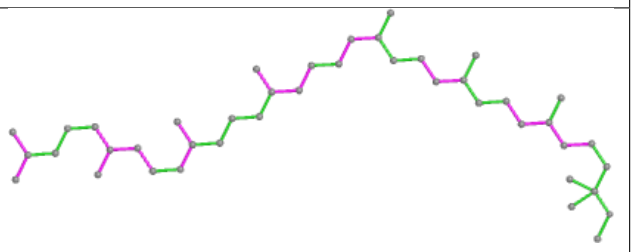
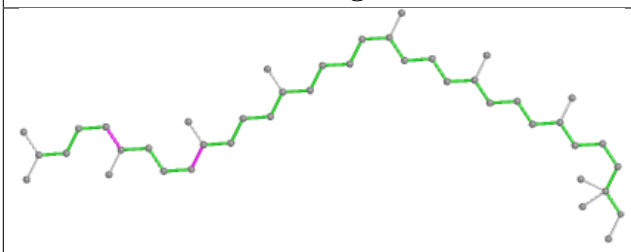


Bond angles



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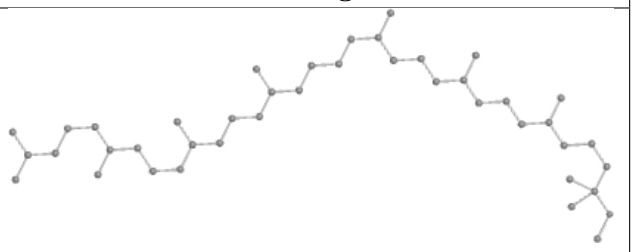
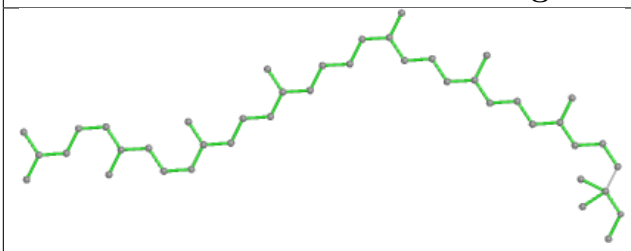


Rings

Ligand SPO r 101



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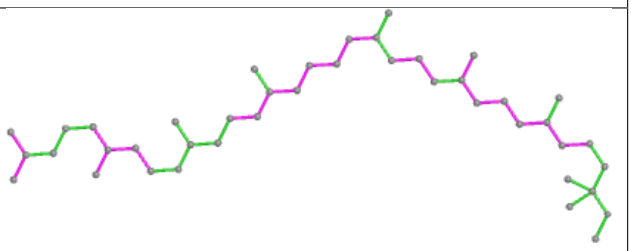
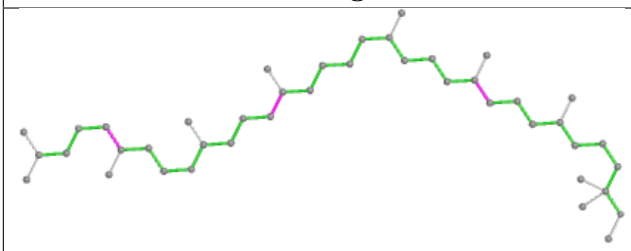


Bond angles



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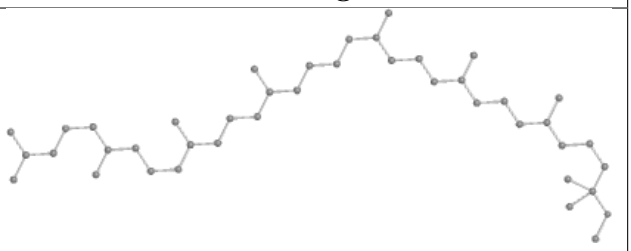
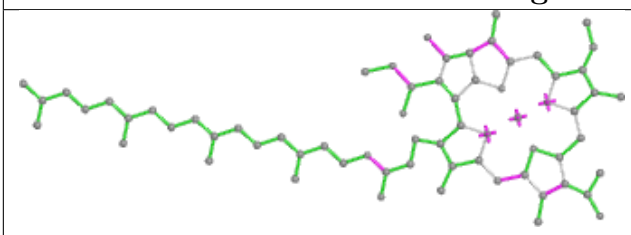
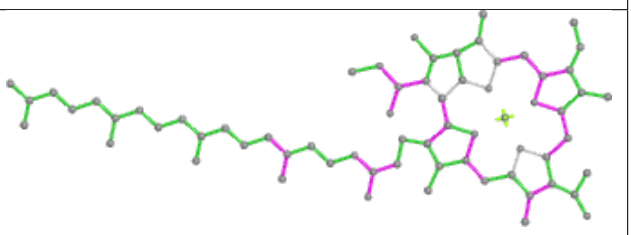


Rings

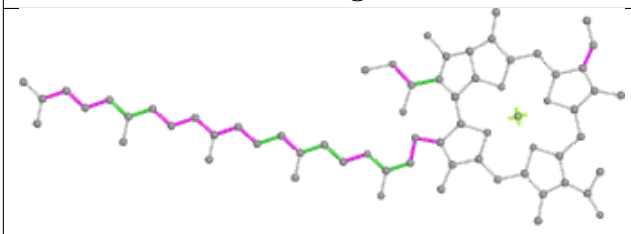
Ligand BCL r 102



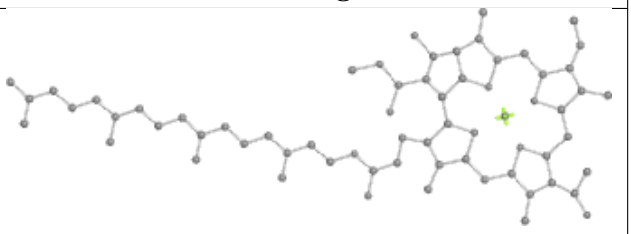
Bond lengths



Bond angles

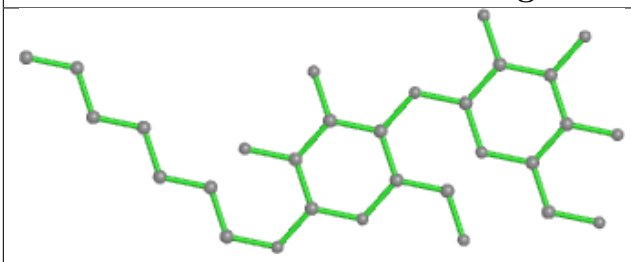


Torsions

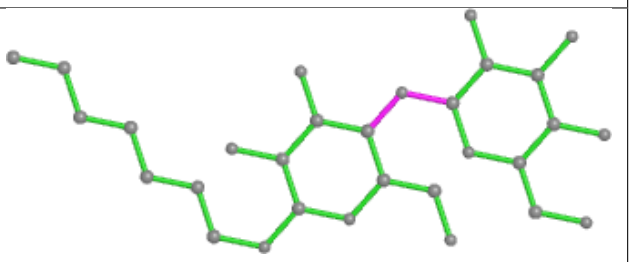


Rings

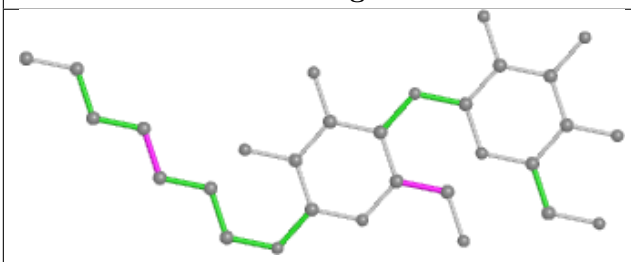
Ligand LMT M 412



Bond lengths



Bond angles



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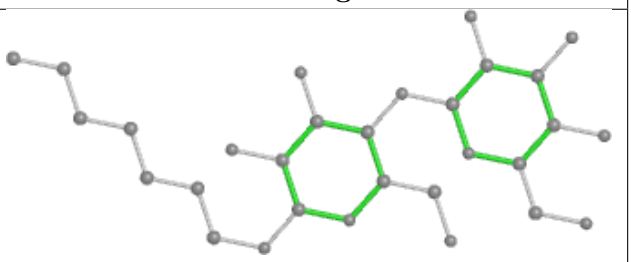
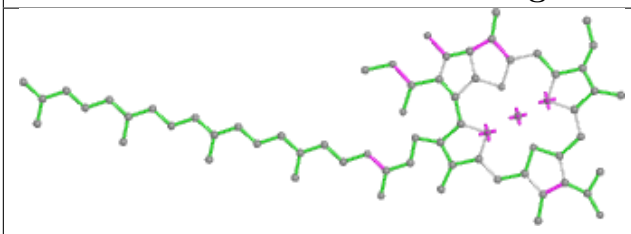
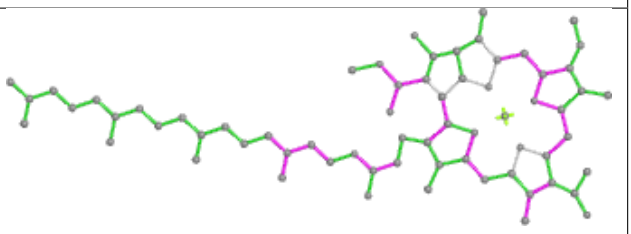


Rings

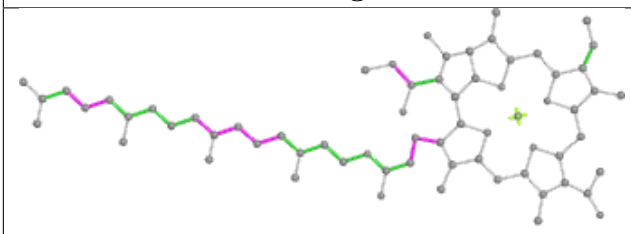
Ligand BCL J 102



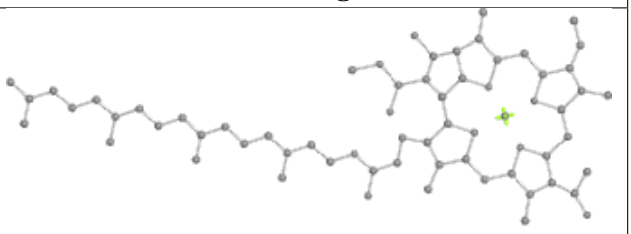
Bond lengths



Bond angles

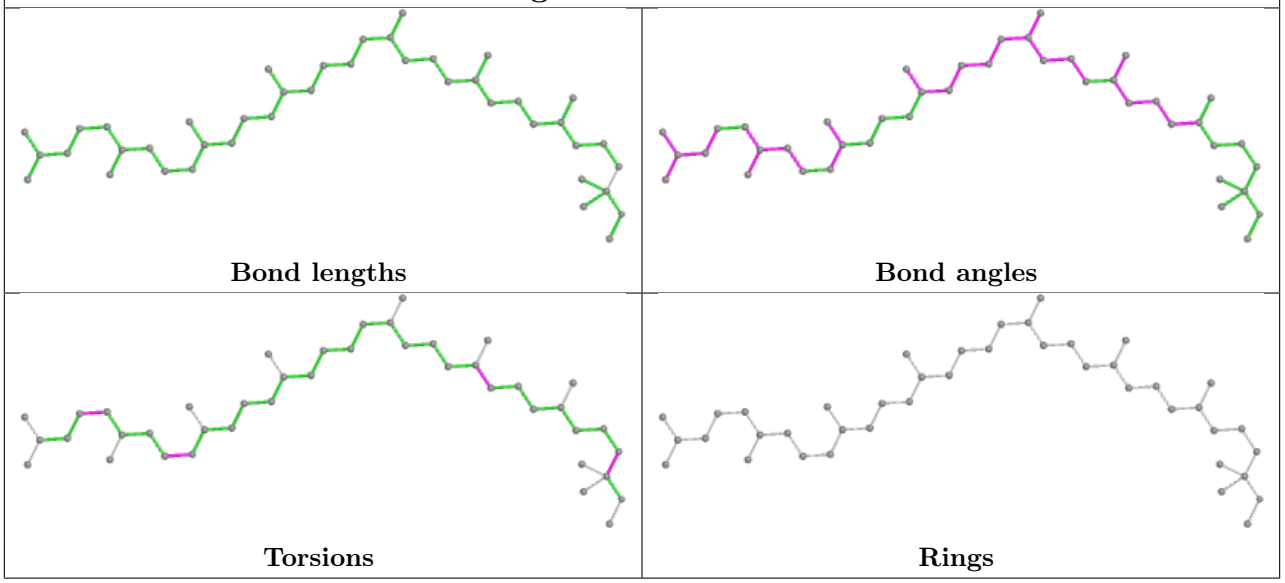


Torsions

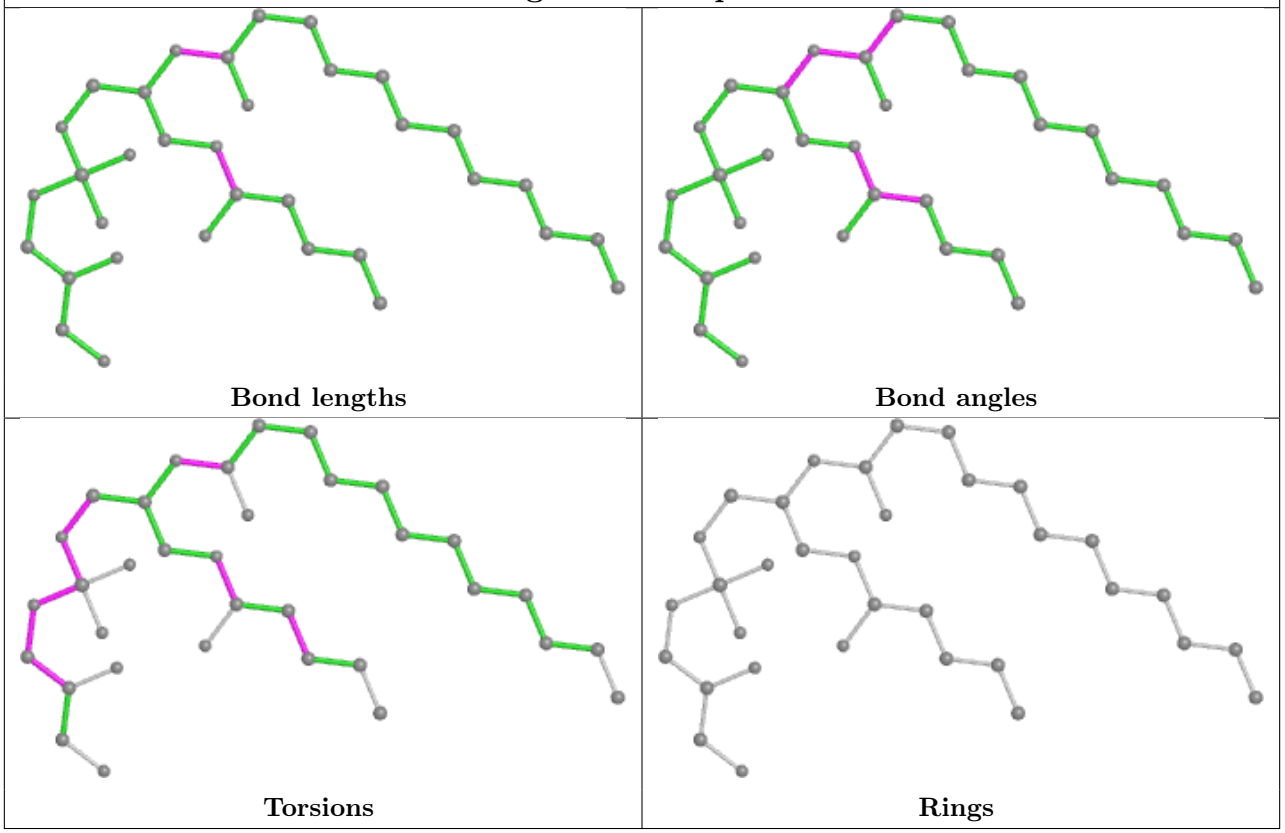


Rings

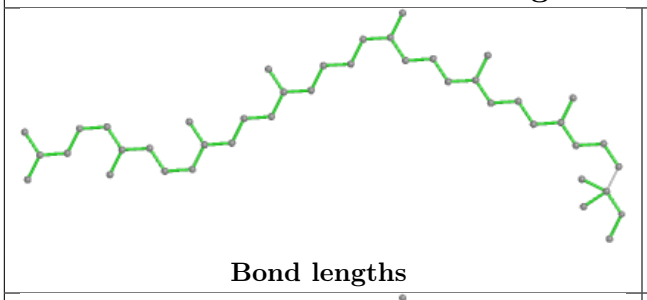
Ligand SPO 5 103



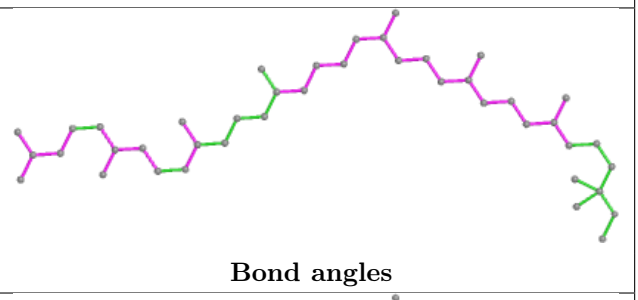
Ligand PGV q 102



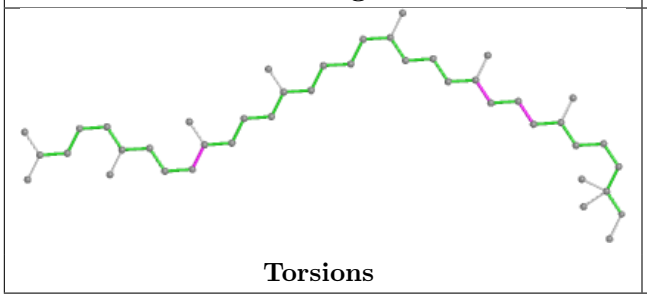
Ligand SPO a 102



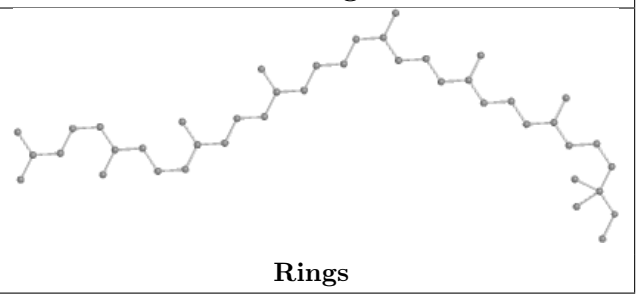
Bond lengths



Bond angles

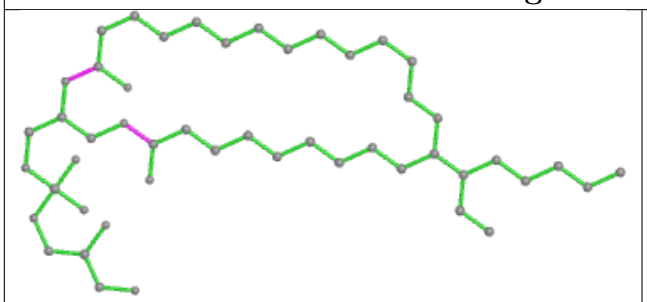


Torsions



Rings

Ligand PGV L 308



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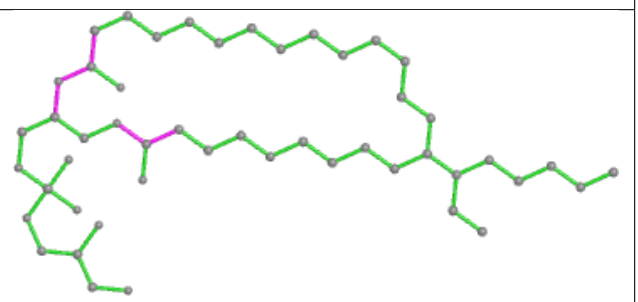
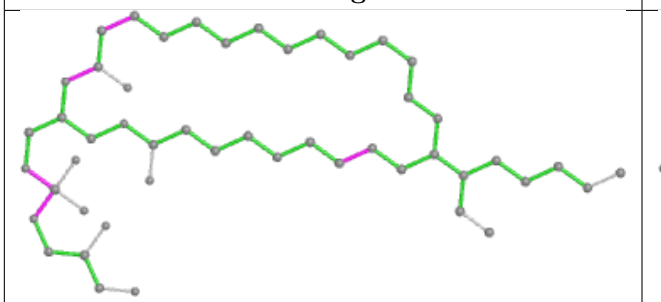


Bond angles



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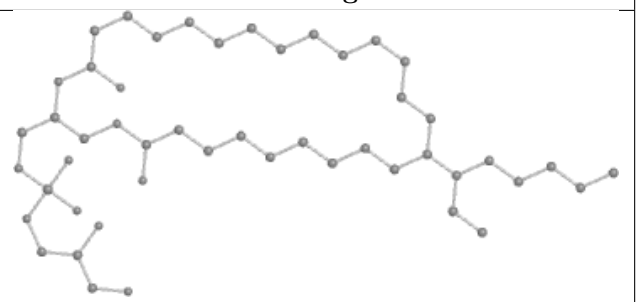
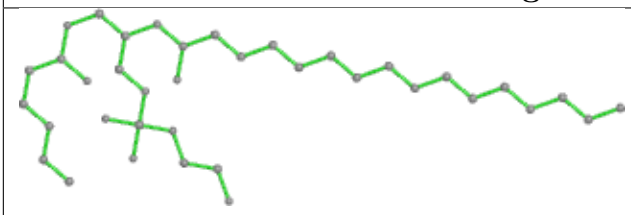
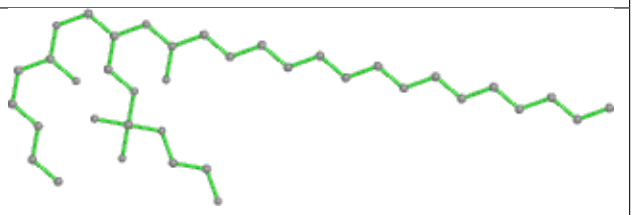


Rings

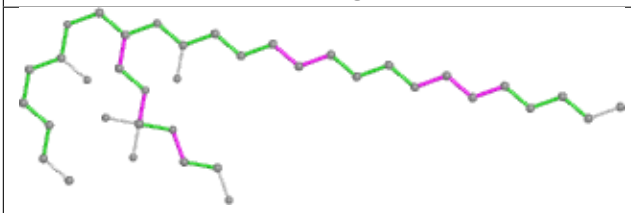
Ligand PTY H 803



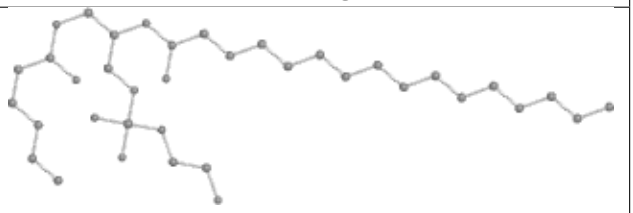
Bond lengths



Bond angles

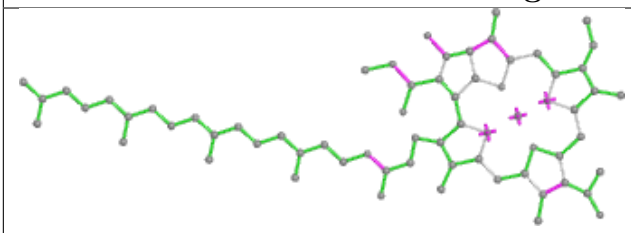


Torsions

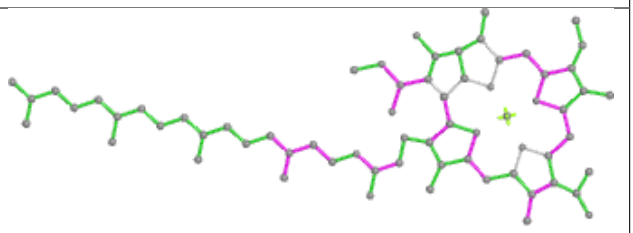


Rings

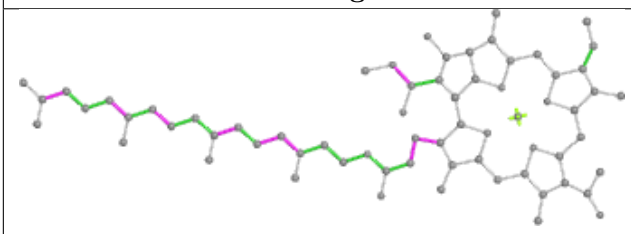
Ligand BCL N 102



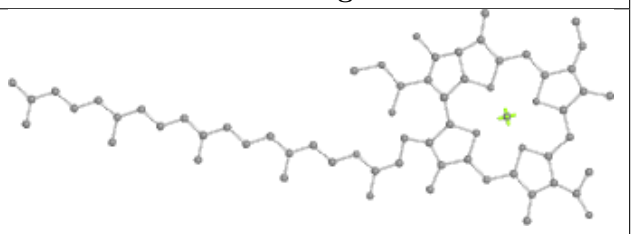
Bond lengths



Bond angles

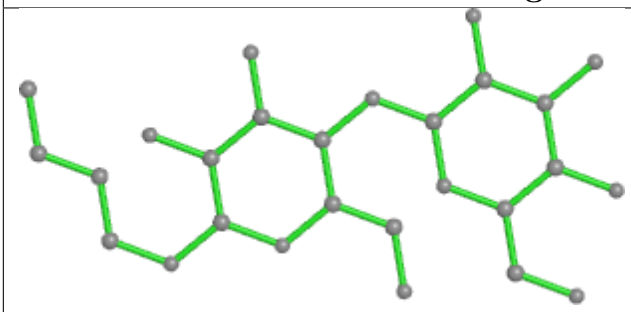


Torsions

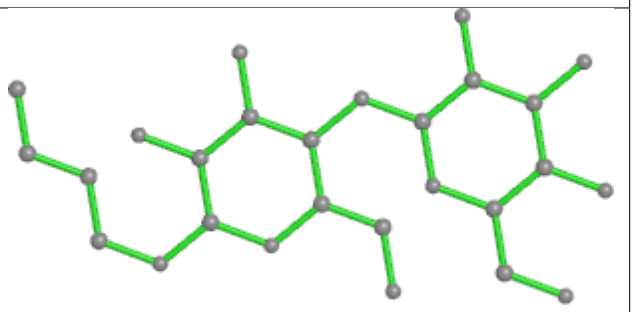


Rings

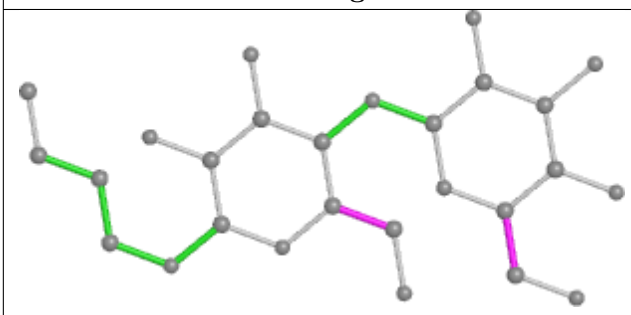
Ligand LMT 3 104



Bond lengths



Bond angles



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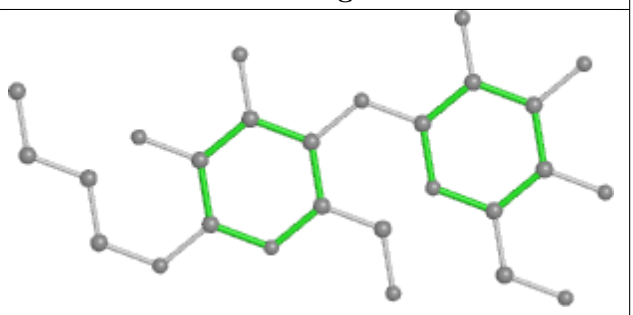
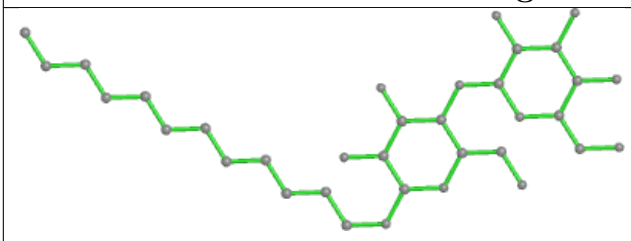
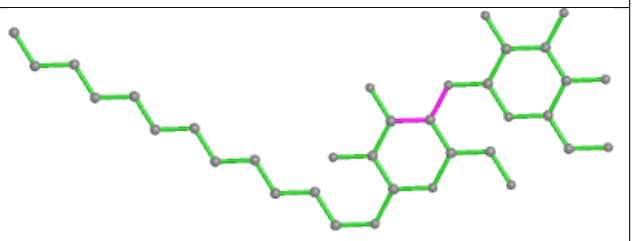


Rings

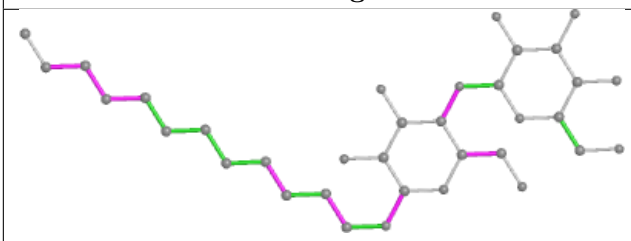
Ligand LMT 03 101



Bond lengths



Bond angles



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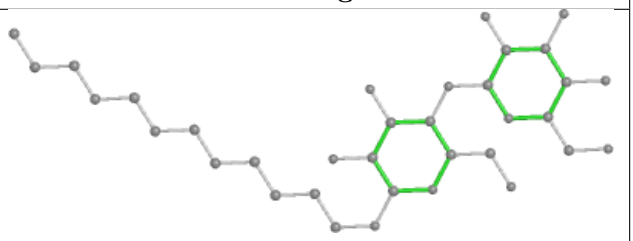
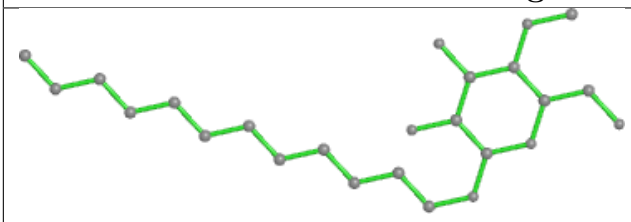
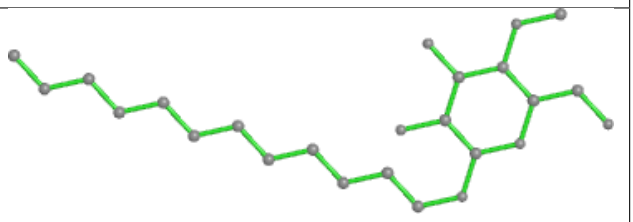


Rings

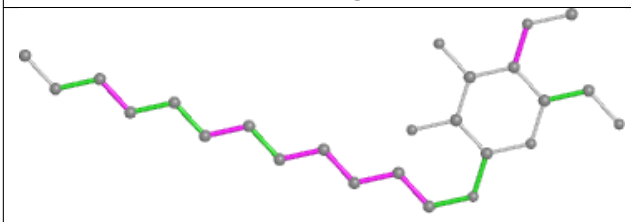
Ligand LMT s 101



Bond lengths



Bond angles



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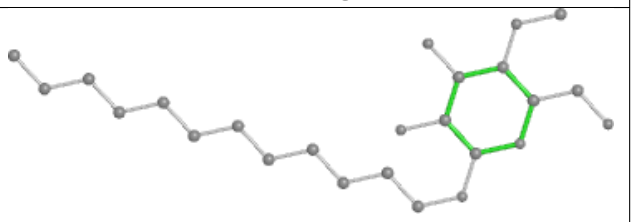
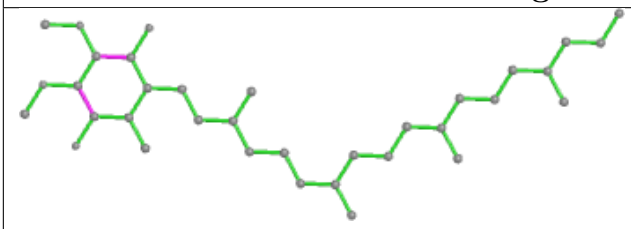


Rings

Ligand U10 L 304



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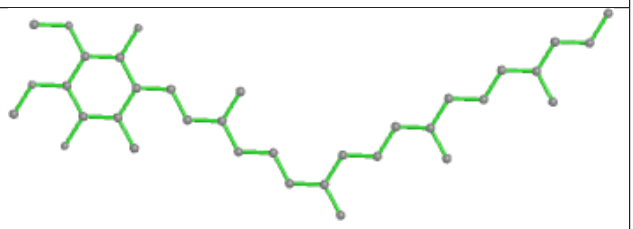
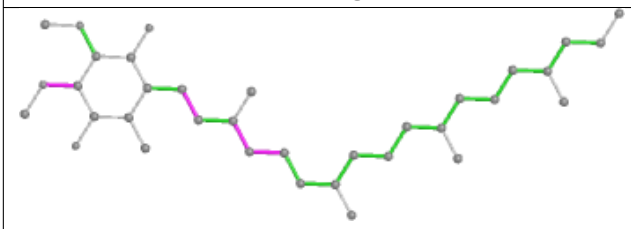
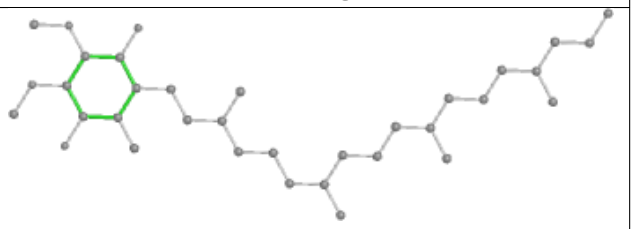


Bond angles

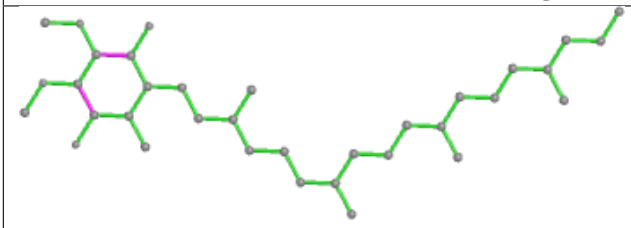


Torsions

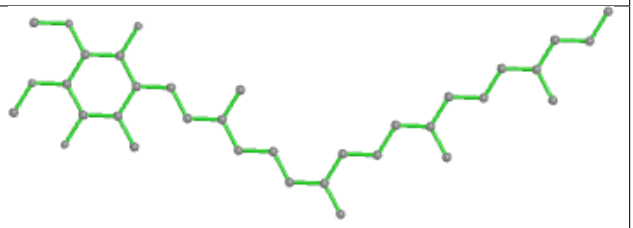


Rings

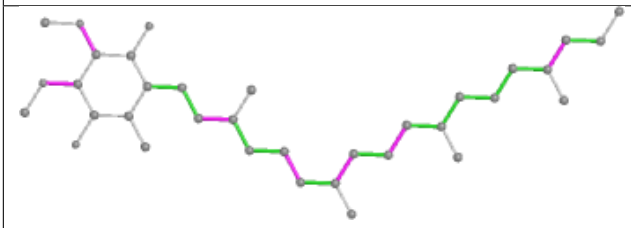
Ligand U10 l 303



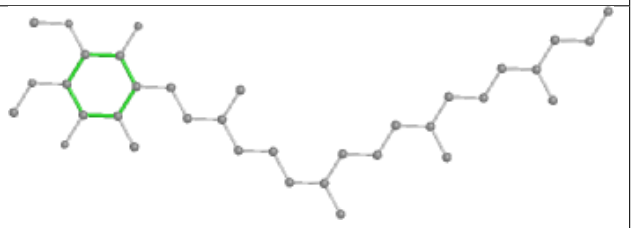
Bond lengths



Bond angles

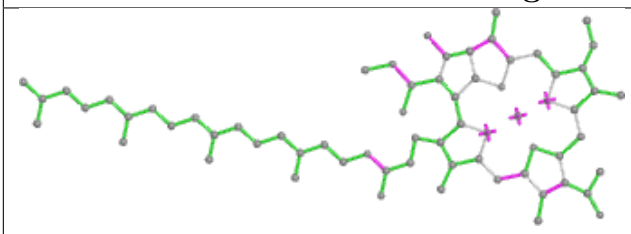


Torsions

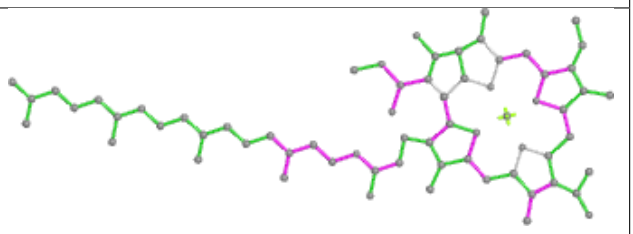


Rings

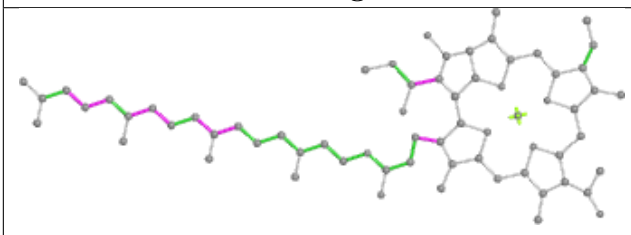
Ligand BCL m 401



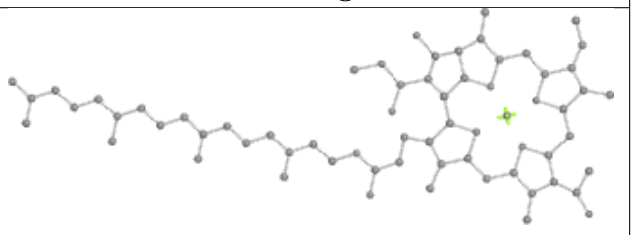
Bond lengths



Bond angles

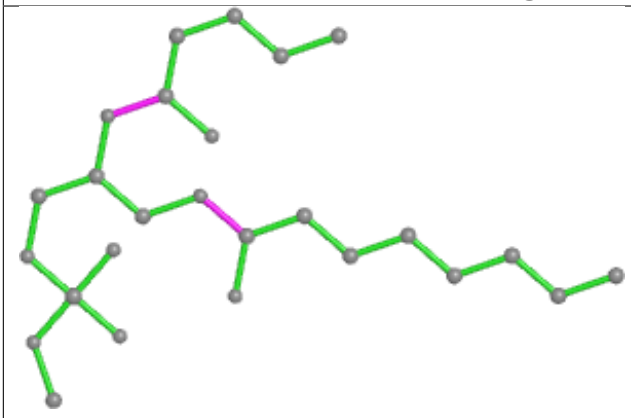


Torsions

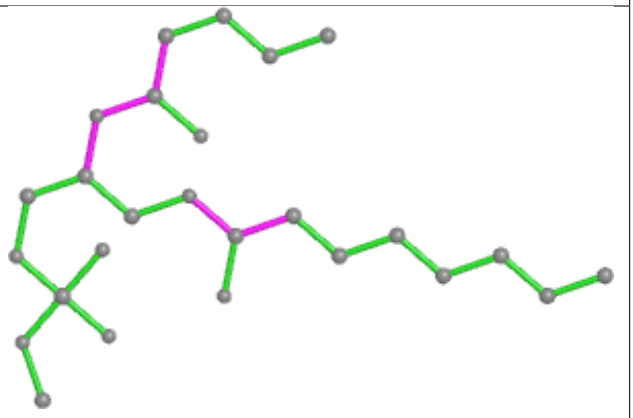


Rings

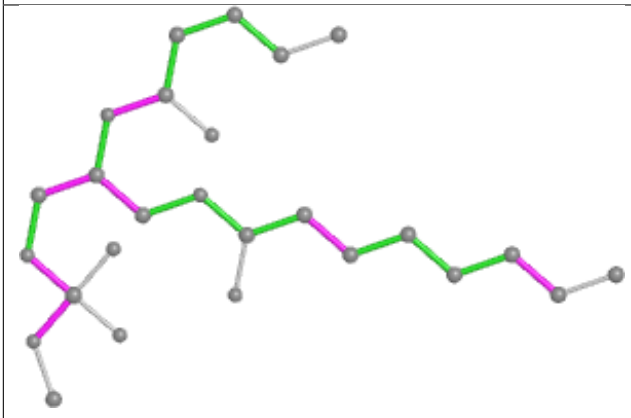
Ligand PGV H 804



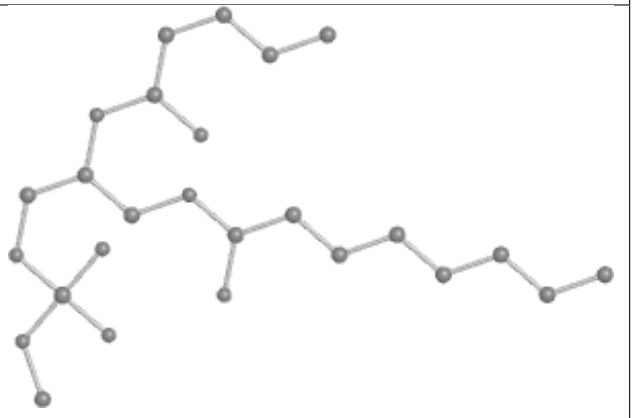
Bond lengths



Bond angles

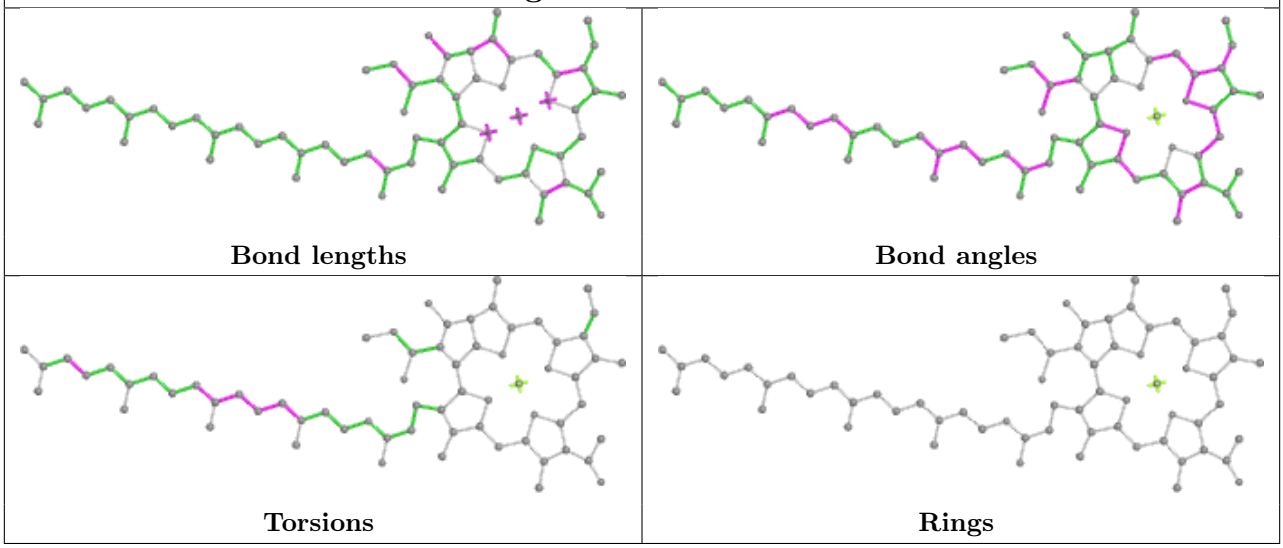


Torsions

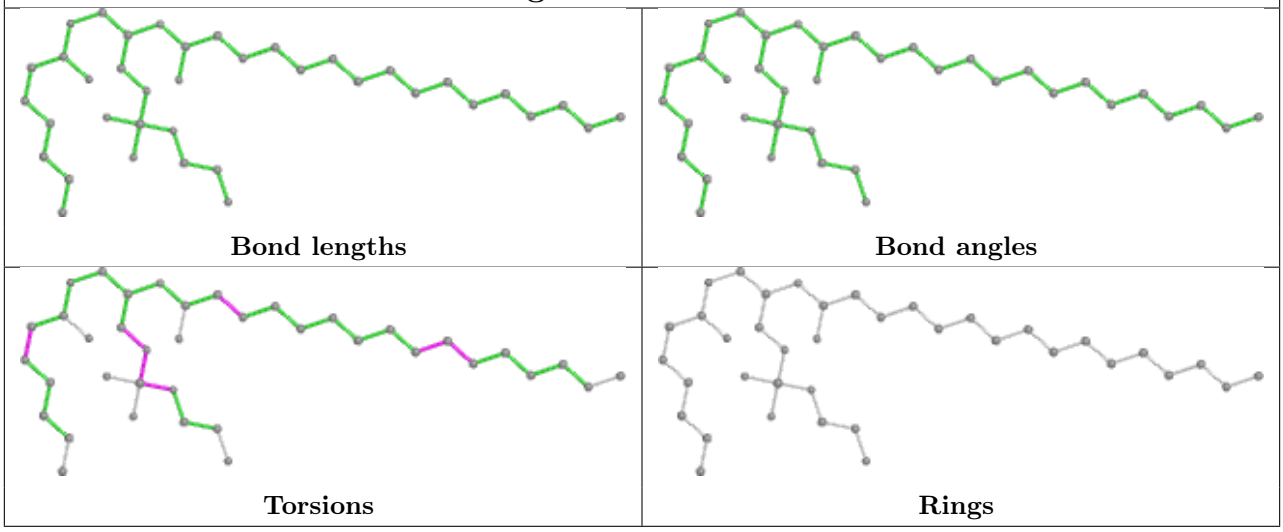


Rings

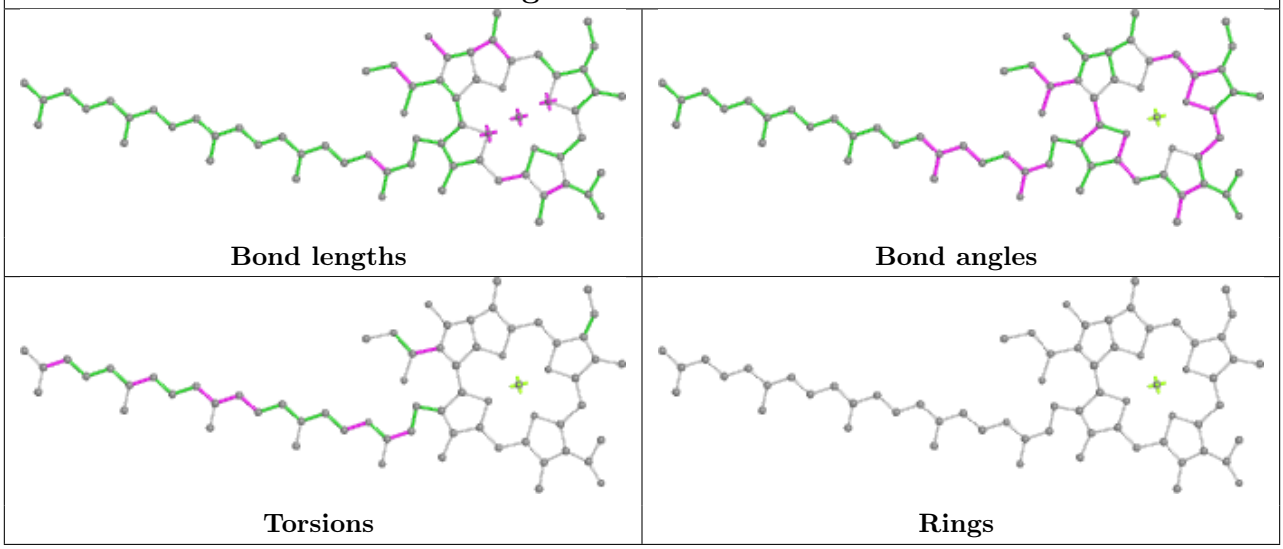
Ligand BCL K 402



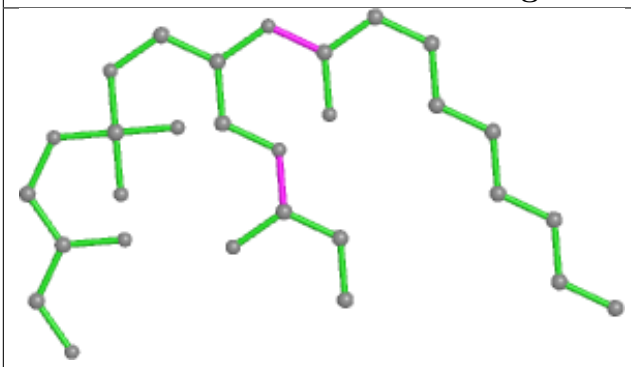
Ligand PTY h 804



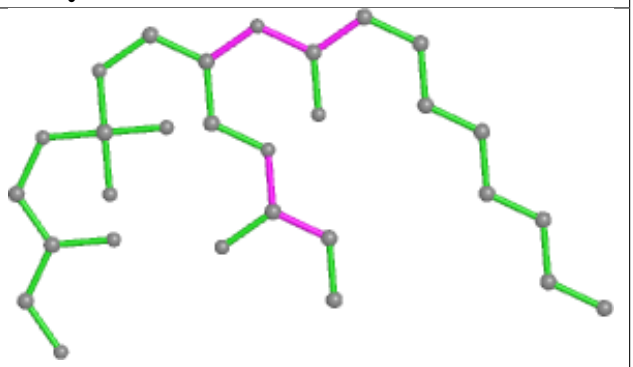
Ligand BCL M 401



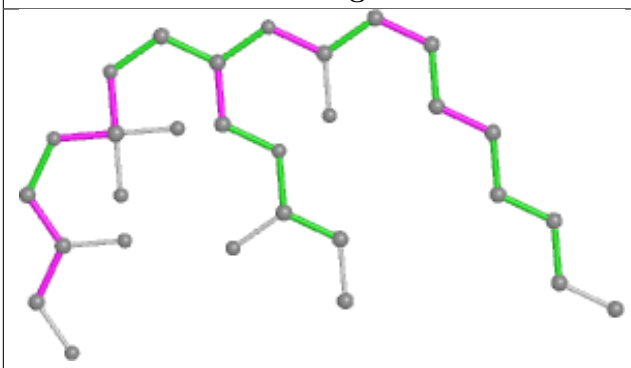
Ligand PGV Q 102



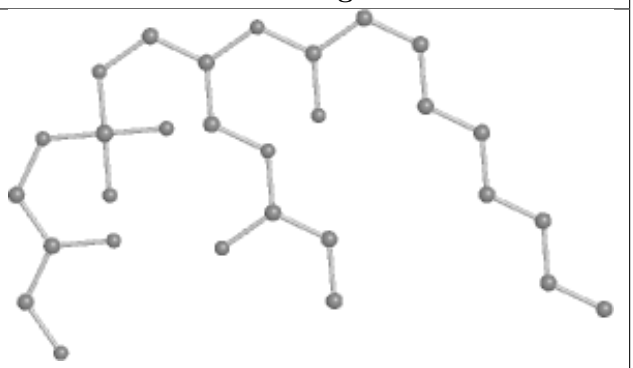
Bond lengths



Bond angles

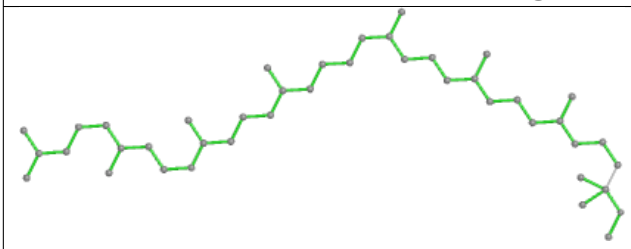


Torsions

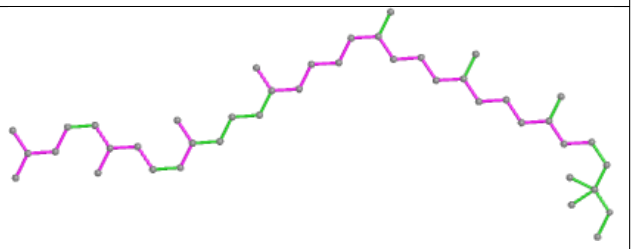


Rings

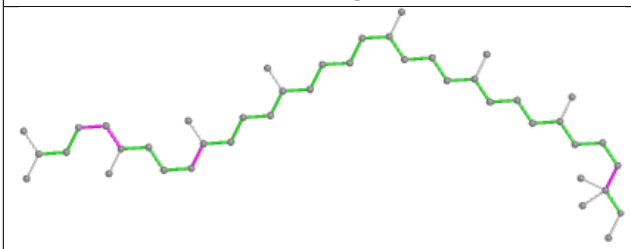
Ligand SPO 6 102



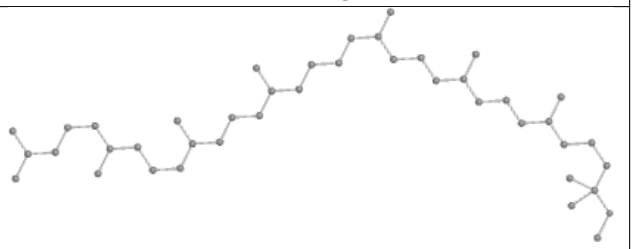
Bond lengths



Bond angles

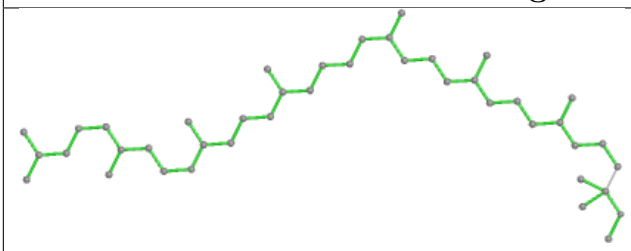


Torsions

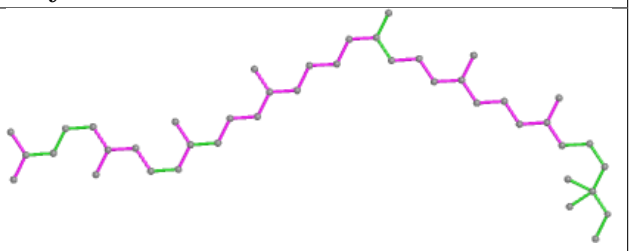


Rings

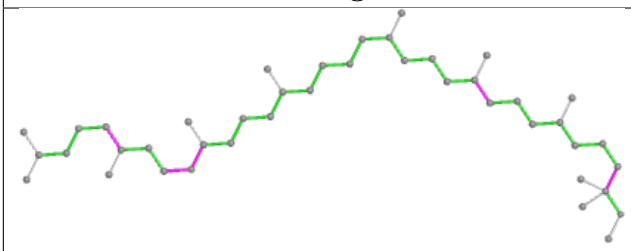
Ligand SPO y 105



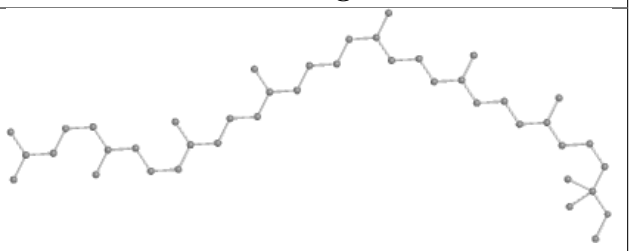
Bond lengths



Bond angles

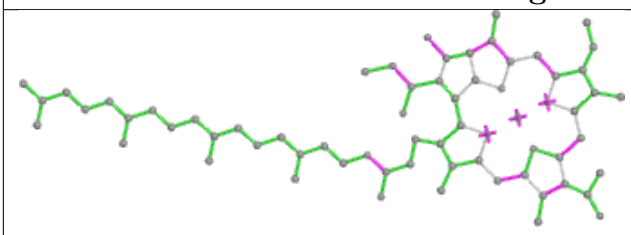


Torsions



Rings

Ligand BCL 5 102



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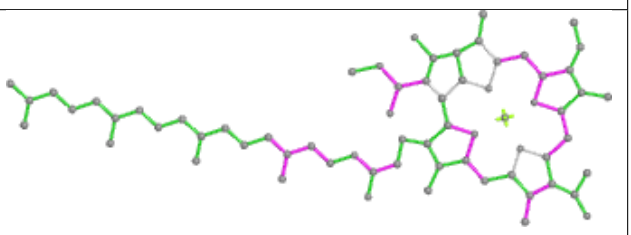
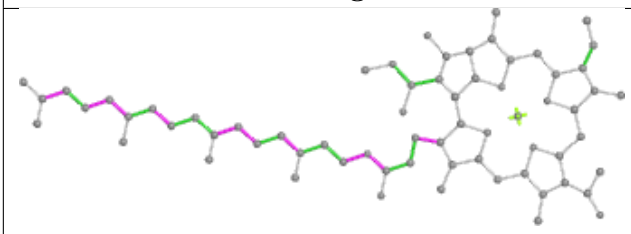


Bond angles



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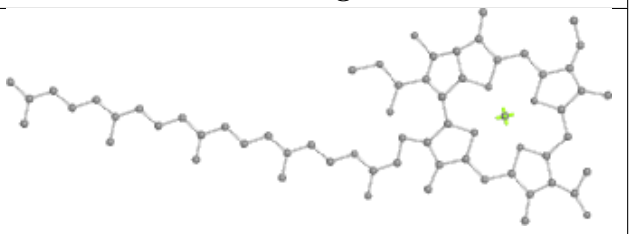
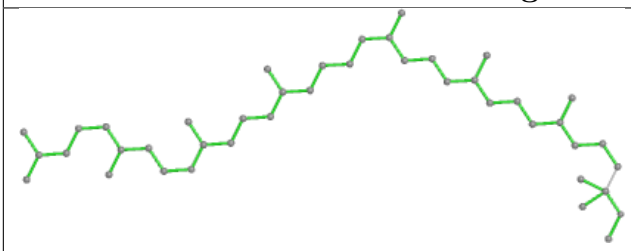
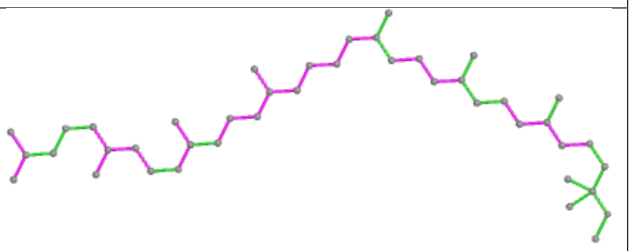


Rings

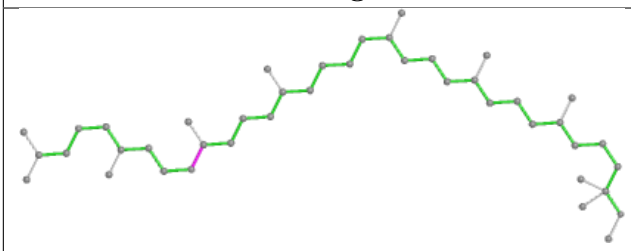
Ligand SPO 02 102



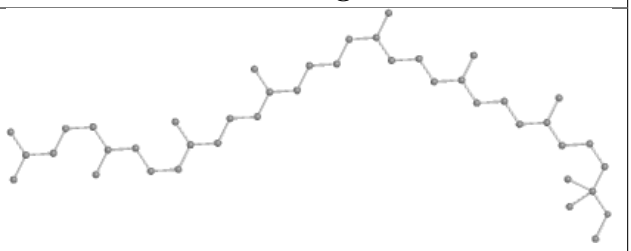
Bond lengths



Bond angles

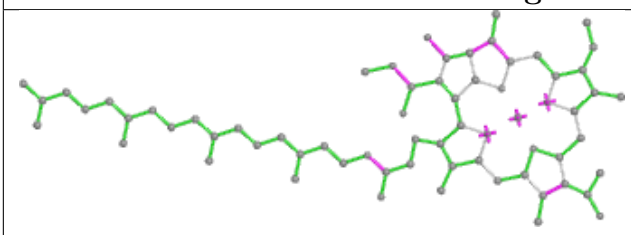


Torsions



Rings

Ligand BCL D 101



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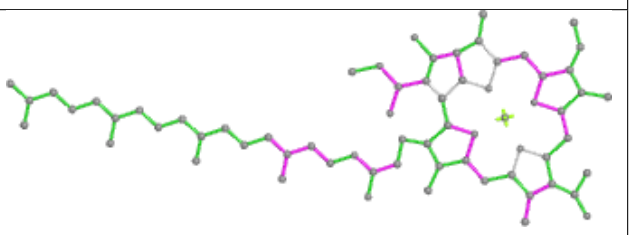
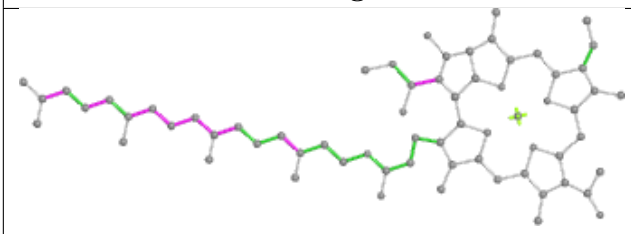
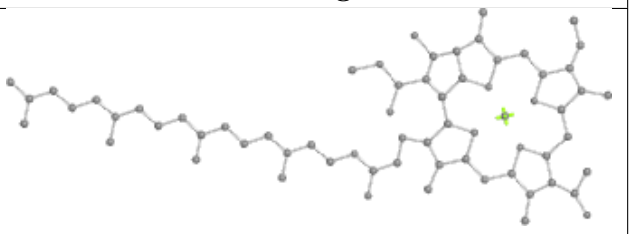


Bond angles

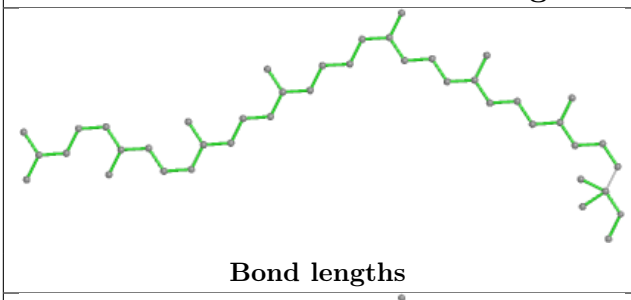


Torsions



Rings

Ligand SPO g 102



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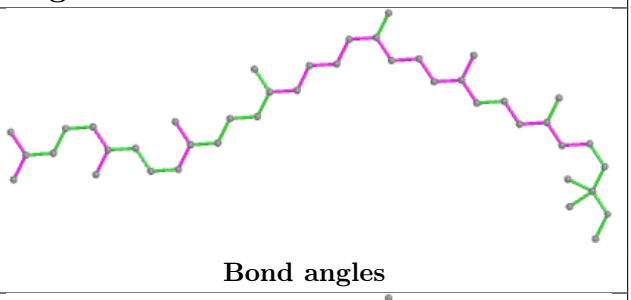
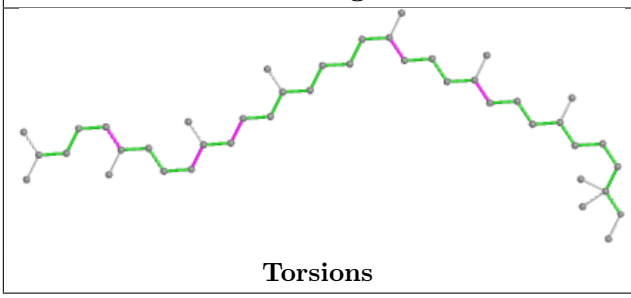


Bond angles



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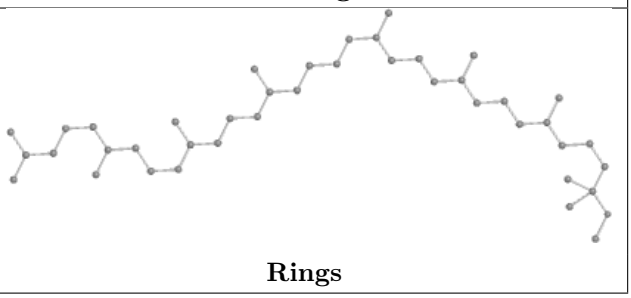
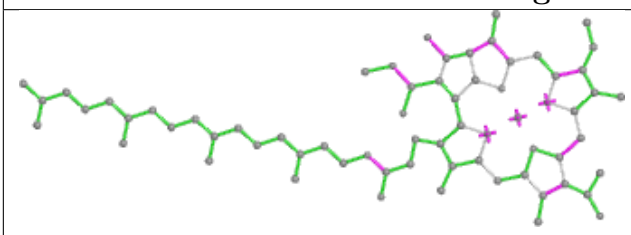


Rings

Ligand BCL l 301



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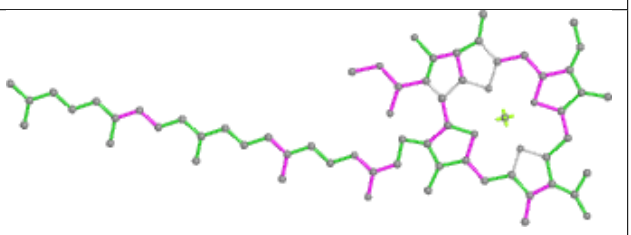
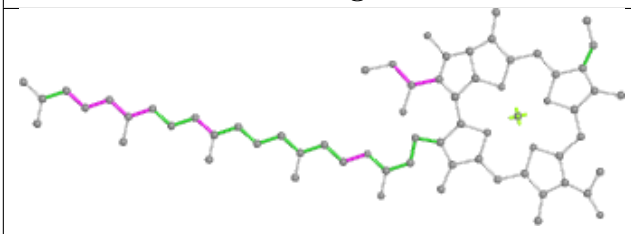


Bond angles



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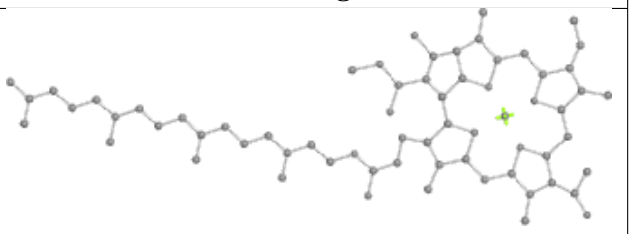
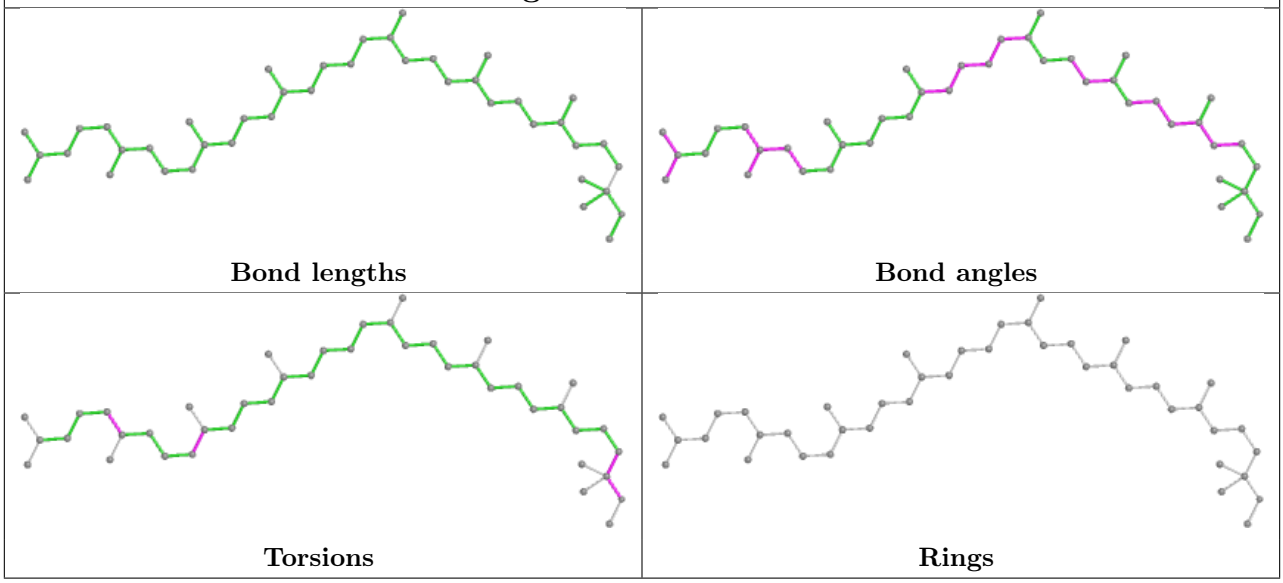
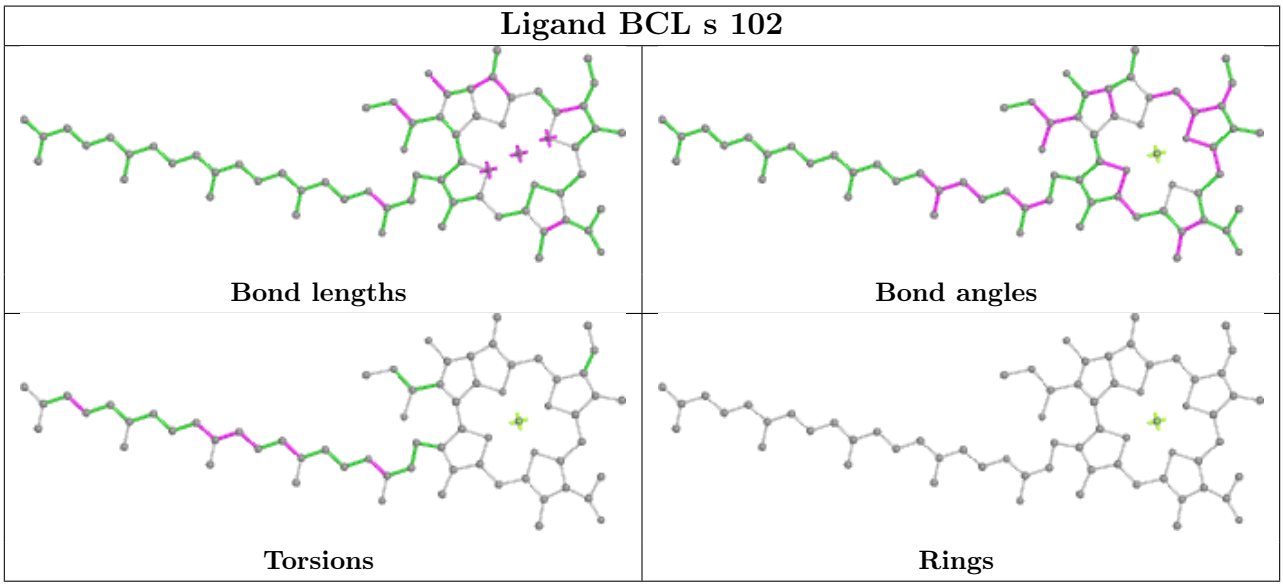


Rings

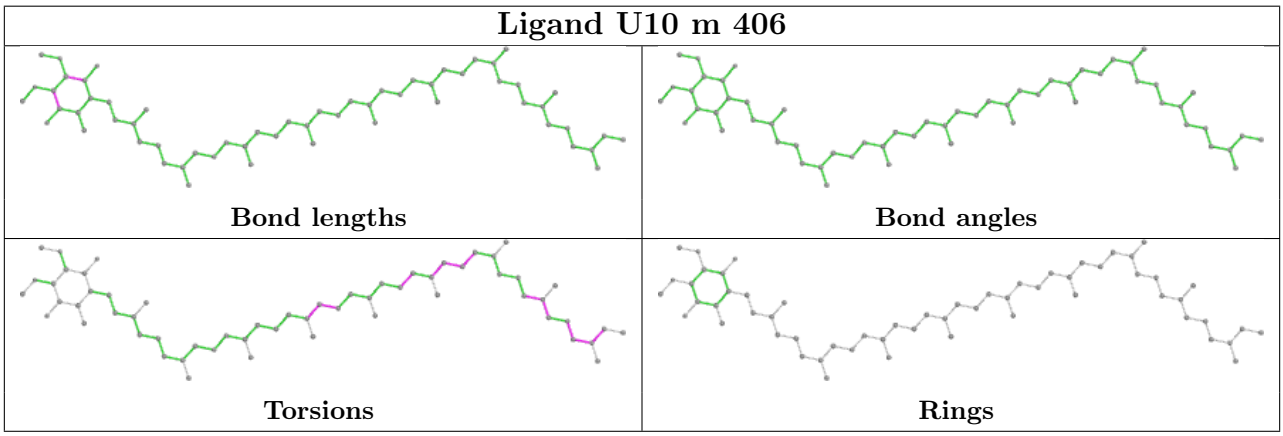
Ligand SPO M 406



Ligand BCL s 102



Ligand U10 m 406



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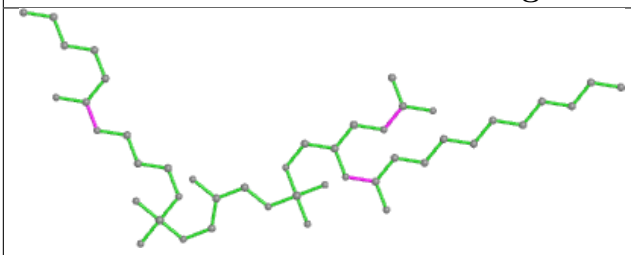
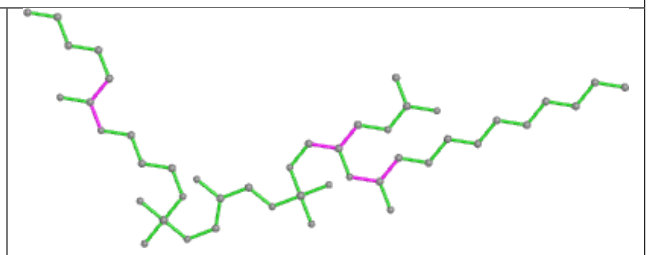
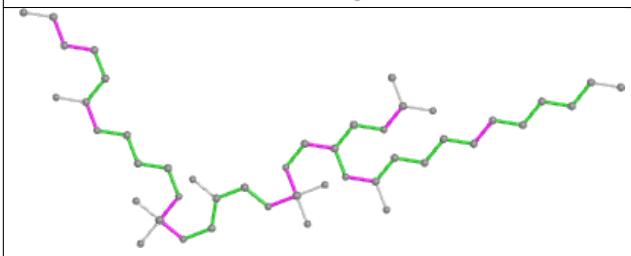


Bond lengths



Bond angles



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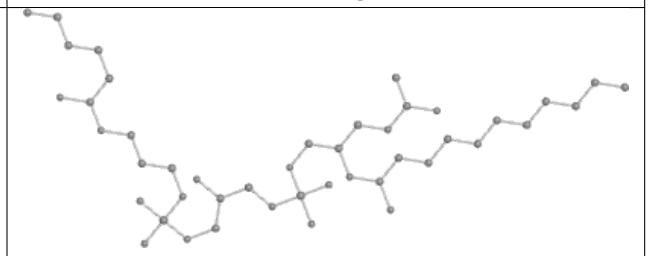
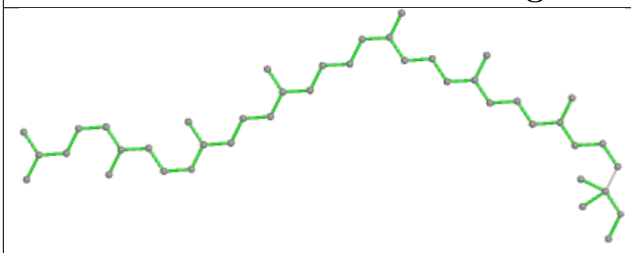


Rings

Ligand SPO T 102



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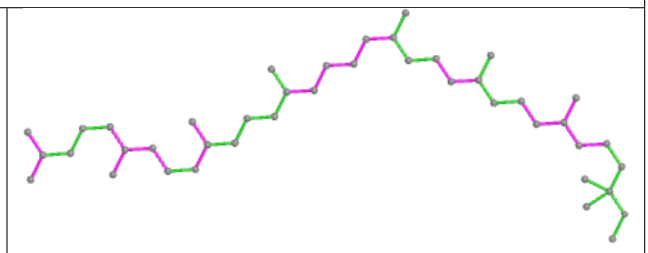
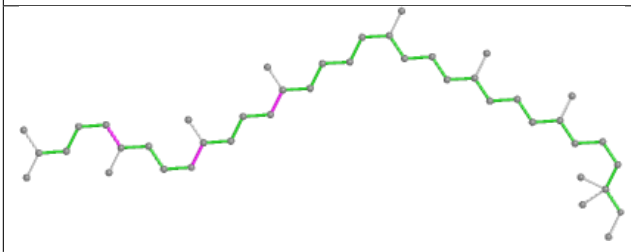
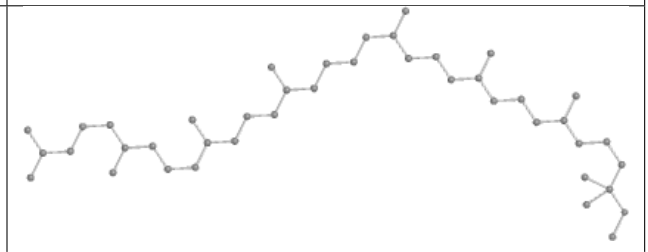


Bond angles

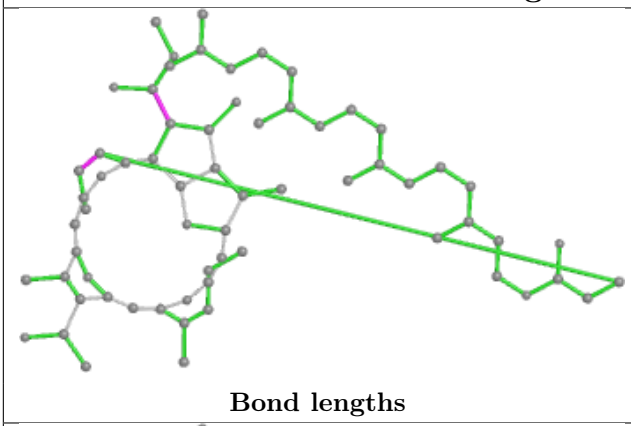


Torsions

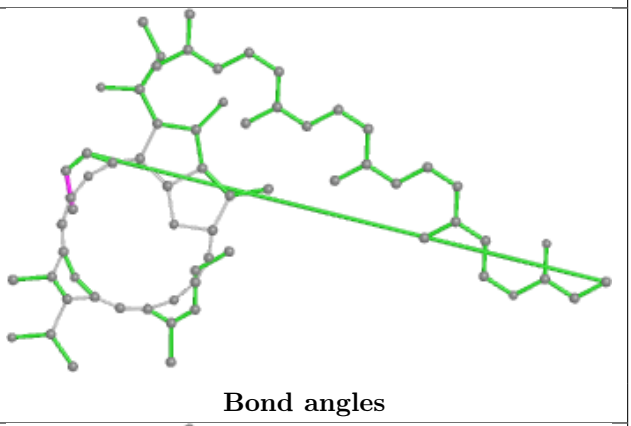


Rings

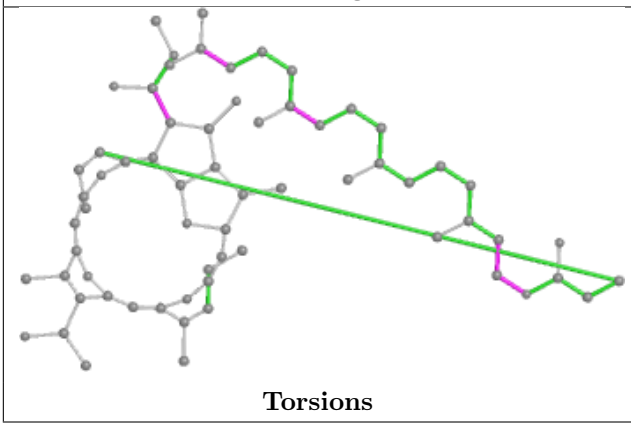
Ligand BPH L 302



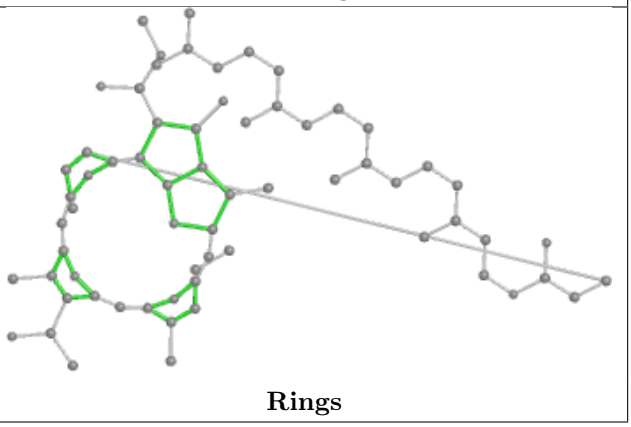
Bond lengths



Bond angles

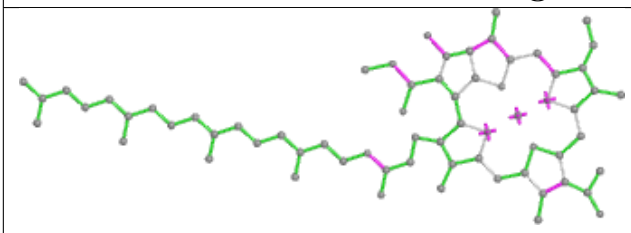


Torsions

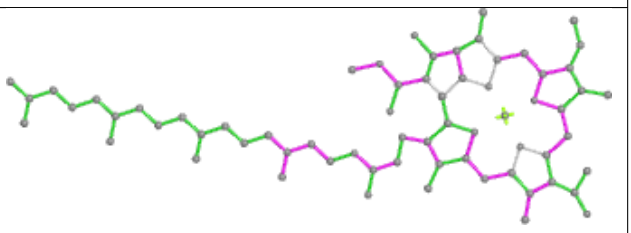


Rings

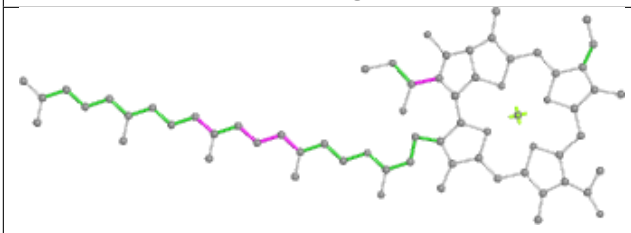
Ligand BCL 3 102



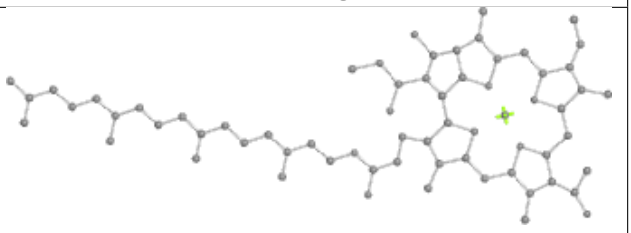
Bond lengths



Bond angles

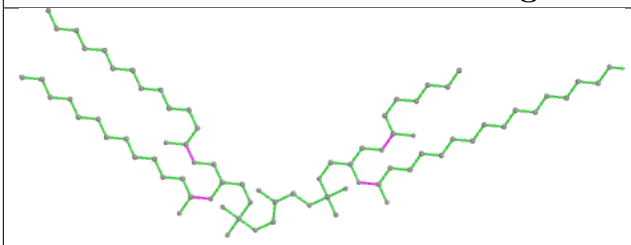


Torsions



Rings

Ligand CDL M 410



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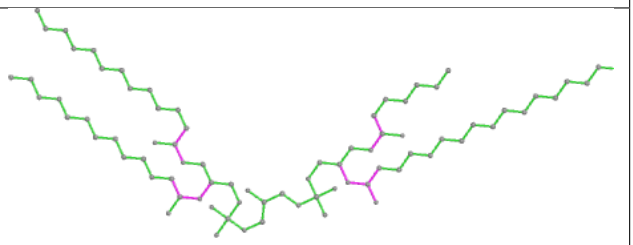
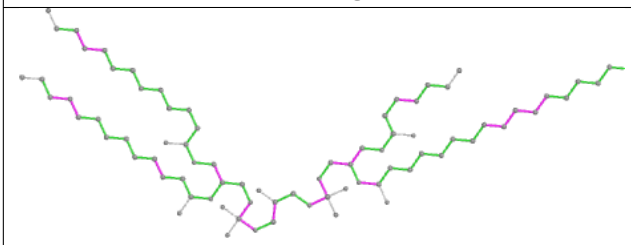


Bond angles



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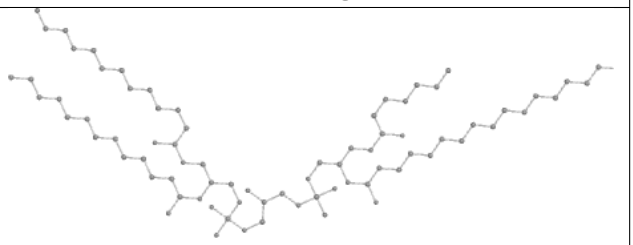
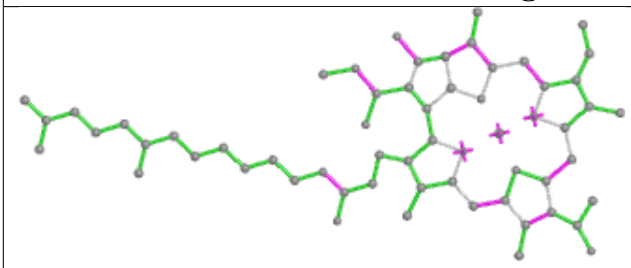


Rings

Ligand BCL 08 102



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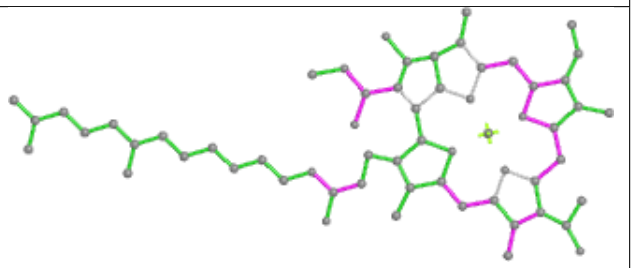
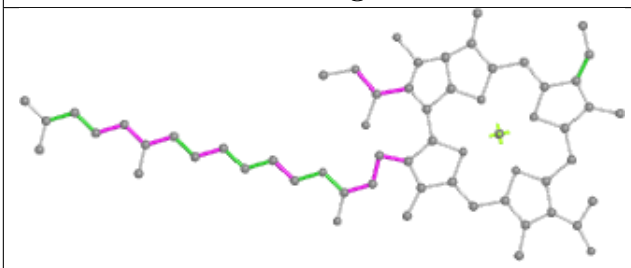


Bond angles



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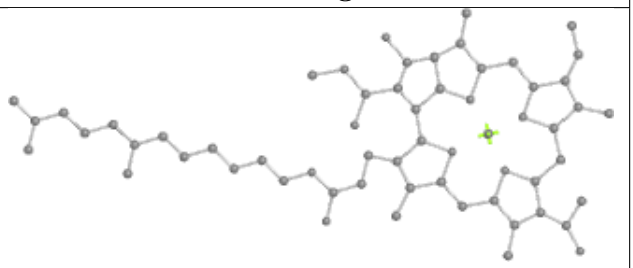
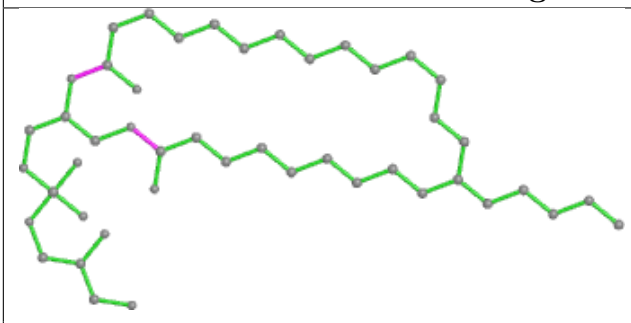
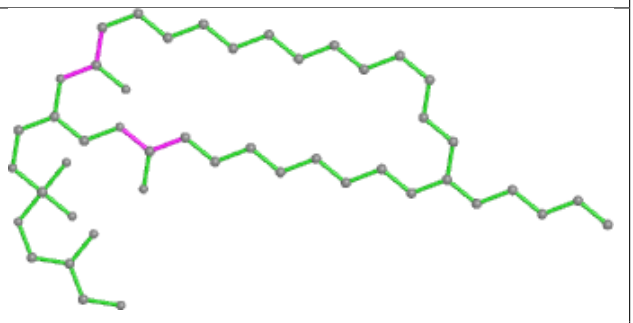


Rings

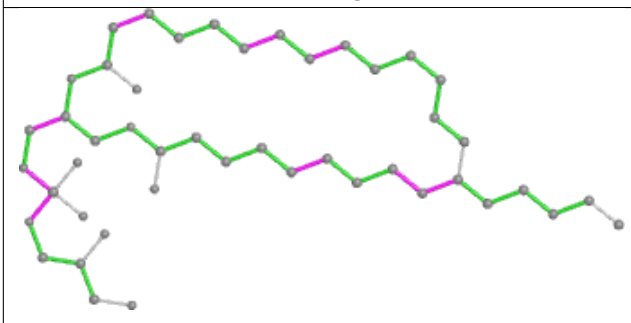
Ligand PGV f 104



Bond lengths



Bond angles



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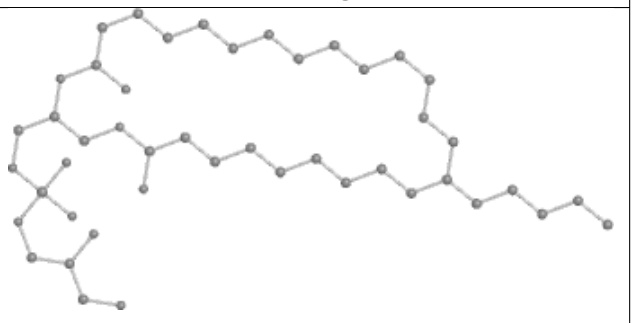
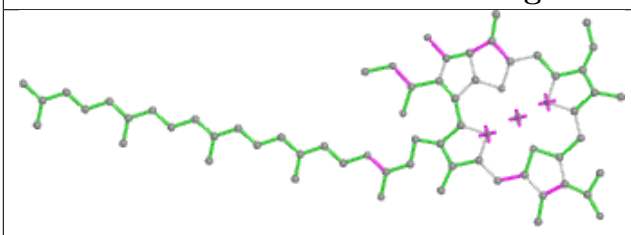
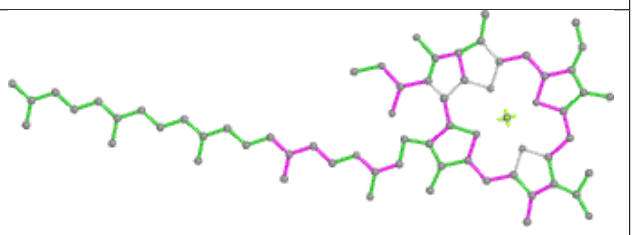


Rings

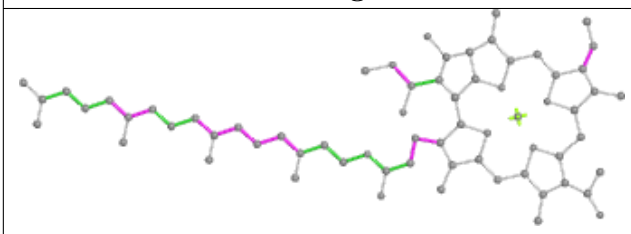
Ligand BCL G 102



Bond lengths



Bond angles



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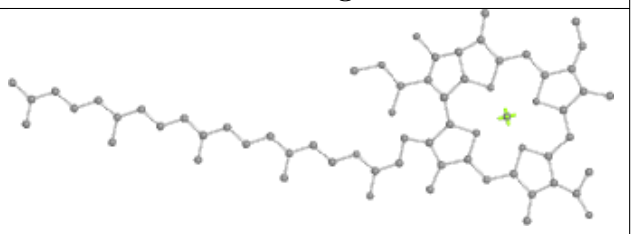
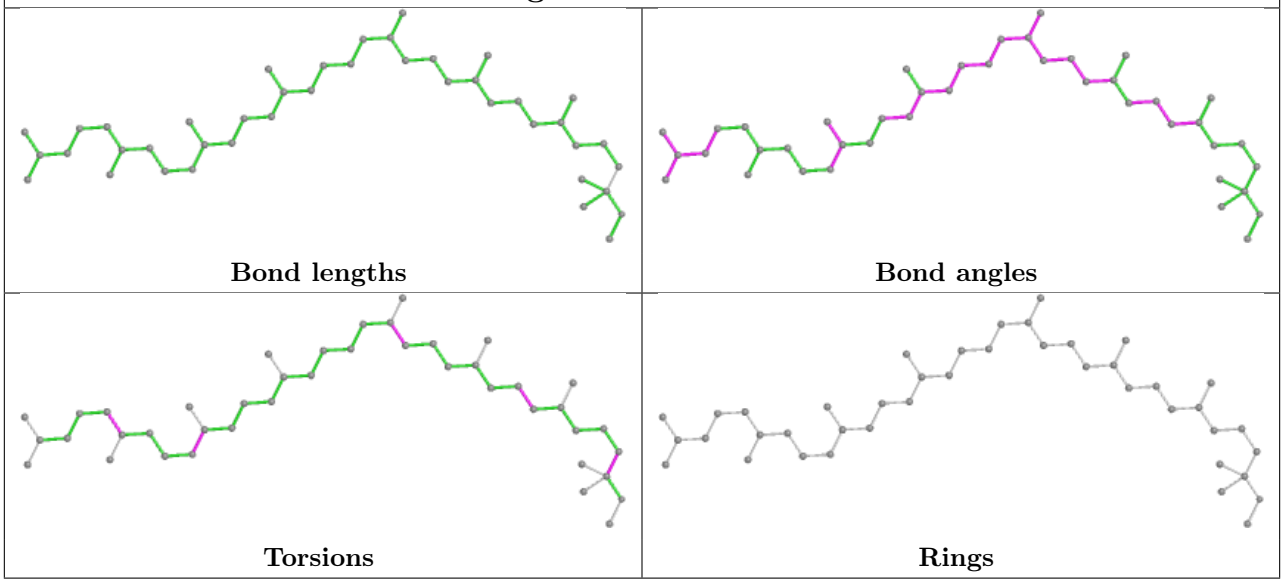
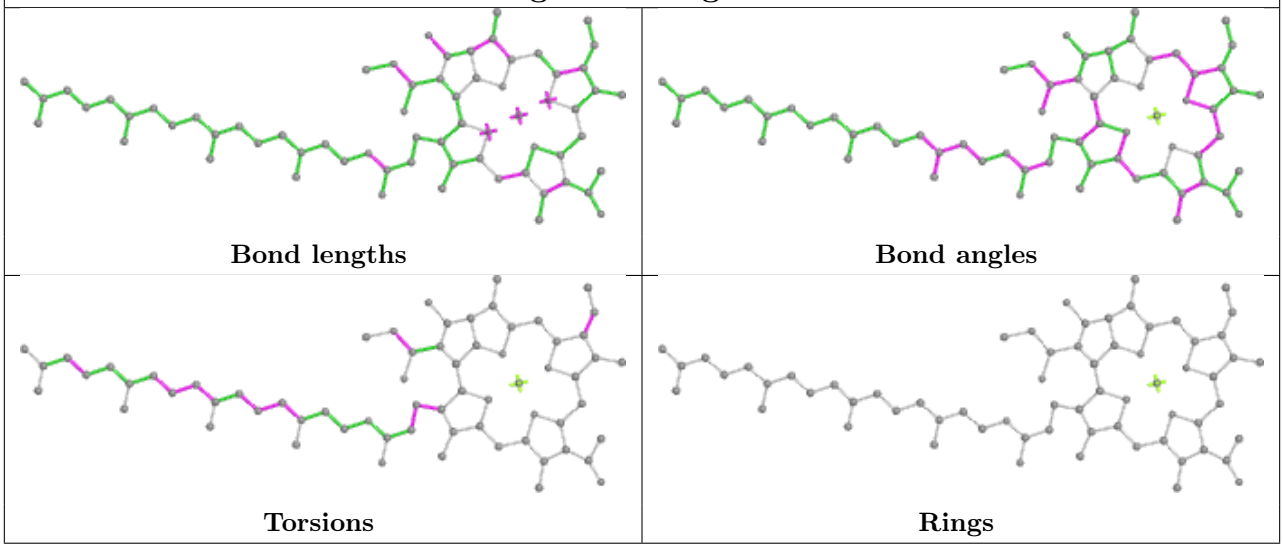


Rings

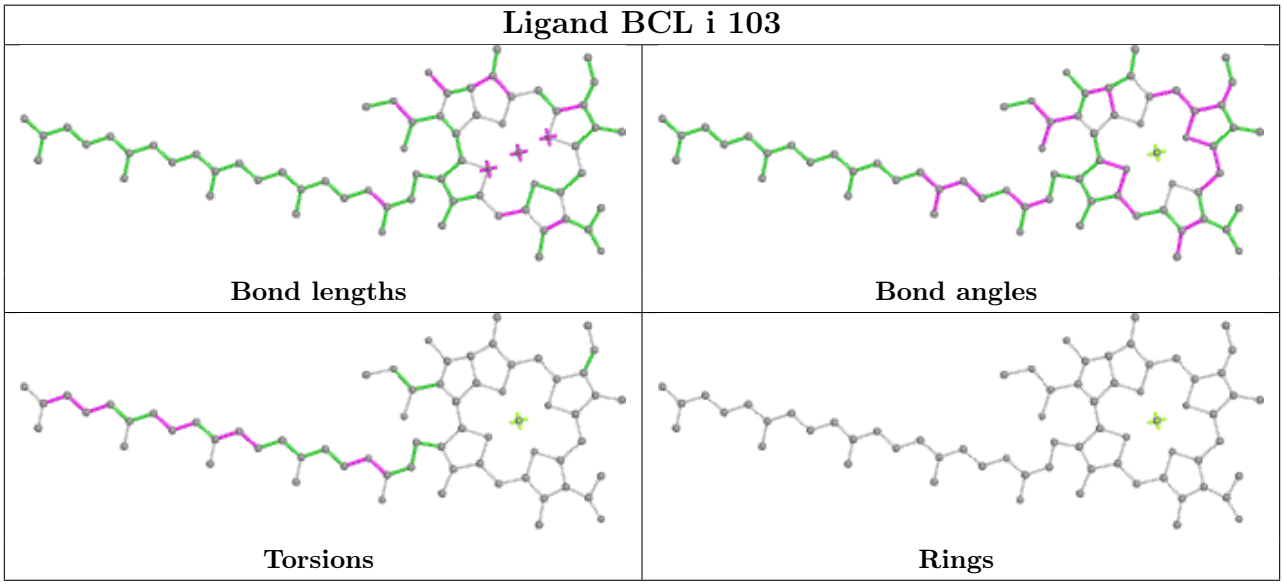
Ligand SPO B 101



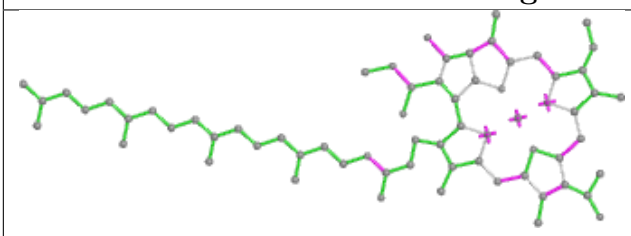
Ligand BCL g 103



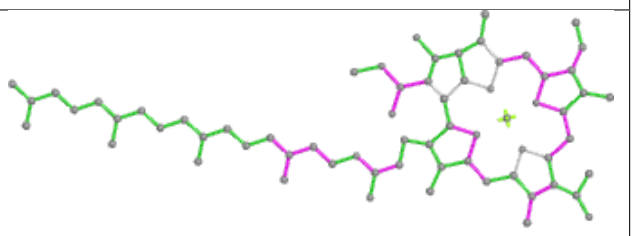
Ligand BCL i 103



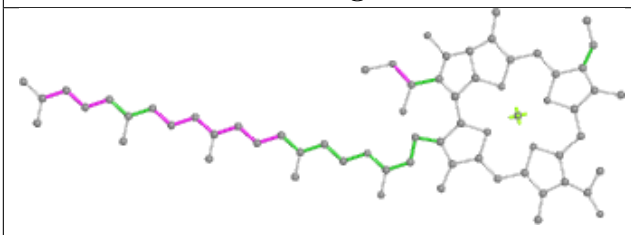
Ligand BCL 07 101



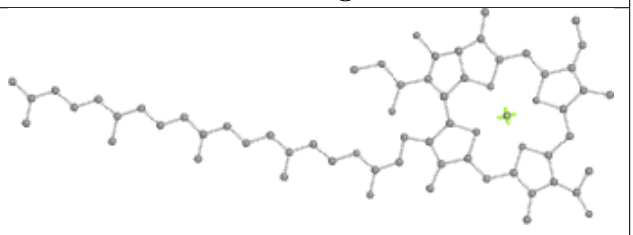
Bond lengths



Bond angles

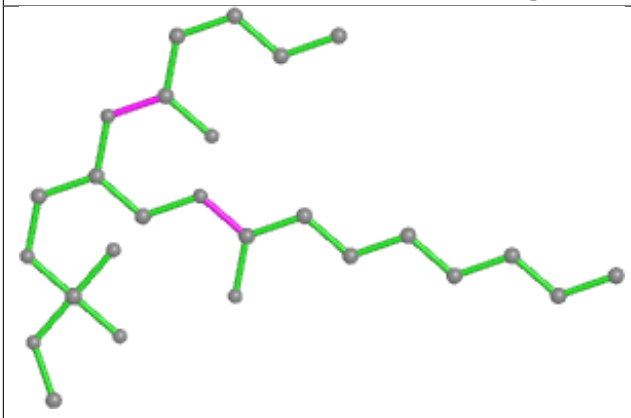


Torsions

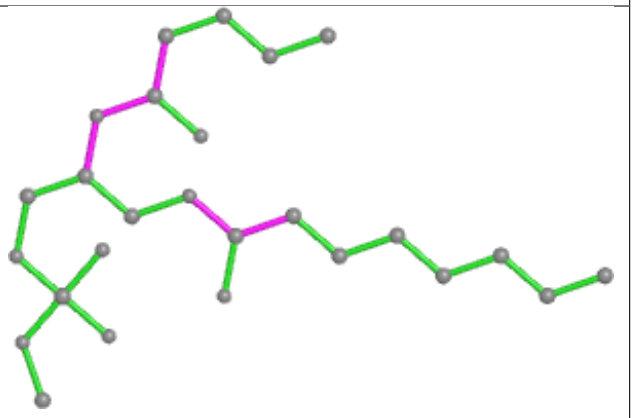


Rings

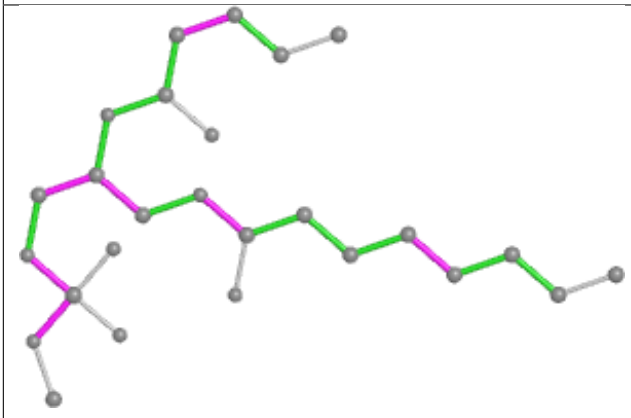
Ligand PGV h 806



Bond lengths



Bond angles



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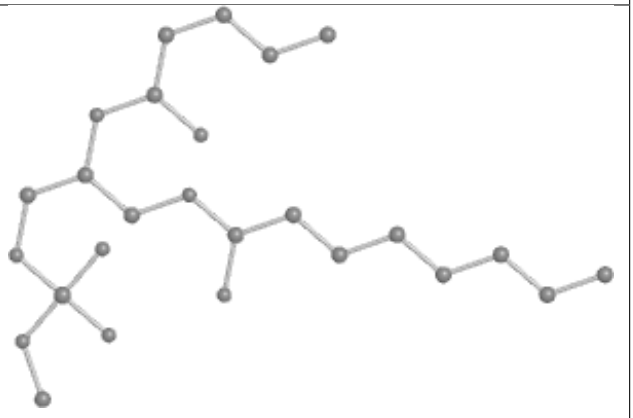
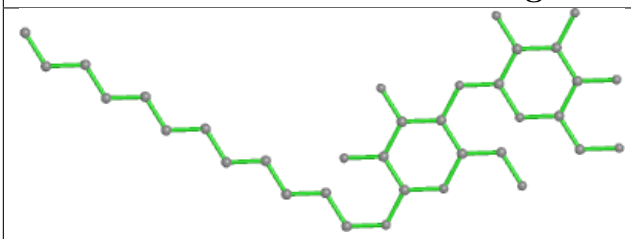
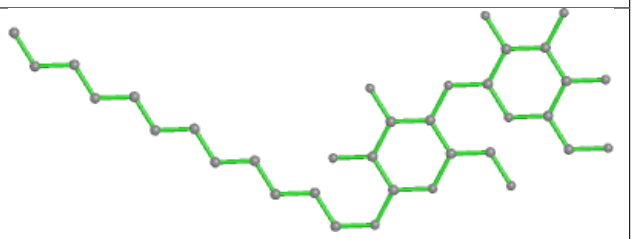


Rings

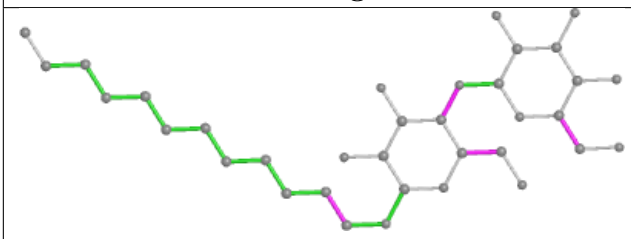
Ligand LMT 3 101



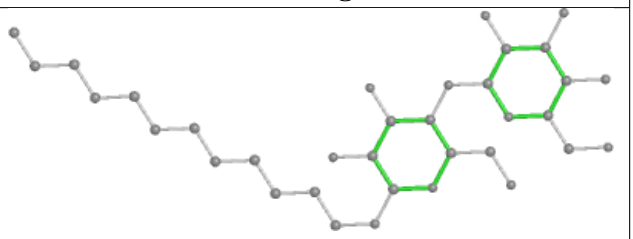
Bond lengths



Bond angles

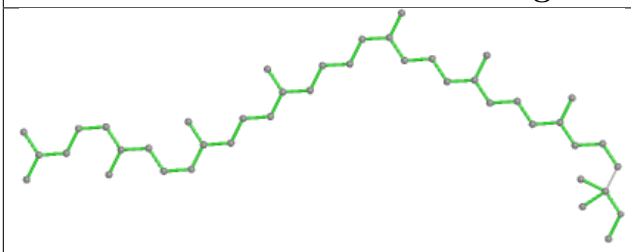


Torsions

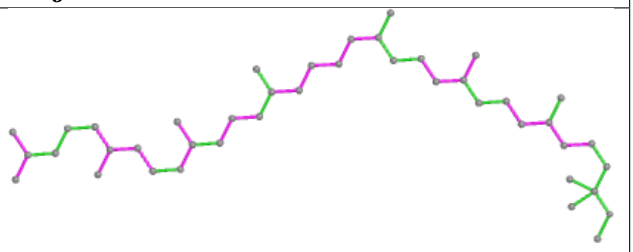


Rings

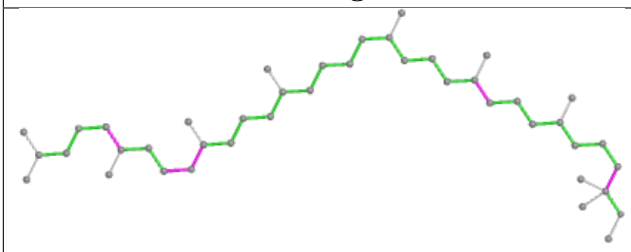
Ligand SPO j 101



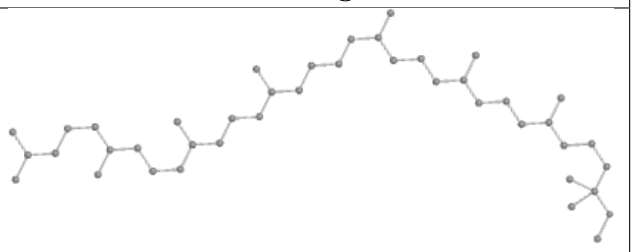
Bond lengths



Bond angles

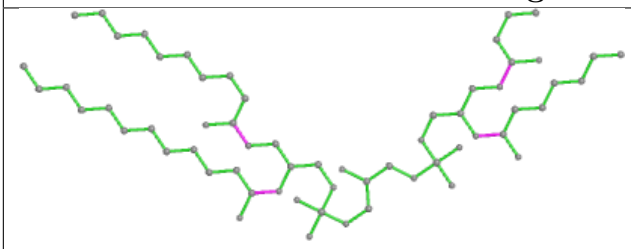


Torsions

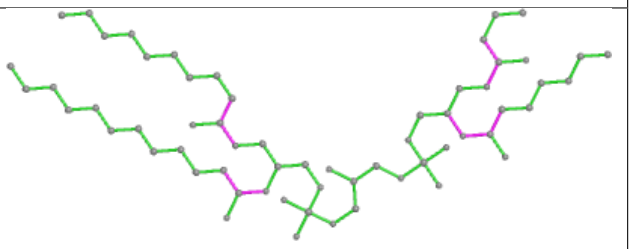


Rings

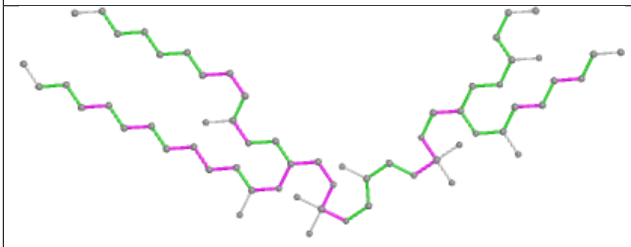
Ligand CDL h 805



Bond lengths



Bond angles



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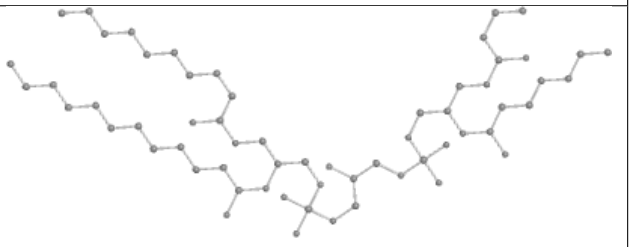
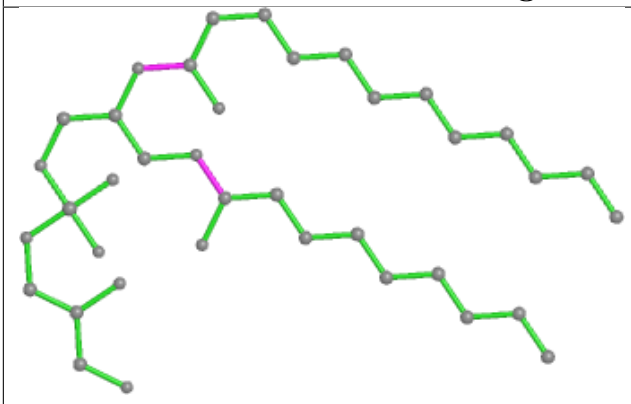
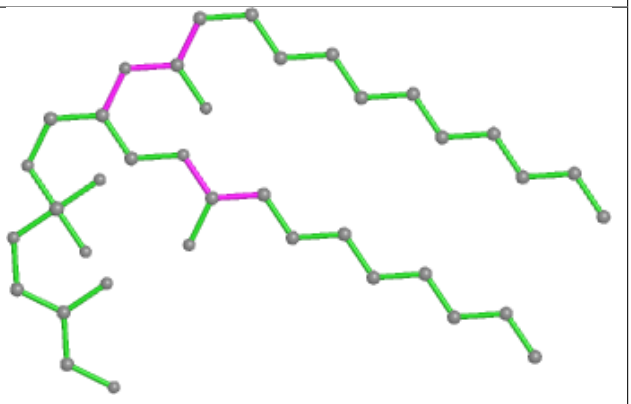


Rings

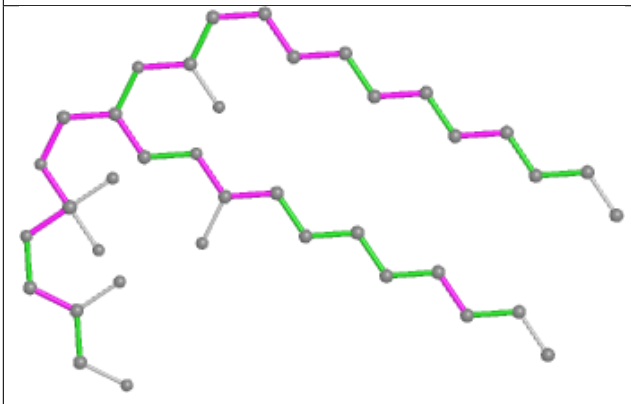
Ligand PGV M 411



Bond lengths



Bond angles



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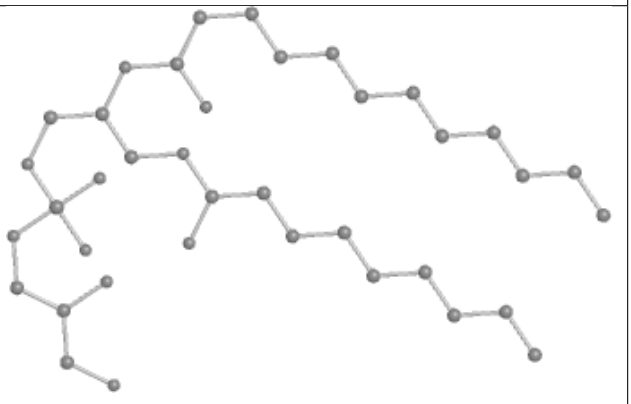
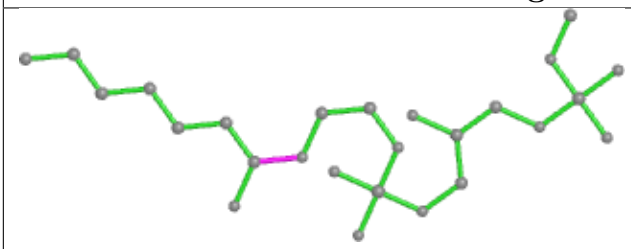


Rings

Ligand CDL x 102



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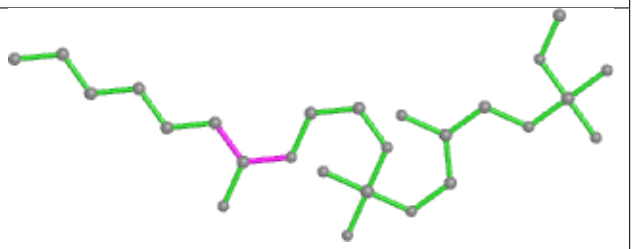
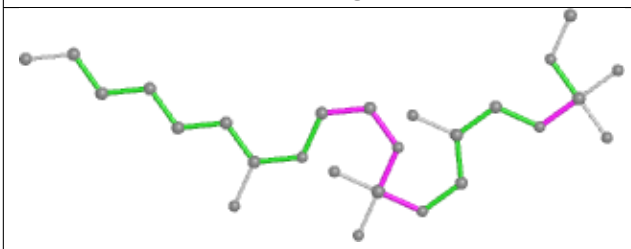


Bond angles



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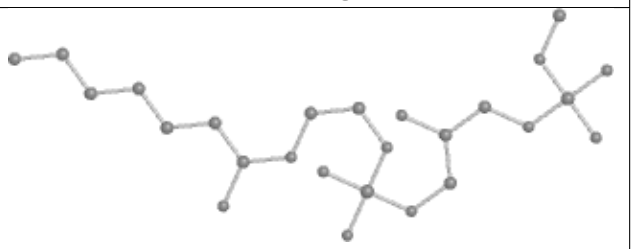
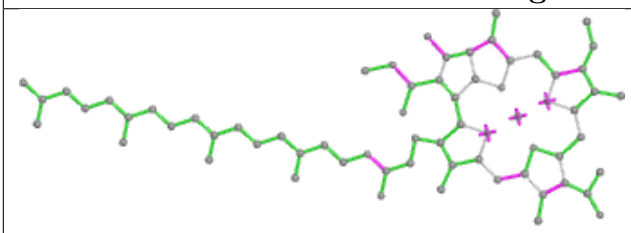
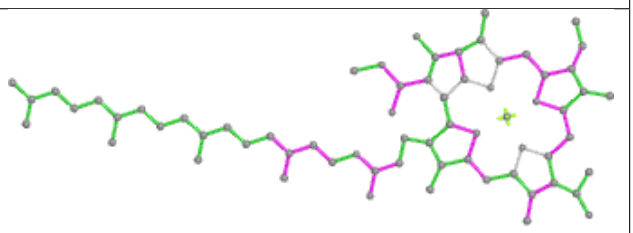


Rings

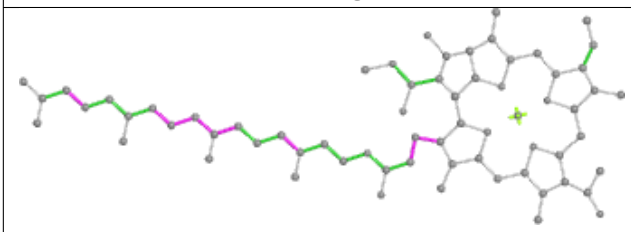
Ligand BCL o 101



Bond lengths



Bond angles



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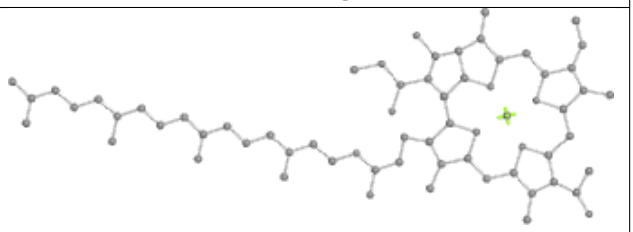
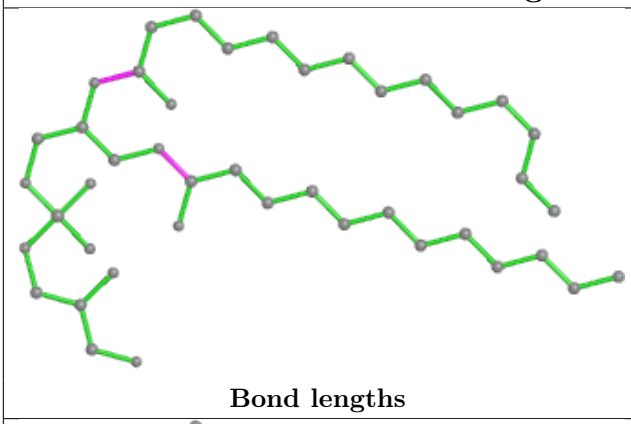


Rings

Ligand PGV y 104



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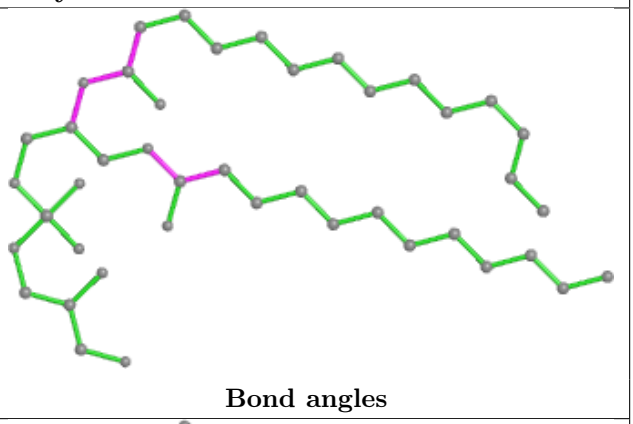
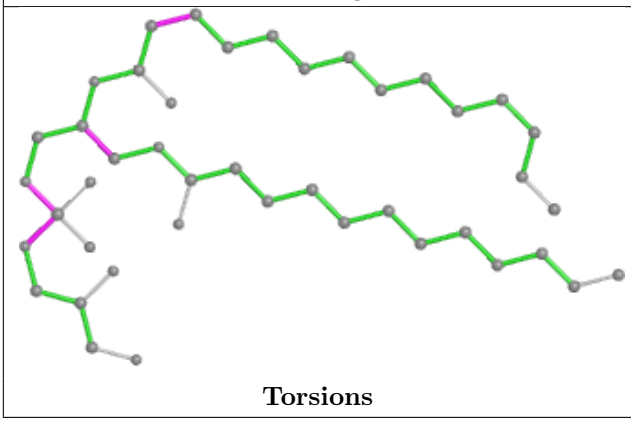
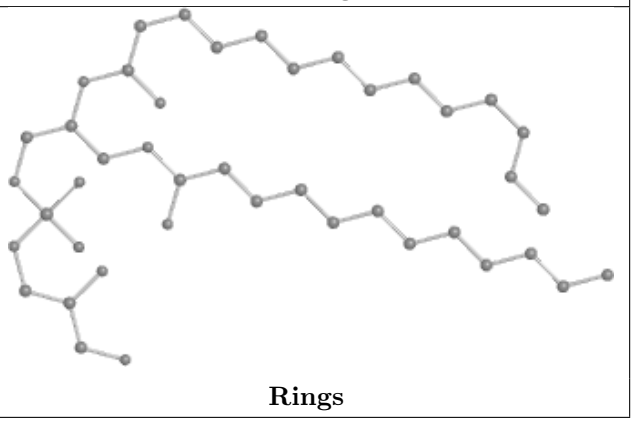


Bond angles

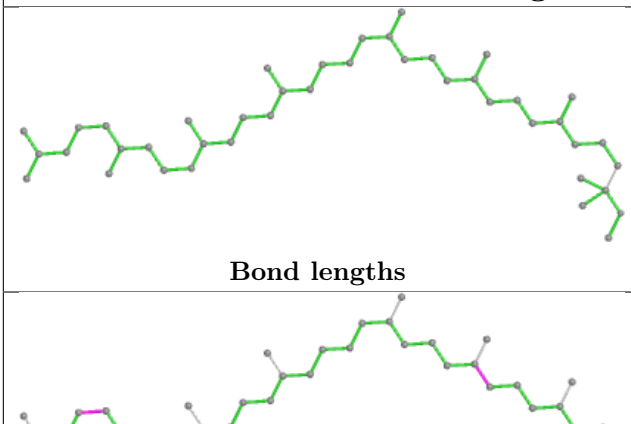


Torsions

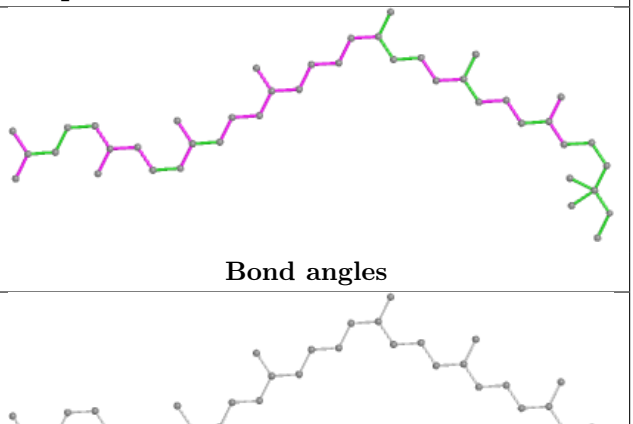


Rings

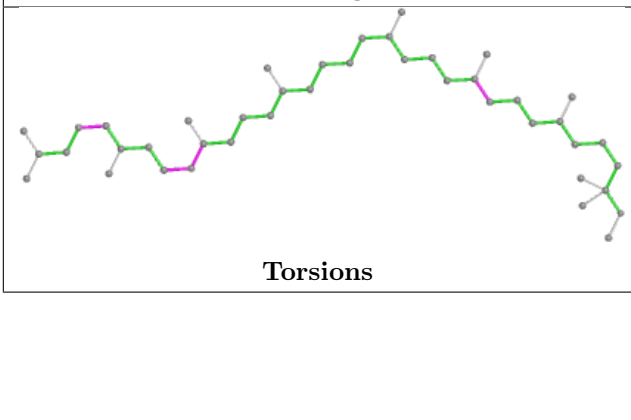
Ligand SPO q 104



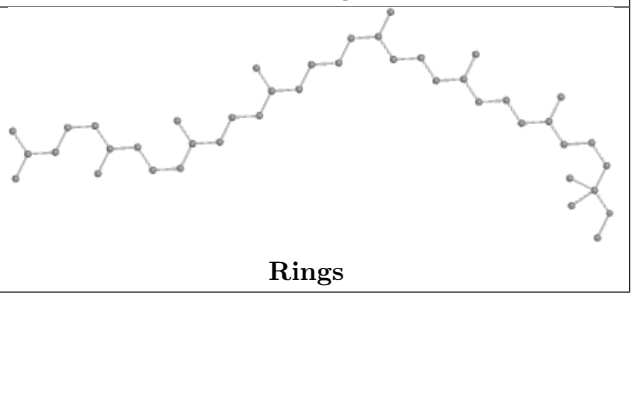
Bond lengths



Bond angles

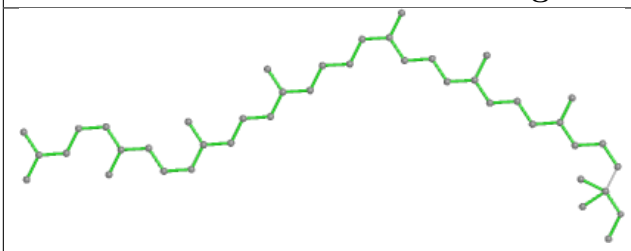


Torsions

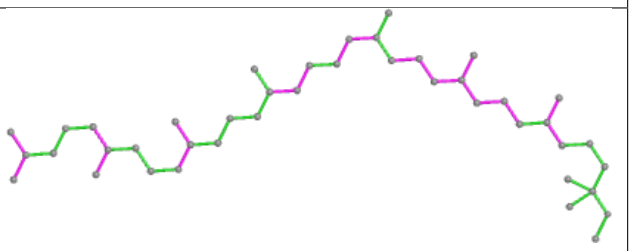


Rings

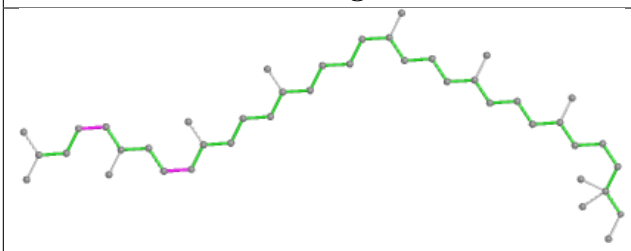
Ligand SPO s 103



Bond lengths



Bond angles



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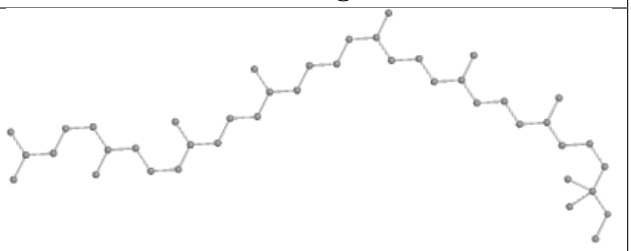
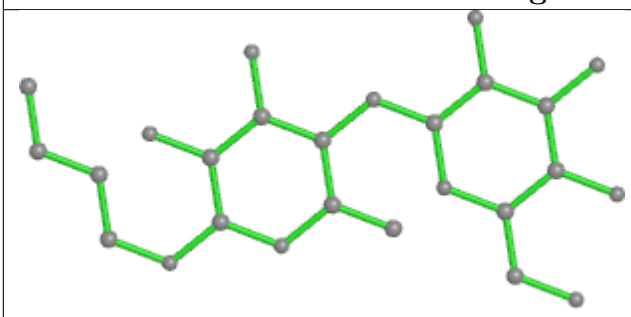


Rings

Ligand LMT i 101



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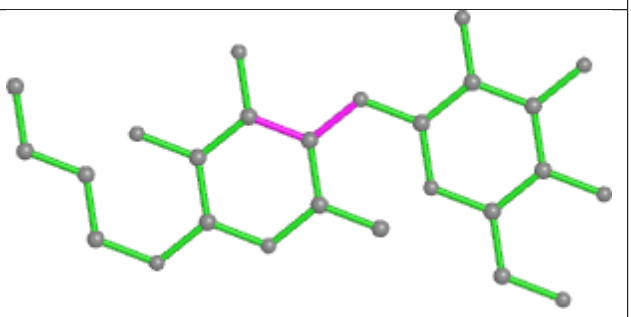
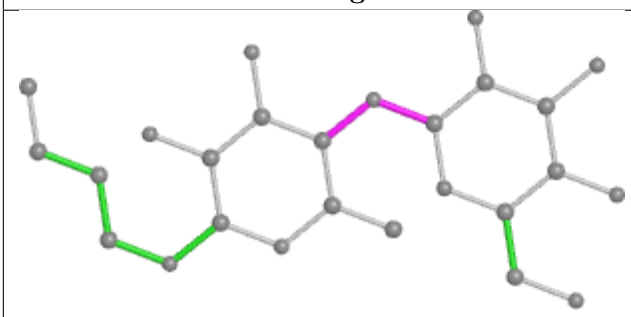
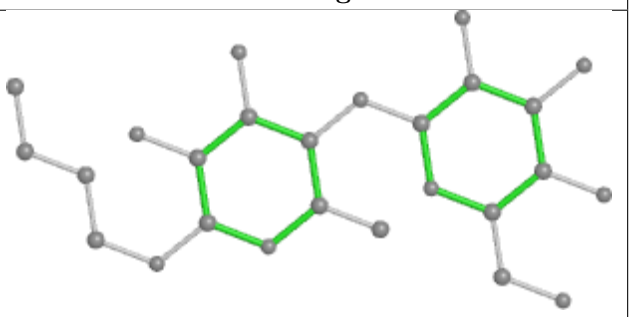


Bond angles

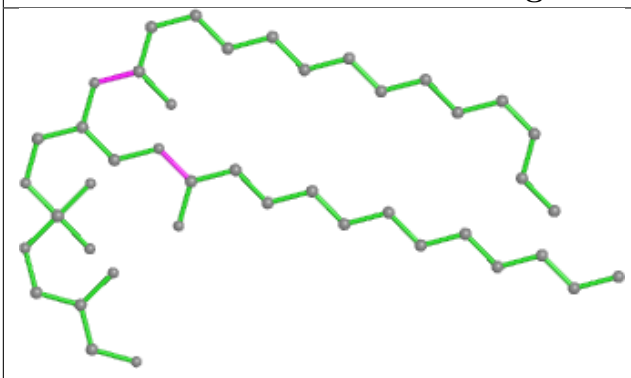


Torsions

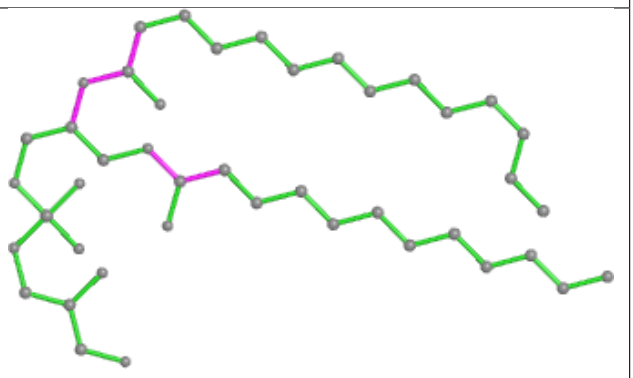


Rings

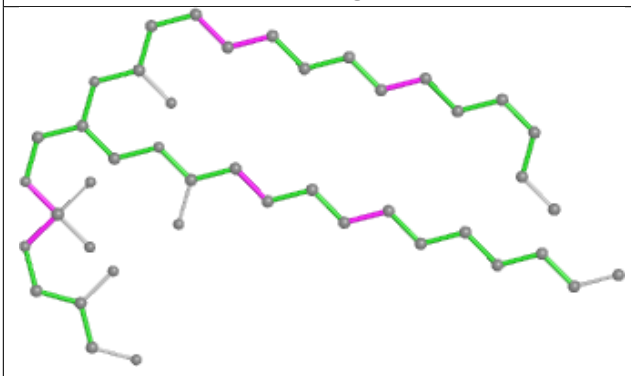
Ligand PGV 1 201



Bond lengths



Bond angles



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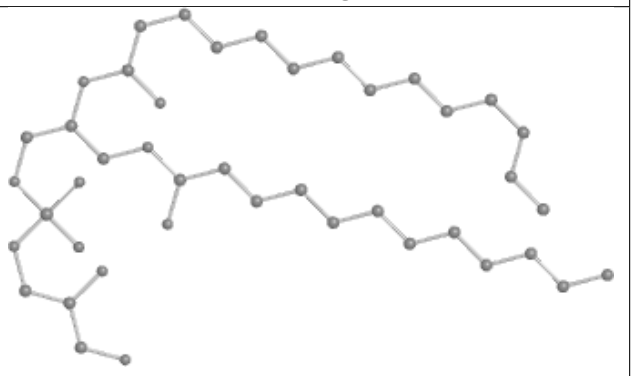
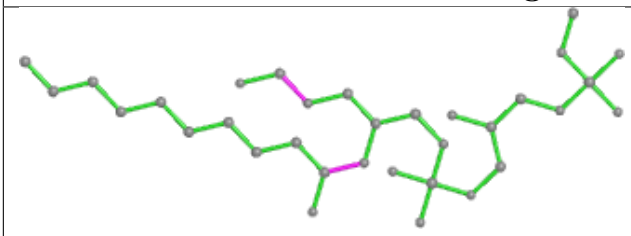
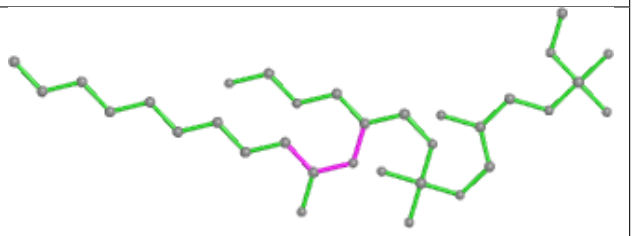


Rings

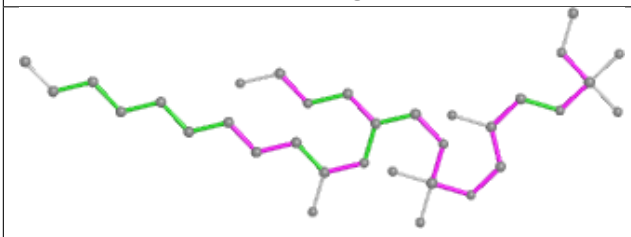
Ligand CDL X 102



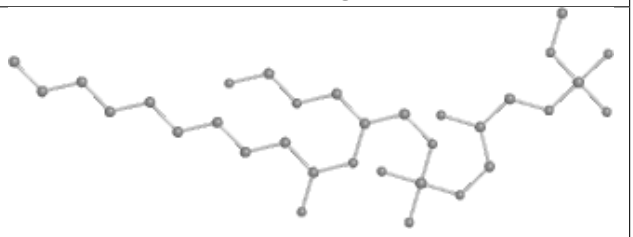
Bond lengths



Bond angles

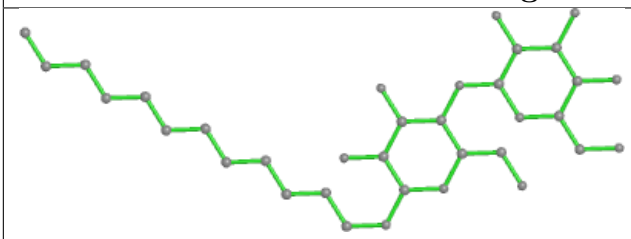


Torsions

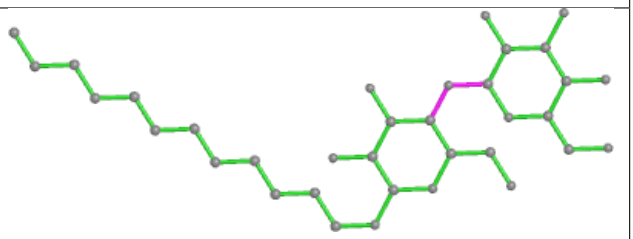


Rings

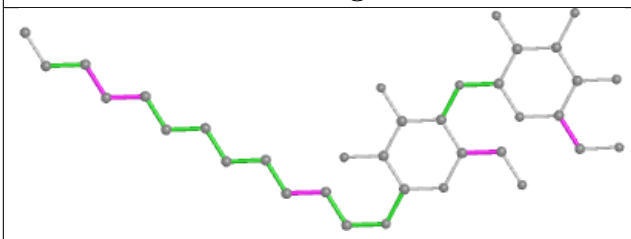
Ligand LMT A 701



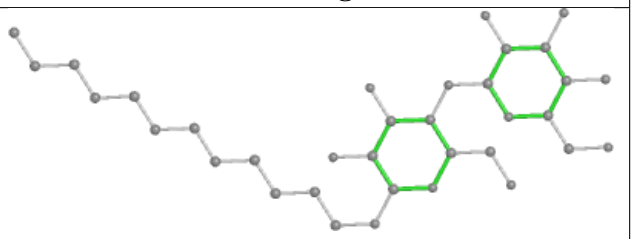
Bond lengths



Bond angles

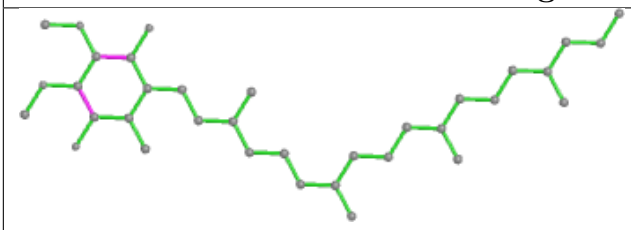


Torsions

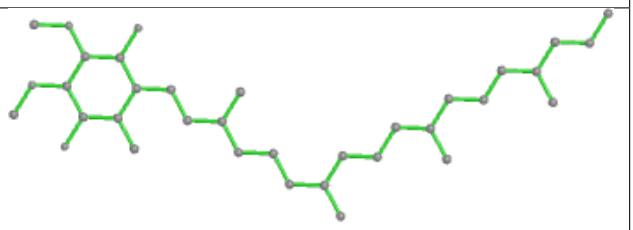


Rings

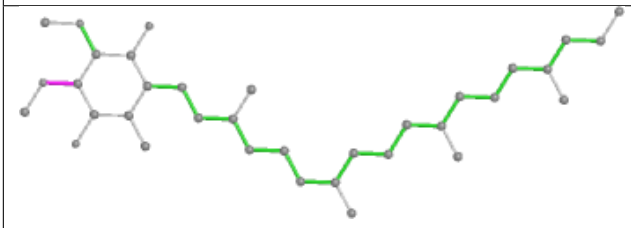
Ligand U10 l 304



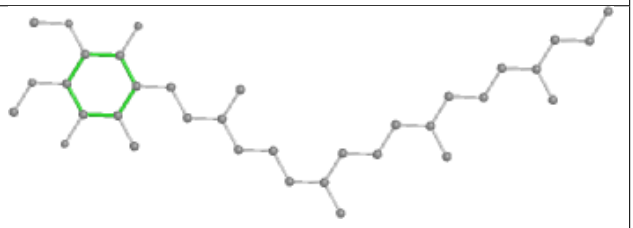
Bond lengths



Bond angles

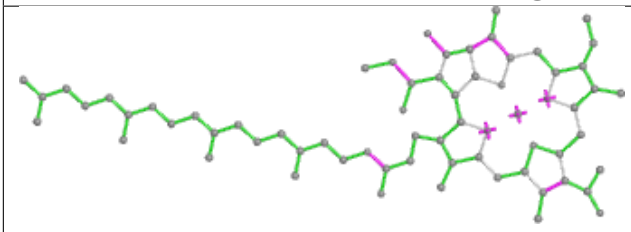


Torsions

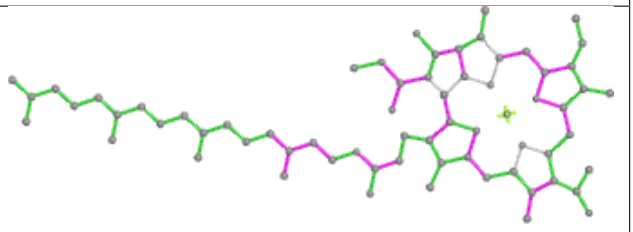


Rings

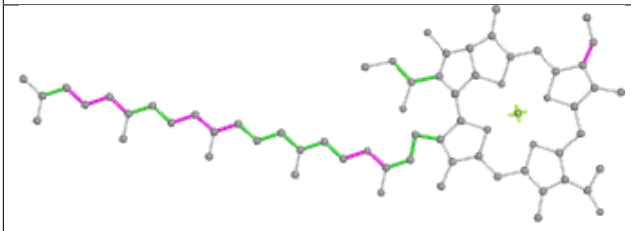
Ligand BCL k 101



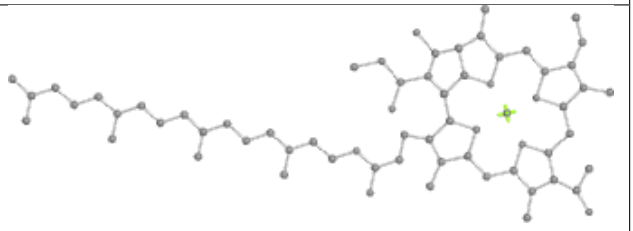
Bond lengths



Bond angles

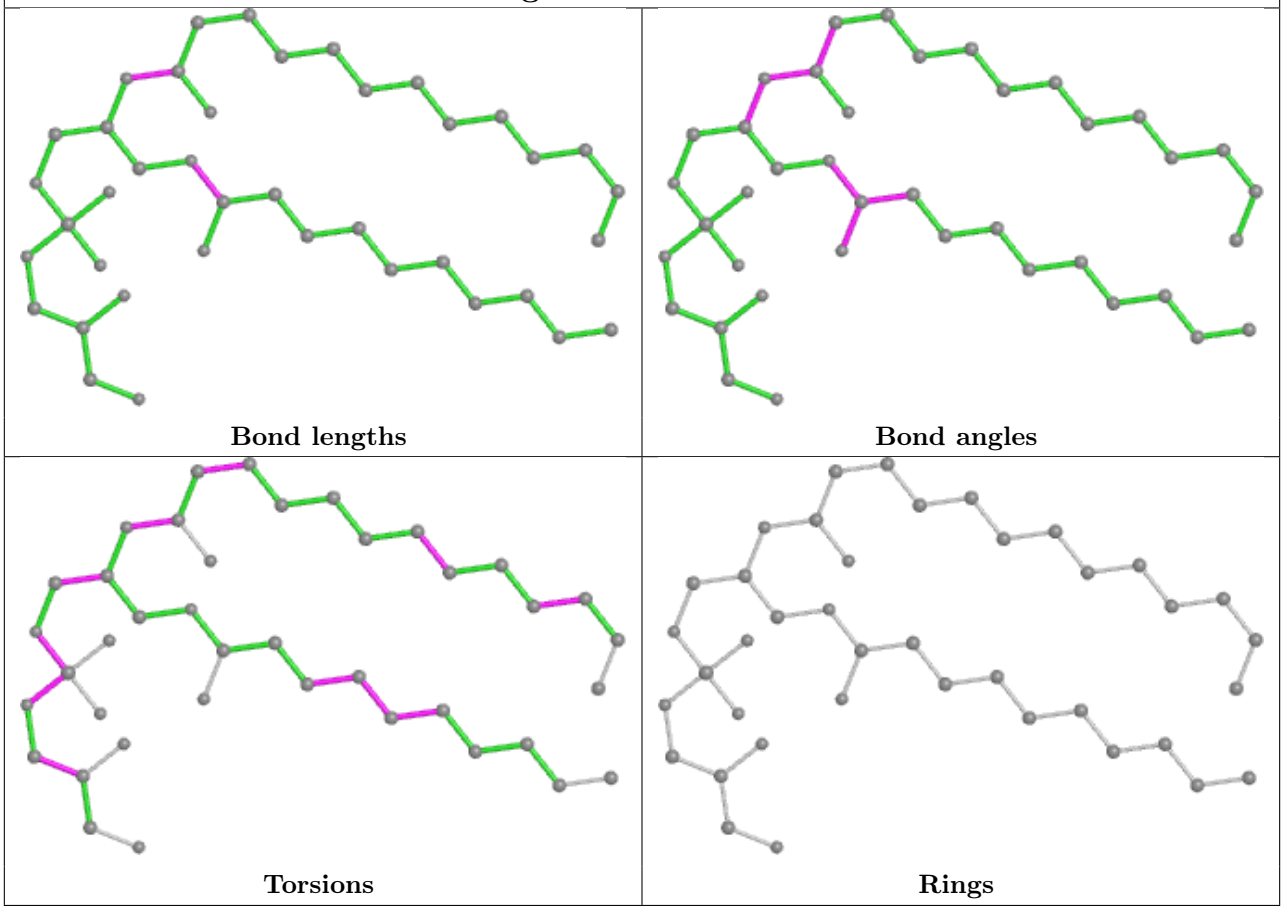


Torsions

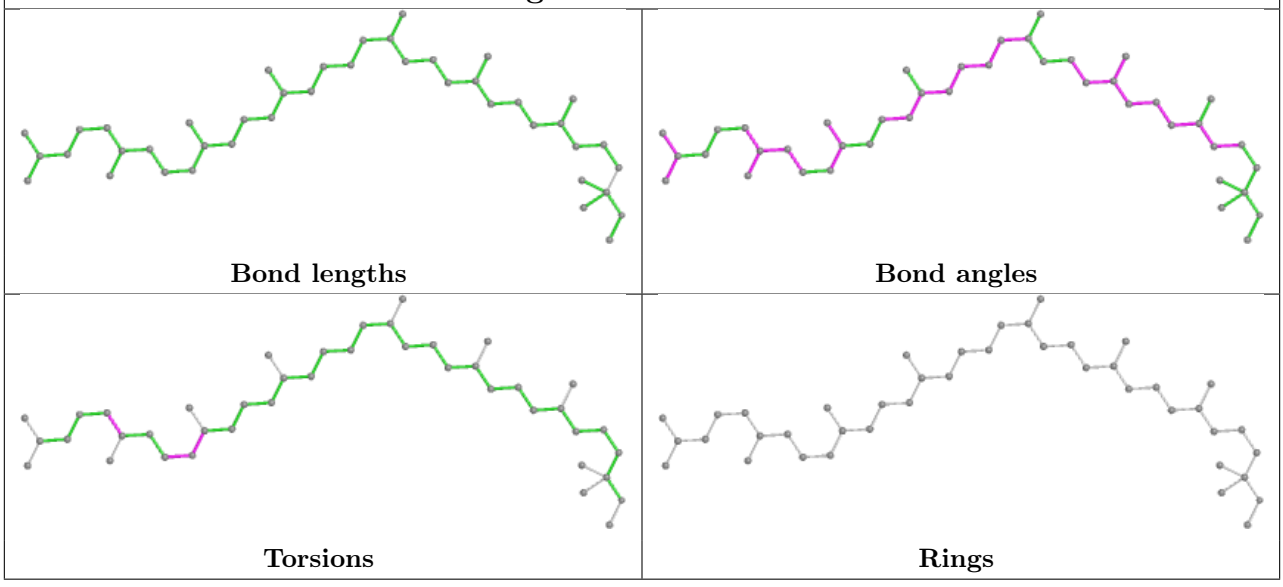


Rings

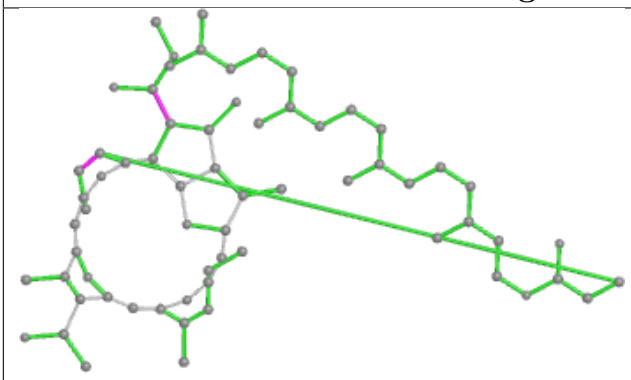
Ligand PGV H 805



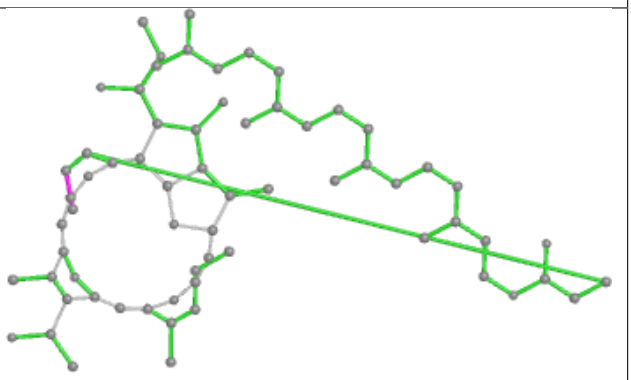
Ligand SPO Y 103



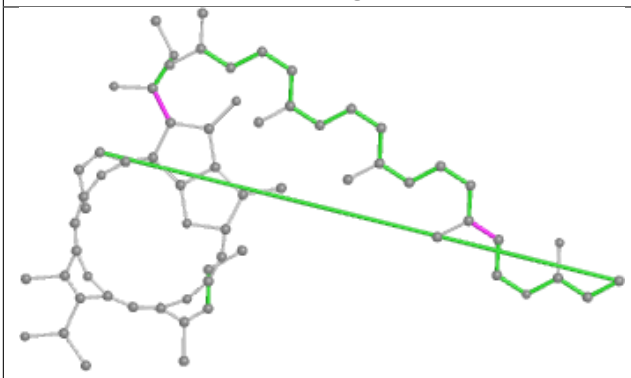
Ligand BPH M 403



Bond lengths



Bond angles



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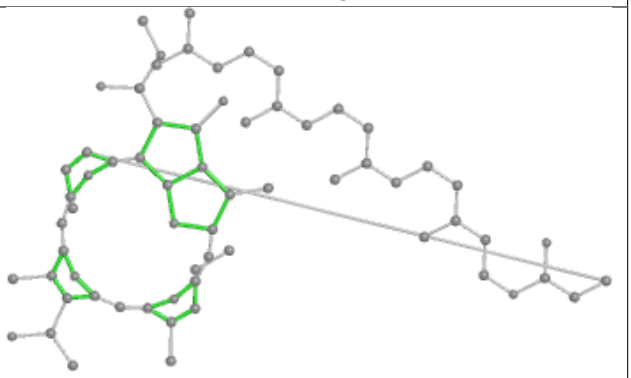
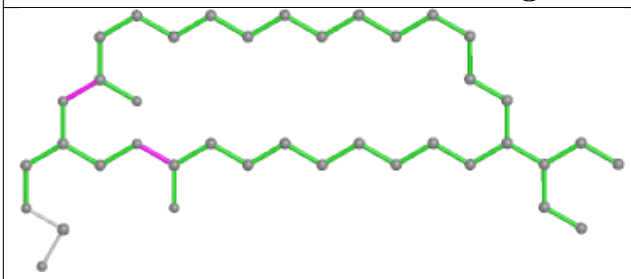


Rings

Ligand PGV K 403



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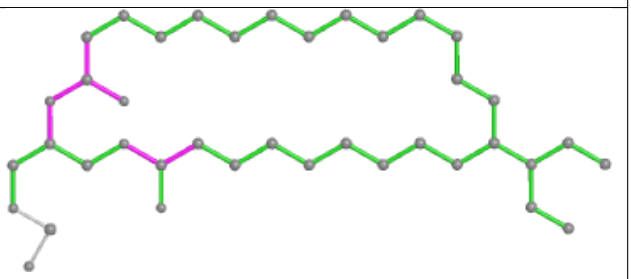
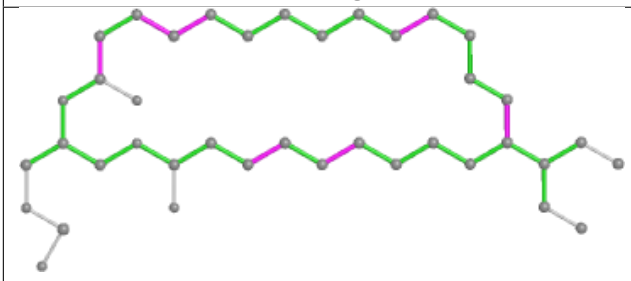


Bond angles



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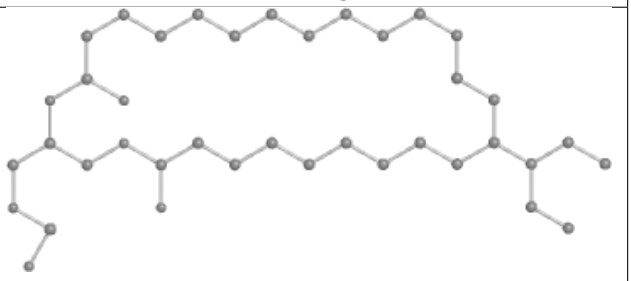
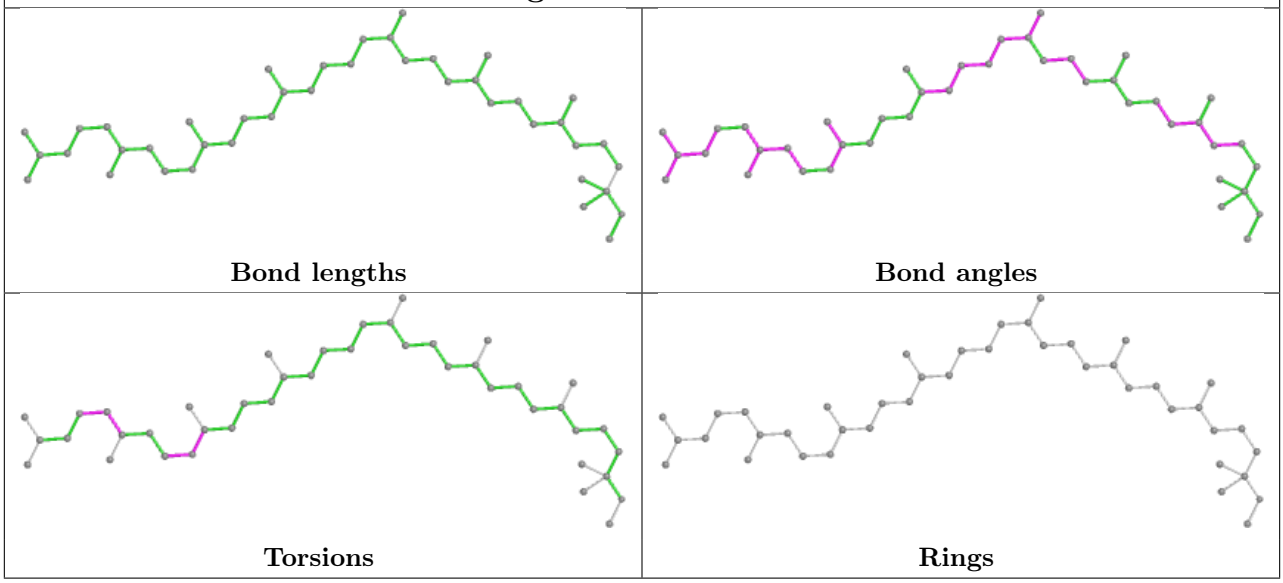
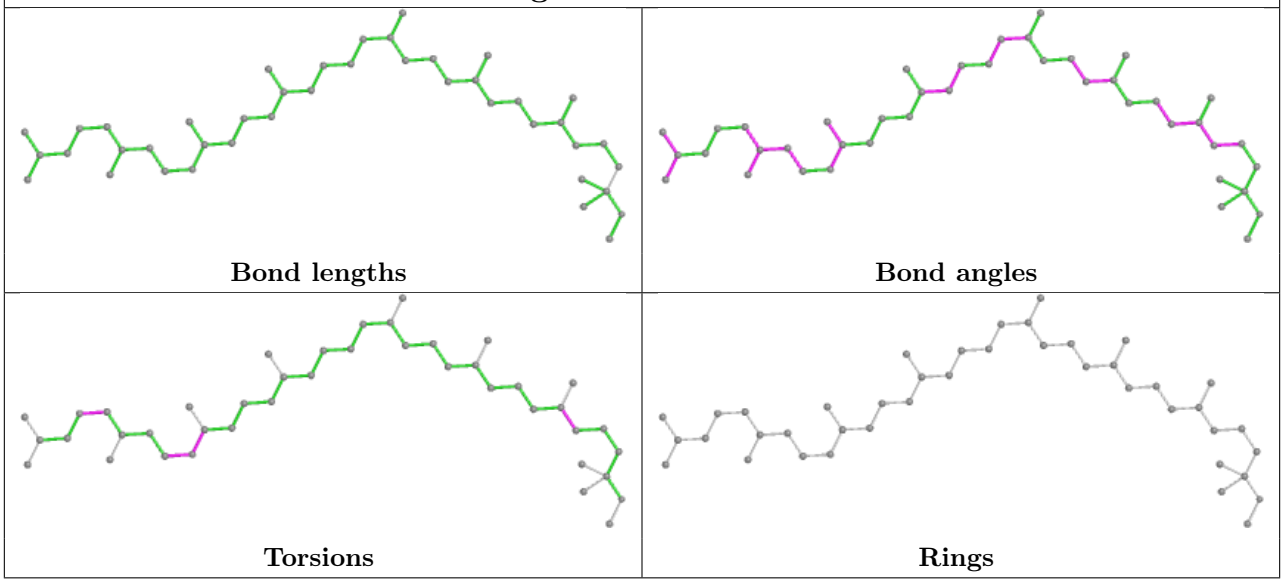


Rings

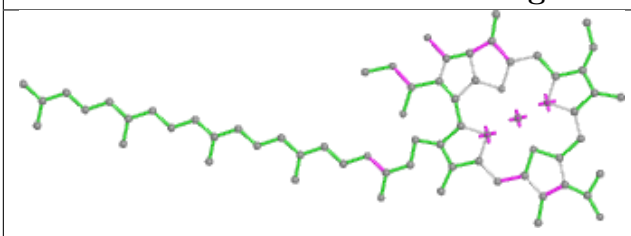
Ligand SPO w 101



Ligand SPO 2 102



Ligand BCL n 102



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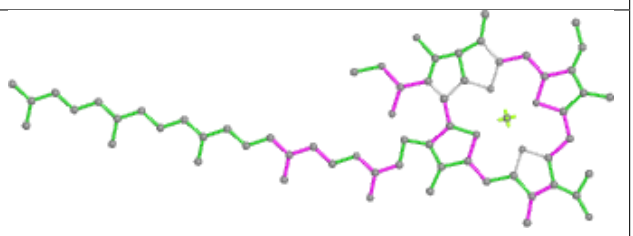
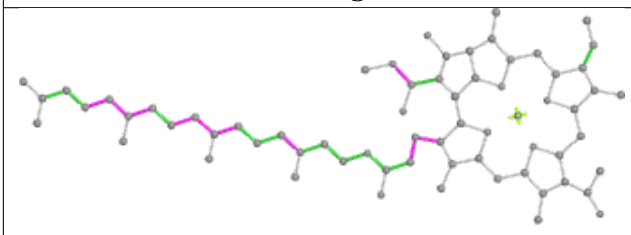
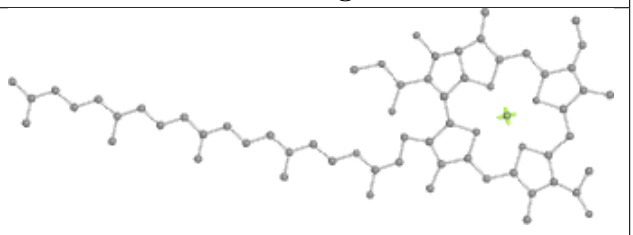


Bond angles

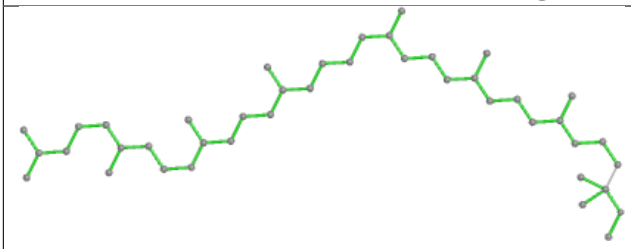


Torsions

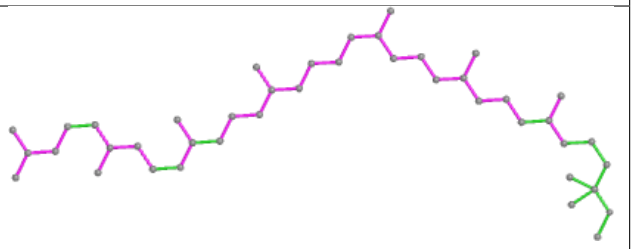


Rings

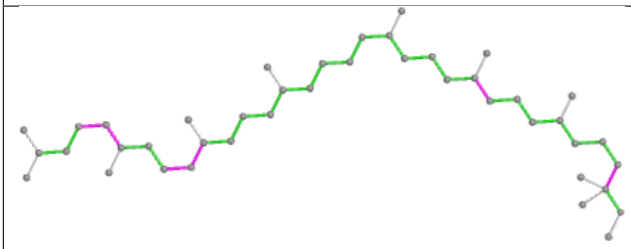
Ligand SPO f 101



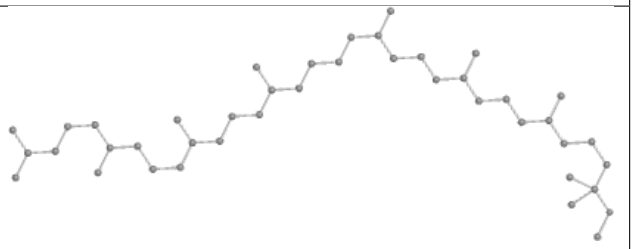
Bond lengths



Bond angles

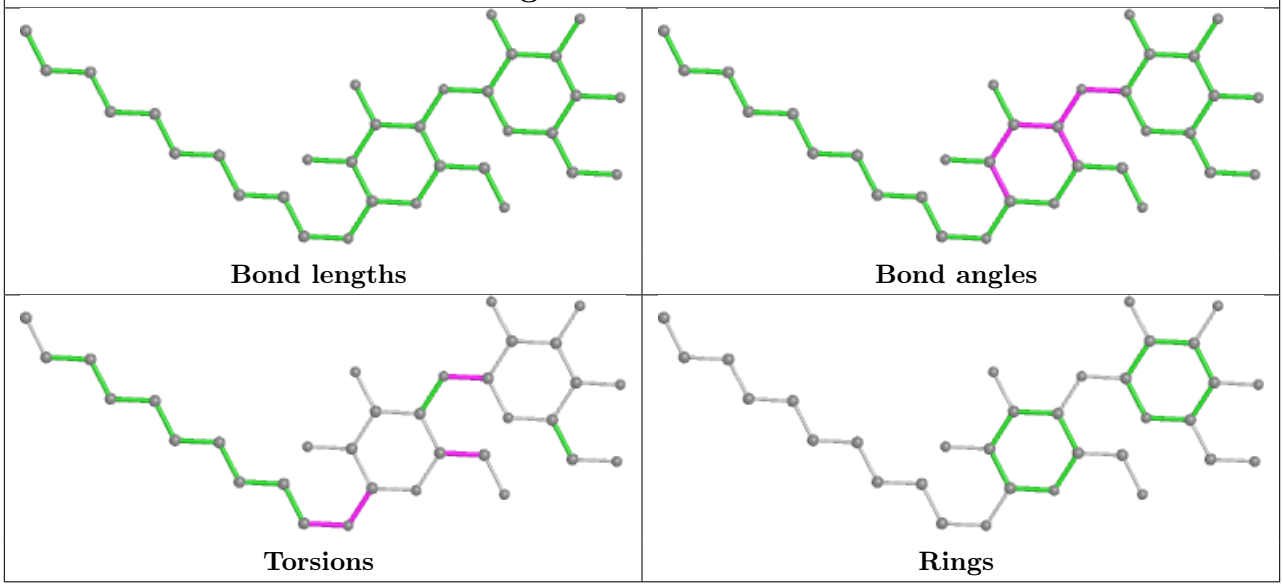


Torsions

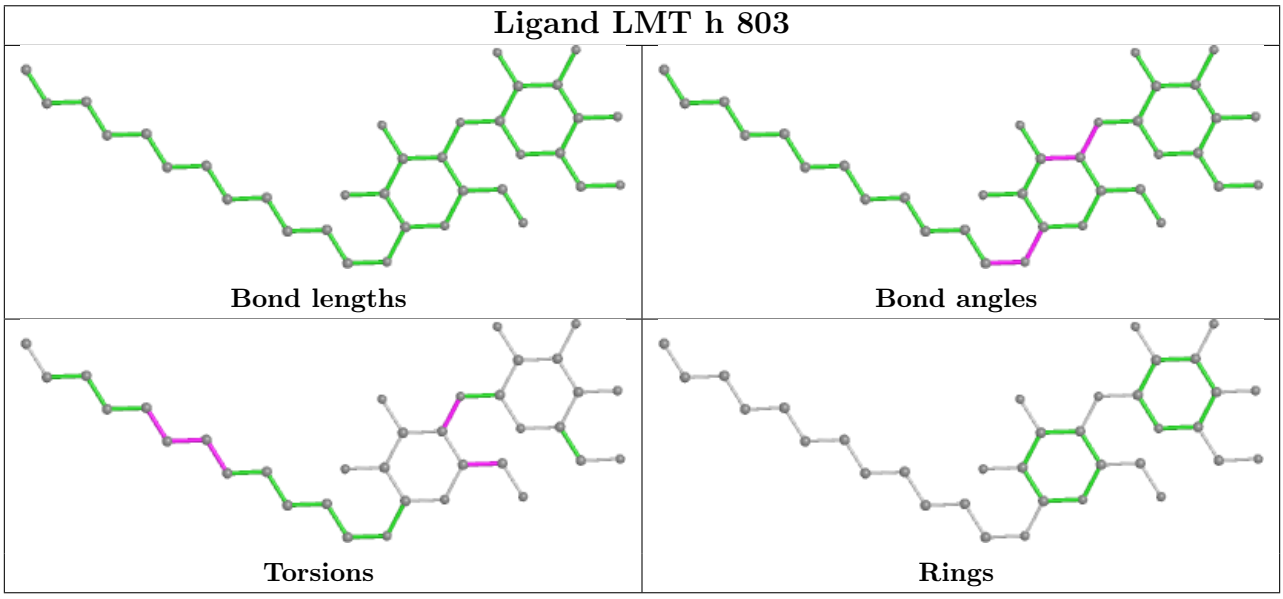


Rings

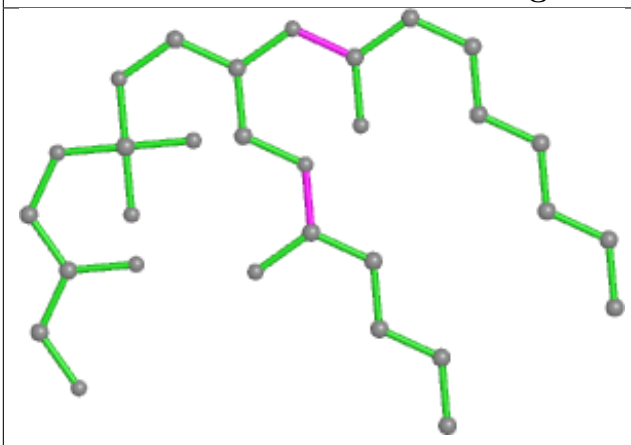
Ligand LMT m 409



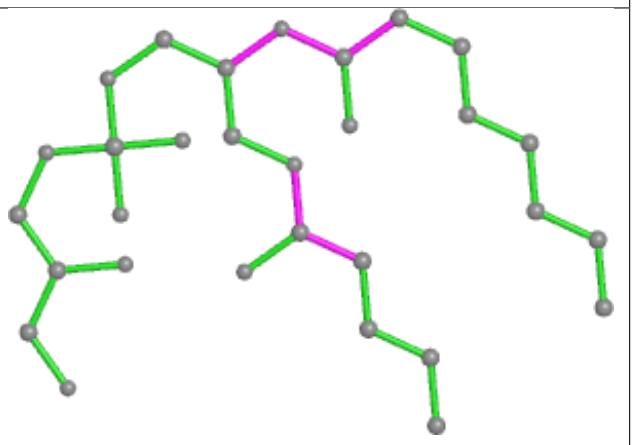
Ligand LMT h 803



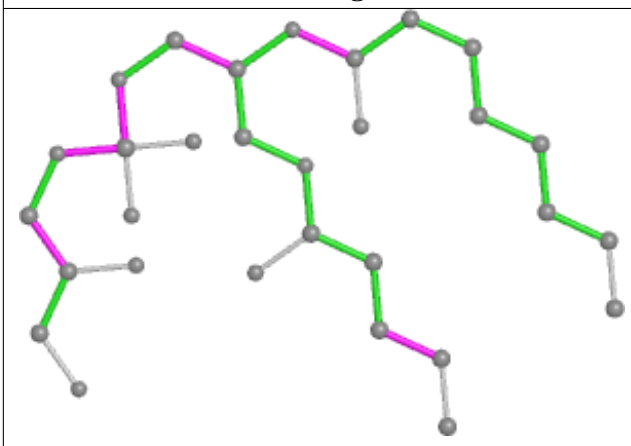
Ligand PGV l 307



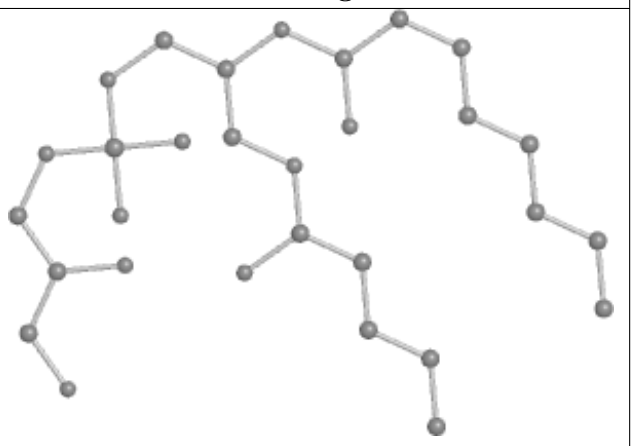
Bond lengths



Bond angles

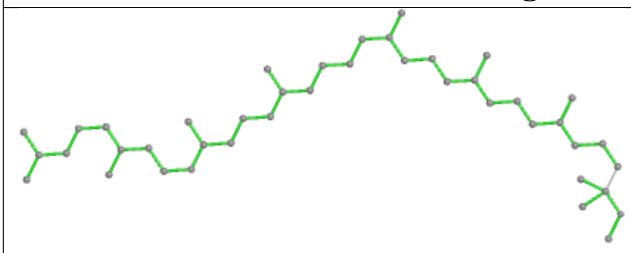


Torsions

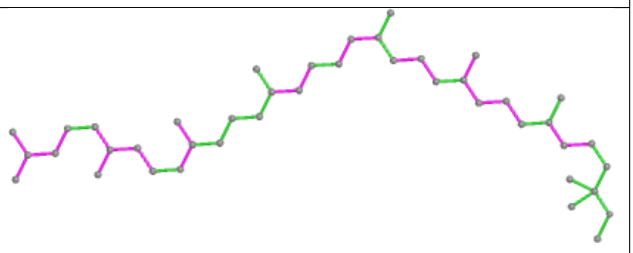


Rings

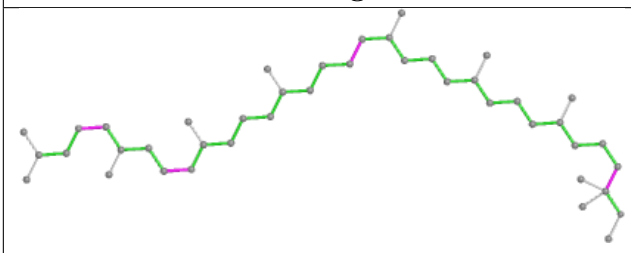
Ligand SPO 05 102



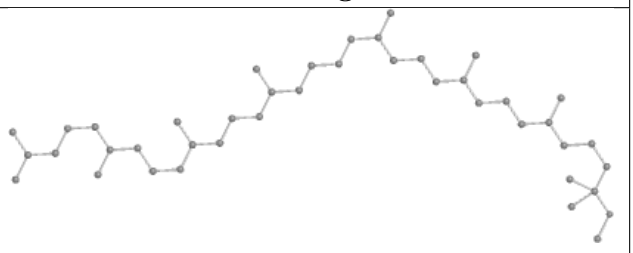
Bond lengths



Bond angles

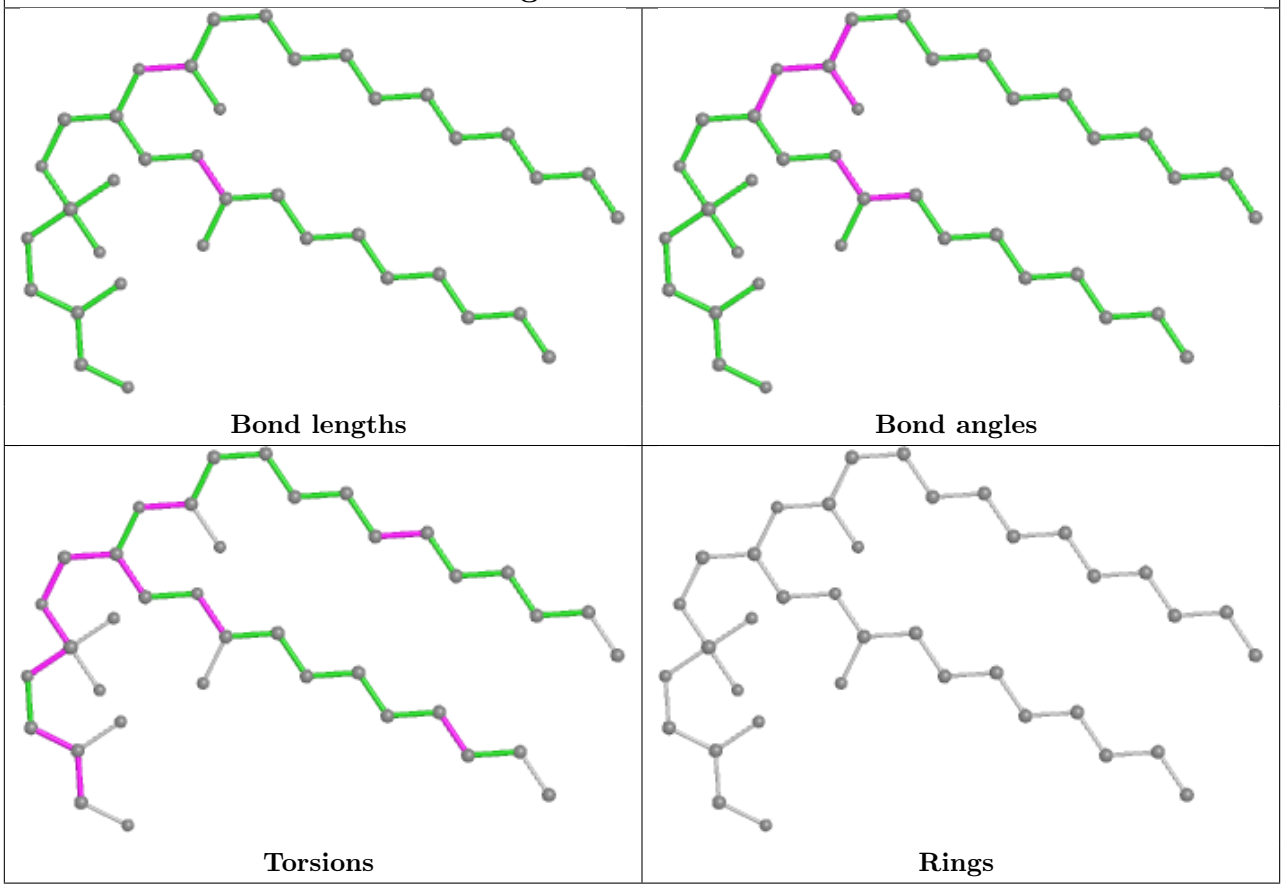


Torsions

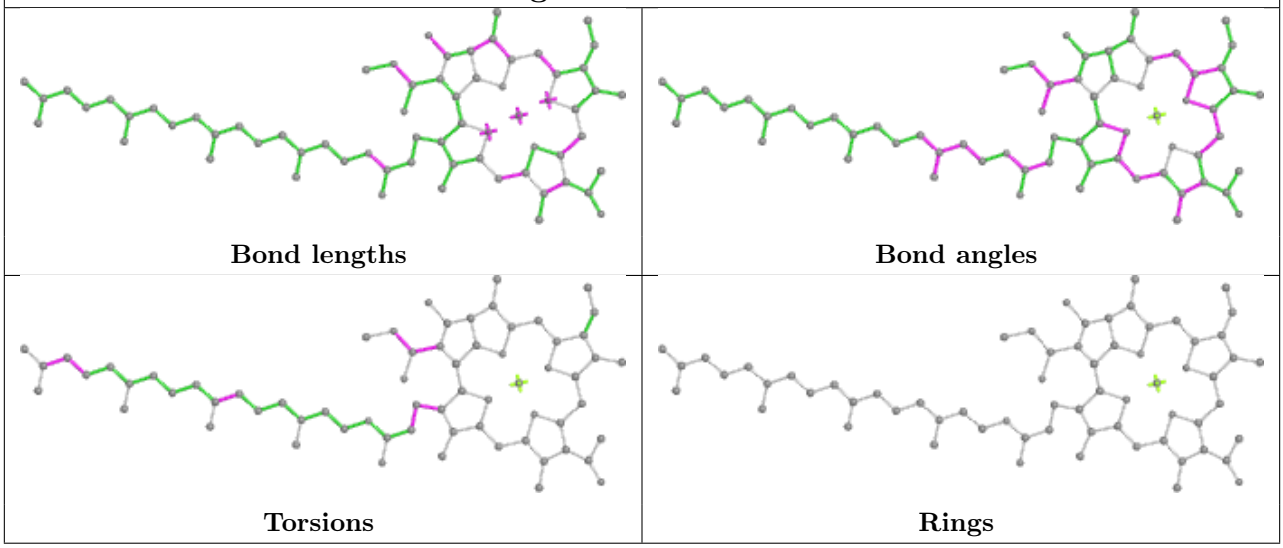


Rings

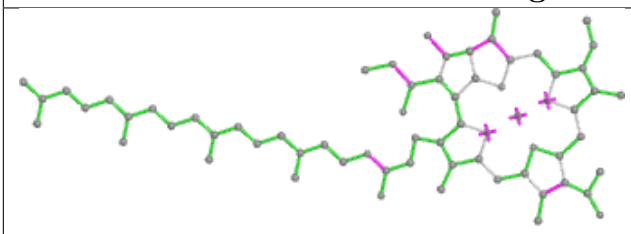
Ligand PGV m 411



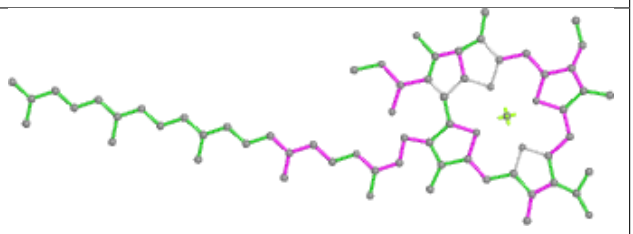
Ligand BCL 4 101



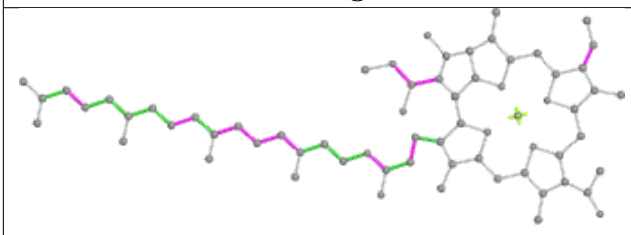
Ligand BCL v 101



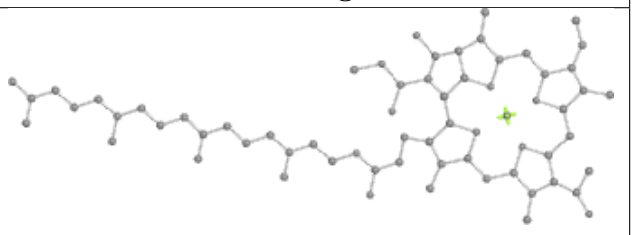
Bond lengths



Bond angles

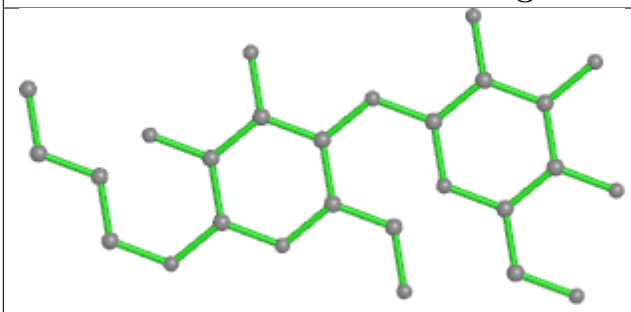


Torsions

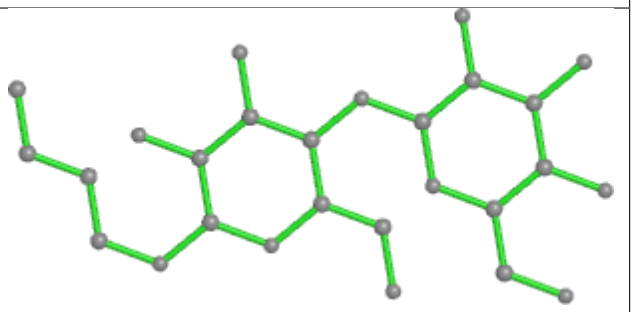


Rings

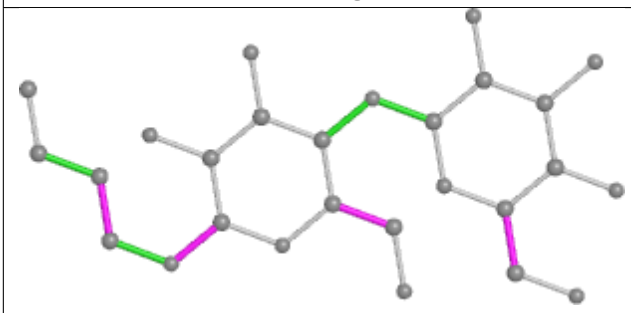
Ligand LMT 03 103



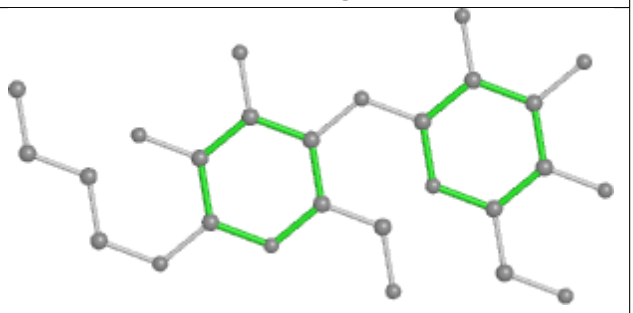
Bond lengths



Bond angles

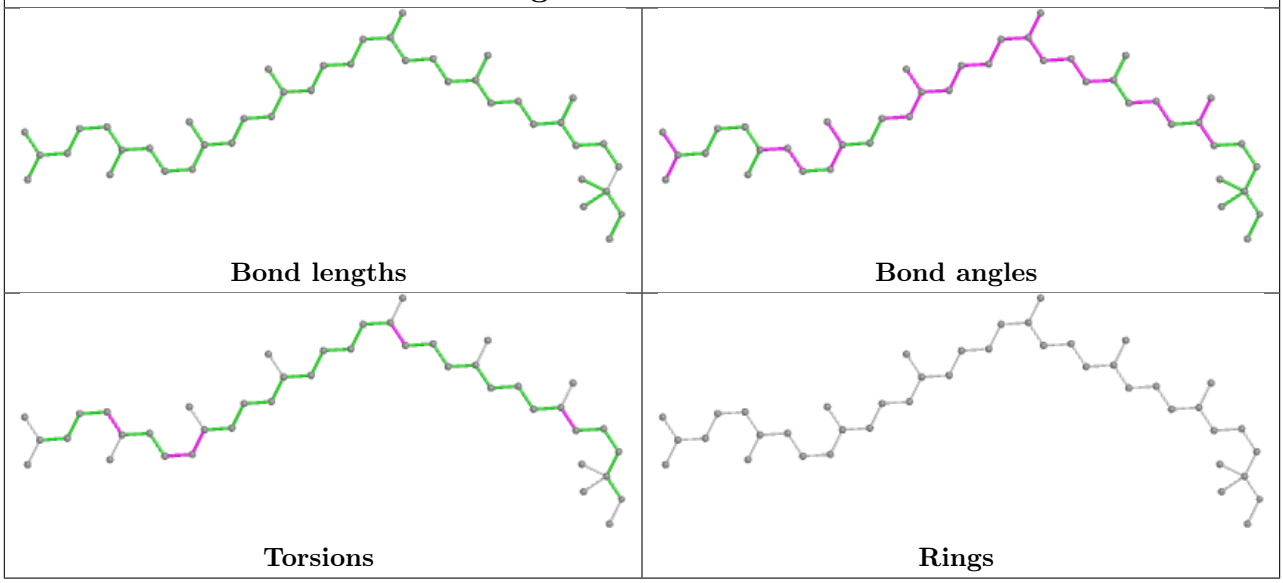


Torsions

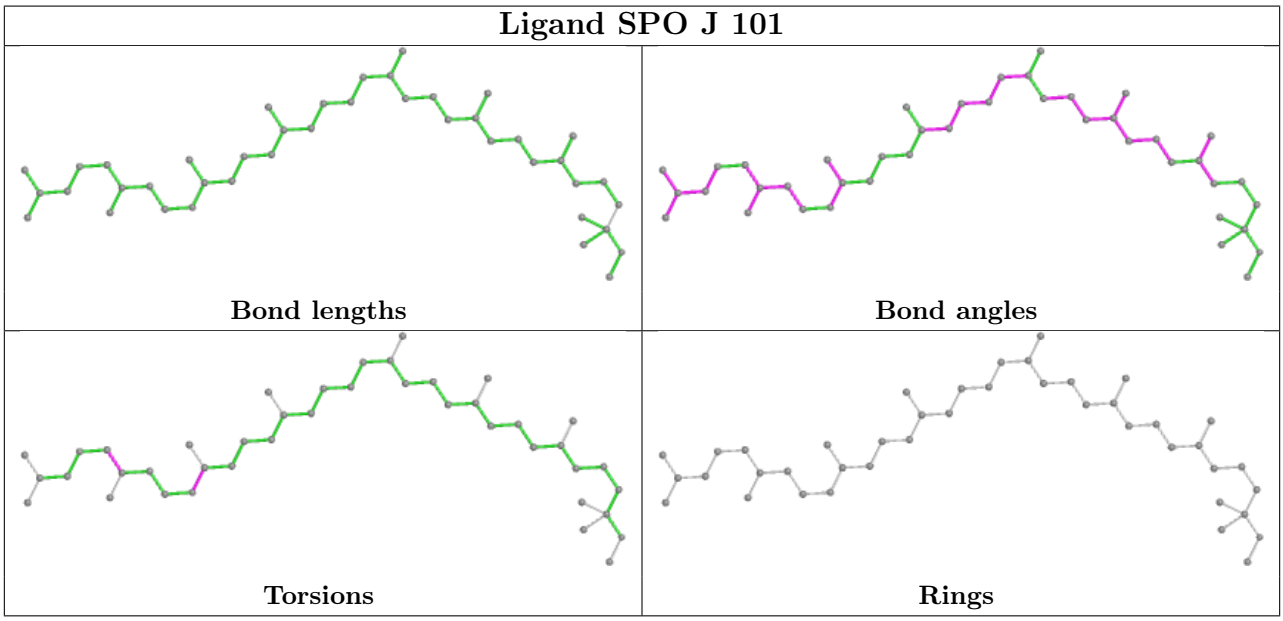


Rings

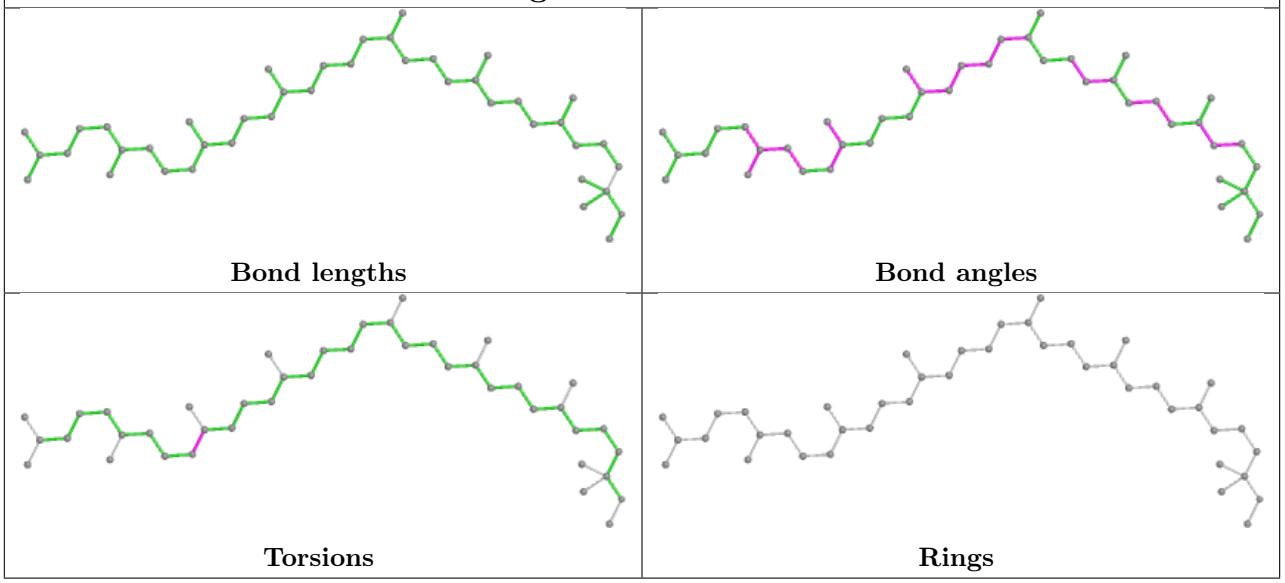
Ligand SPO 2 101



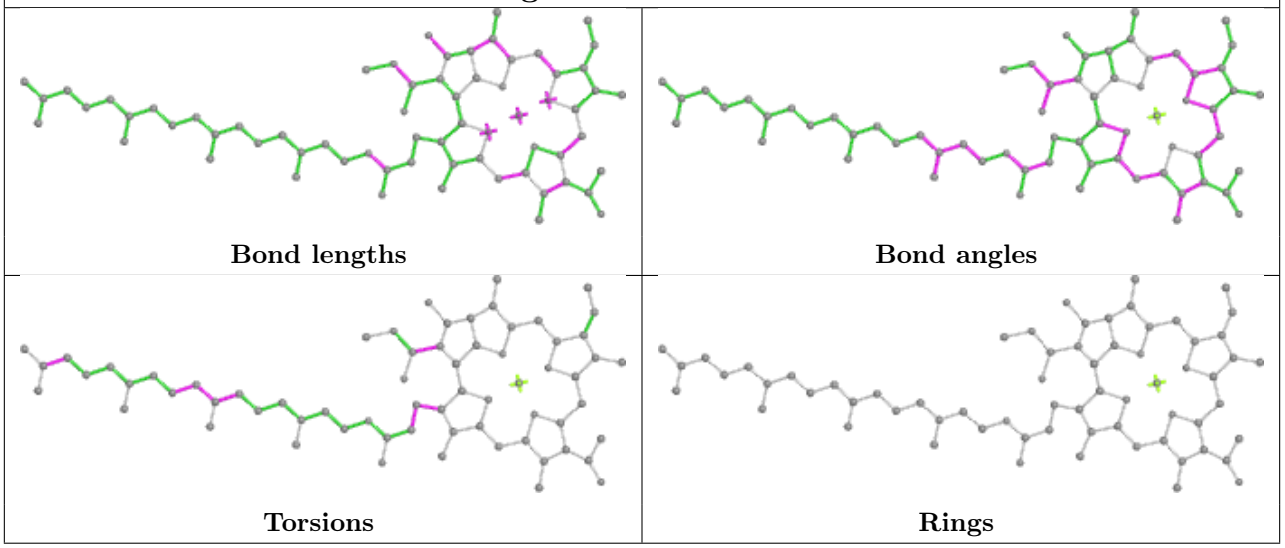
Ligand SPO J 101



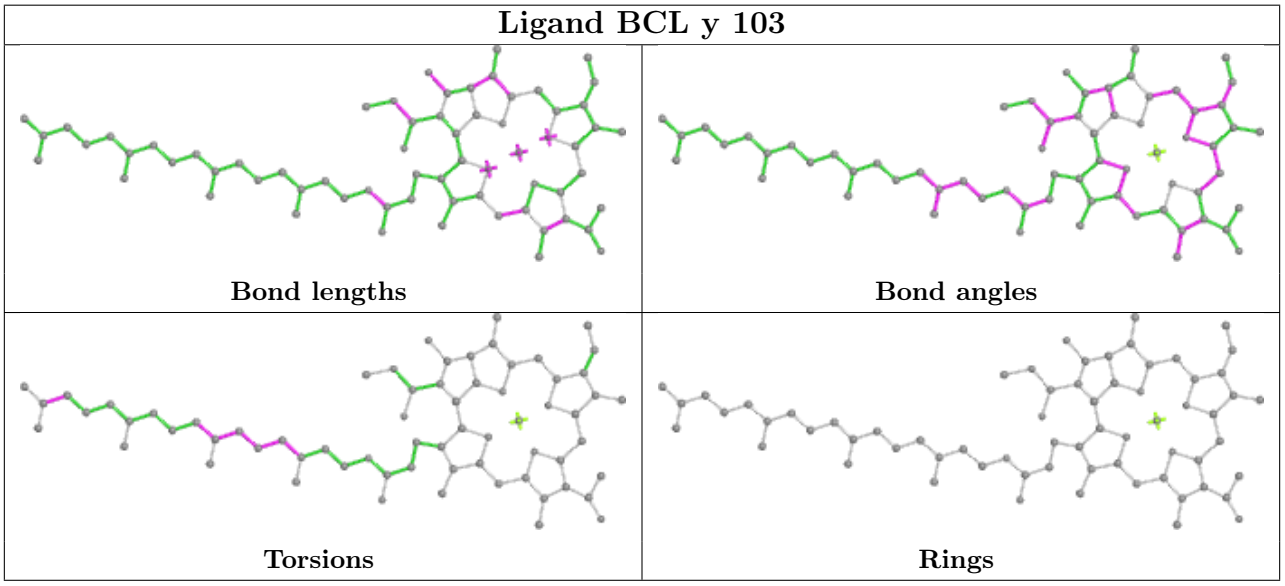
Ligand SPO S 103



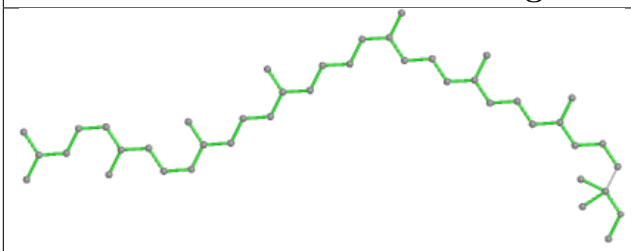
Ligand BCL 04 101



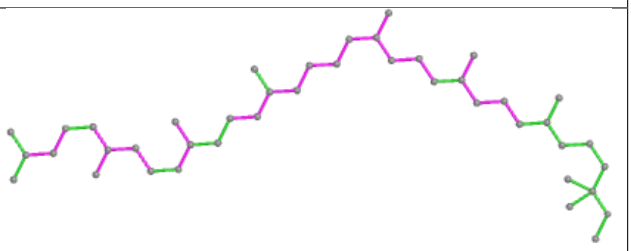
Ligand BCL y 103



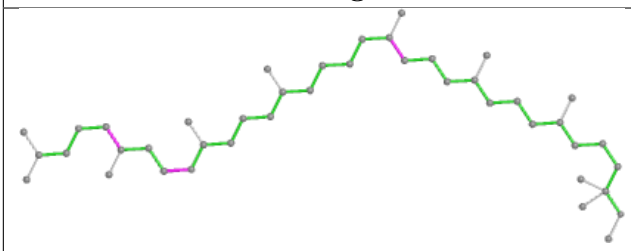
Ligand SPO V 102



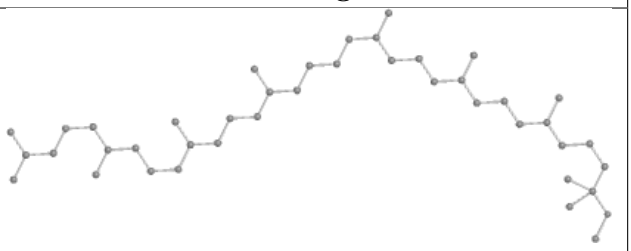
Bond lengths



Bond angles

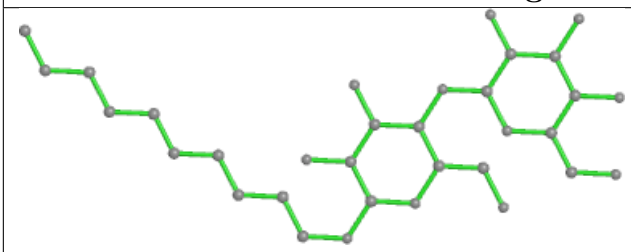


Torsions

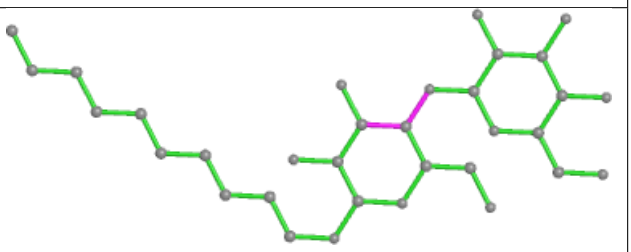


Rings

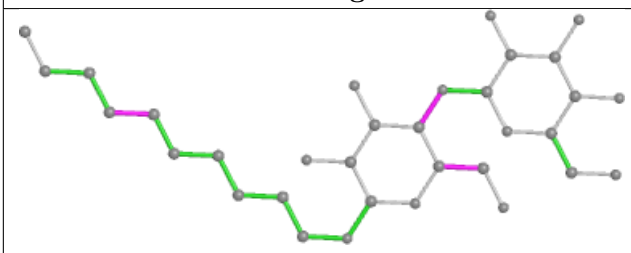
Ligand LMT 5 101



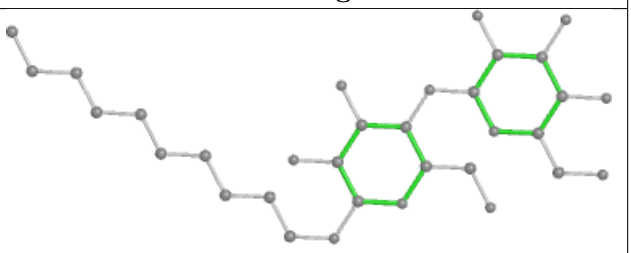
Bond lengths



Bond angles

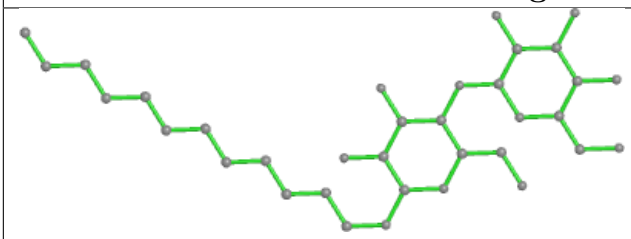


Torsions



Rings

Ligand LMT i 102



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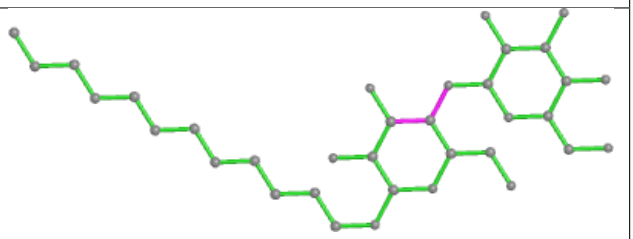

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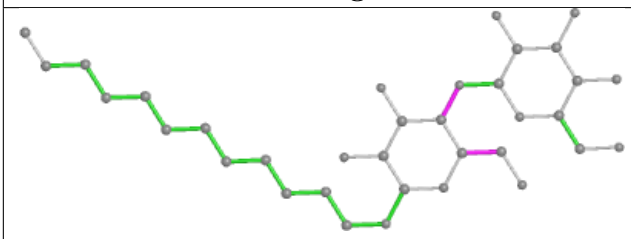

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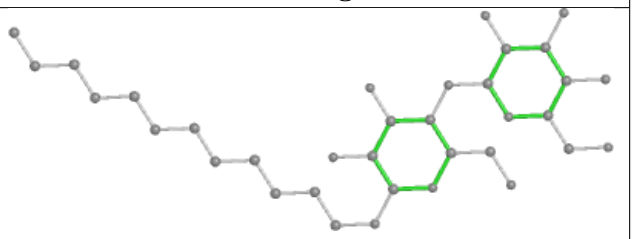
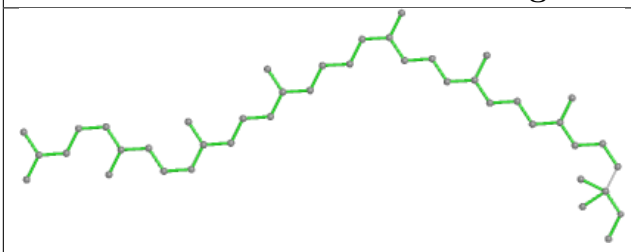


Rings

Ligand SPO v 102



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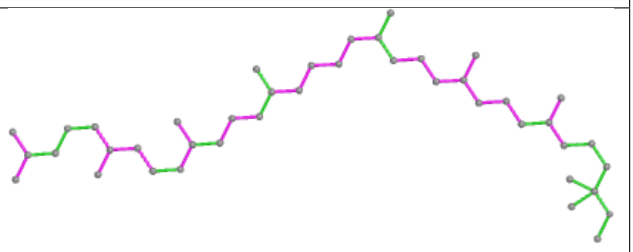

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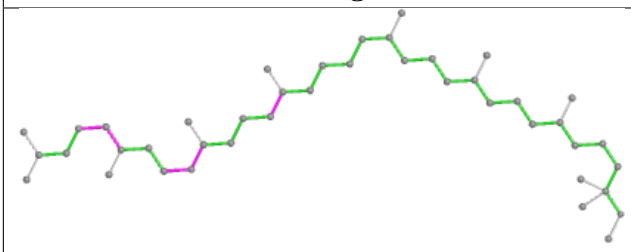

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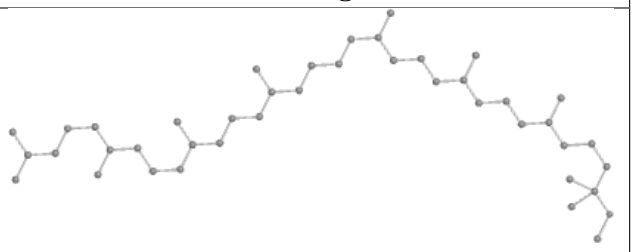
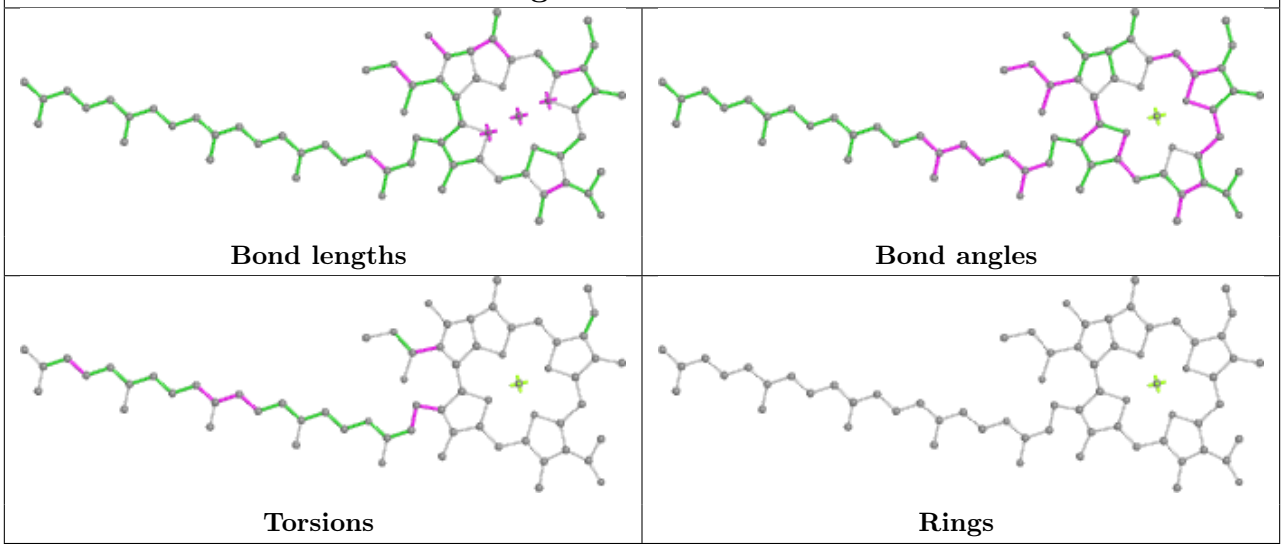


Rings

Ligand BCL e 102



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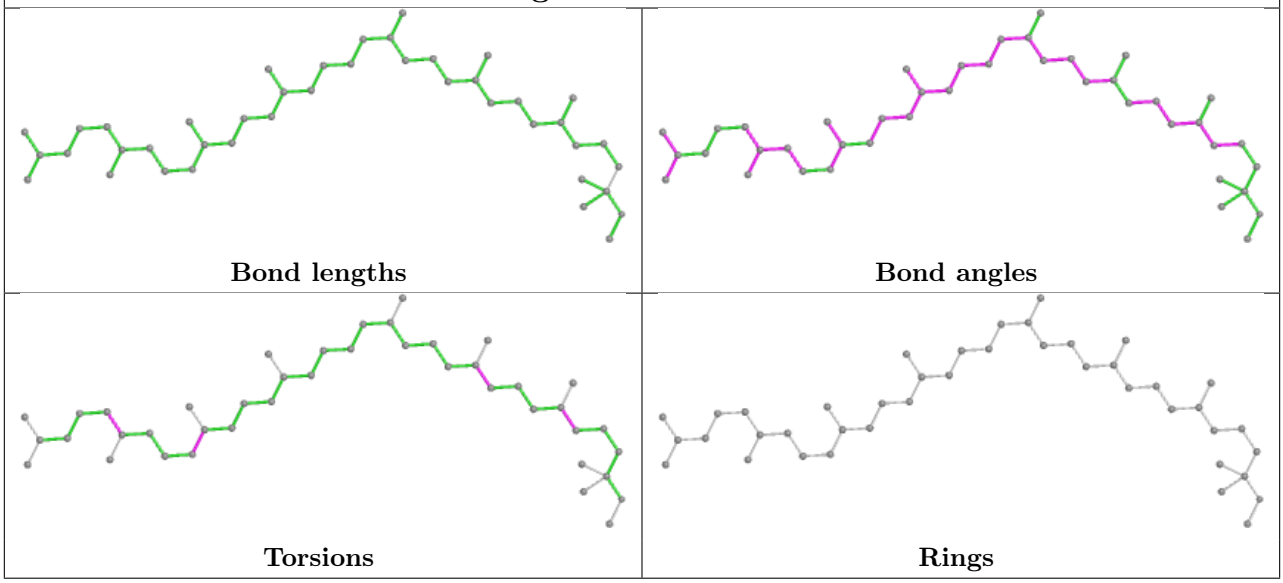

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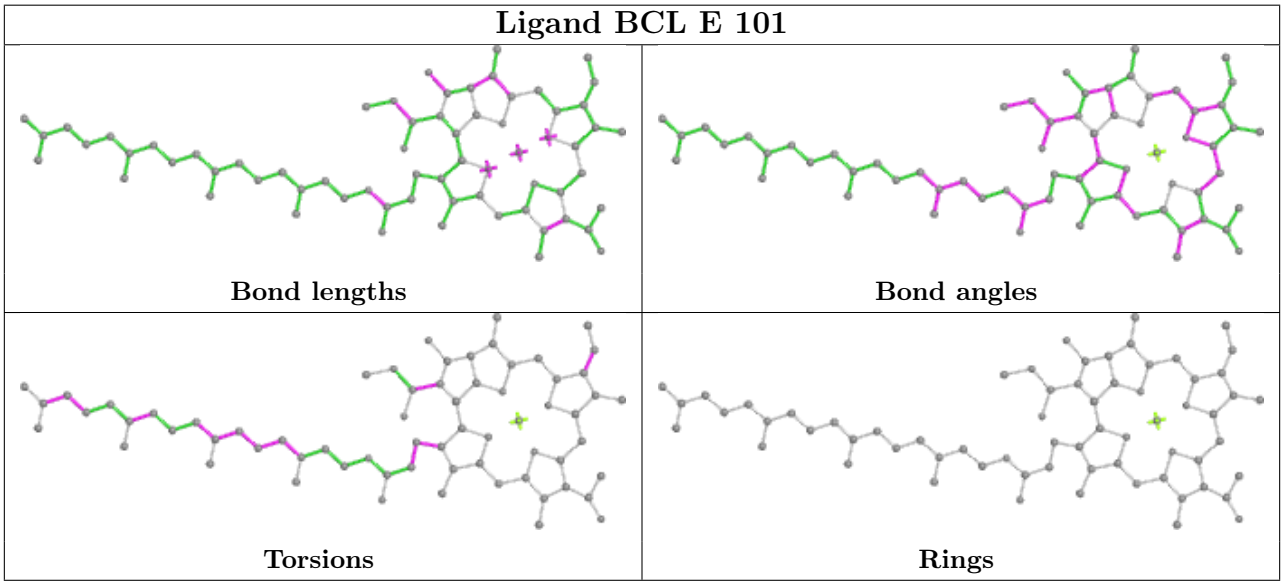

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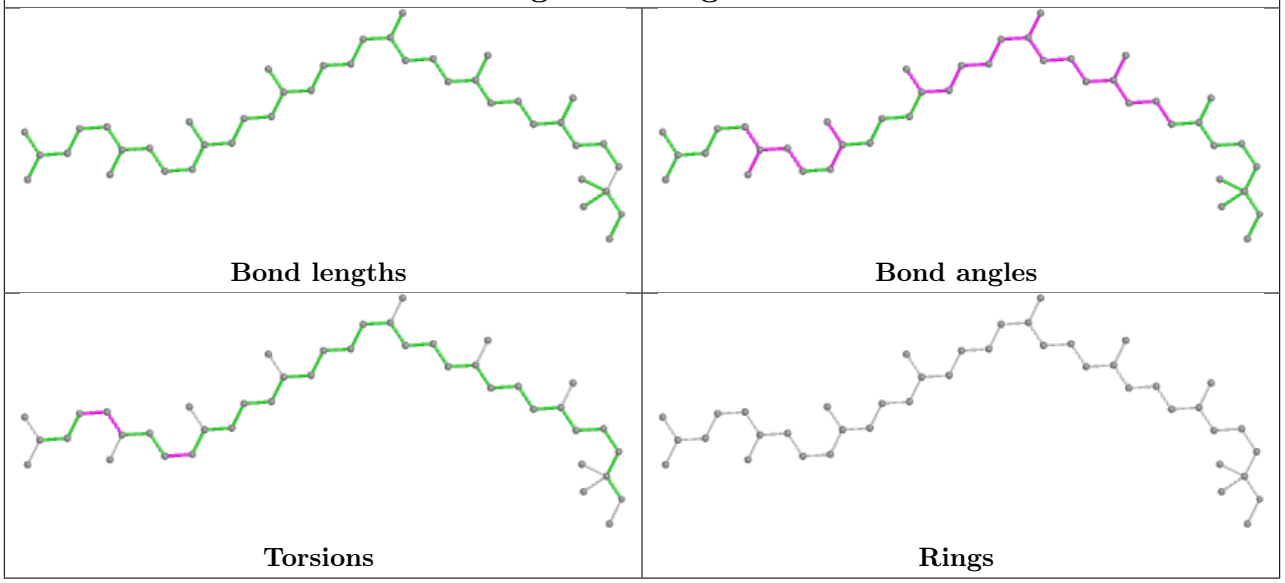

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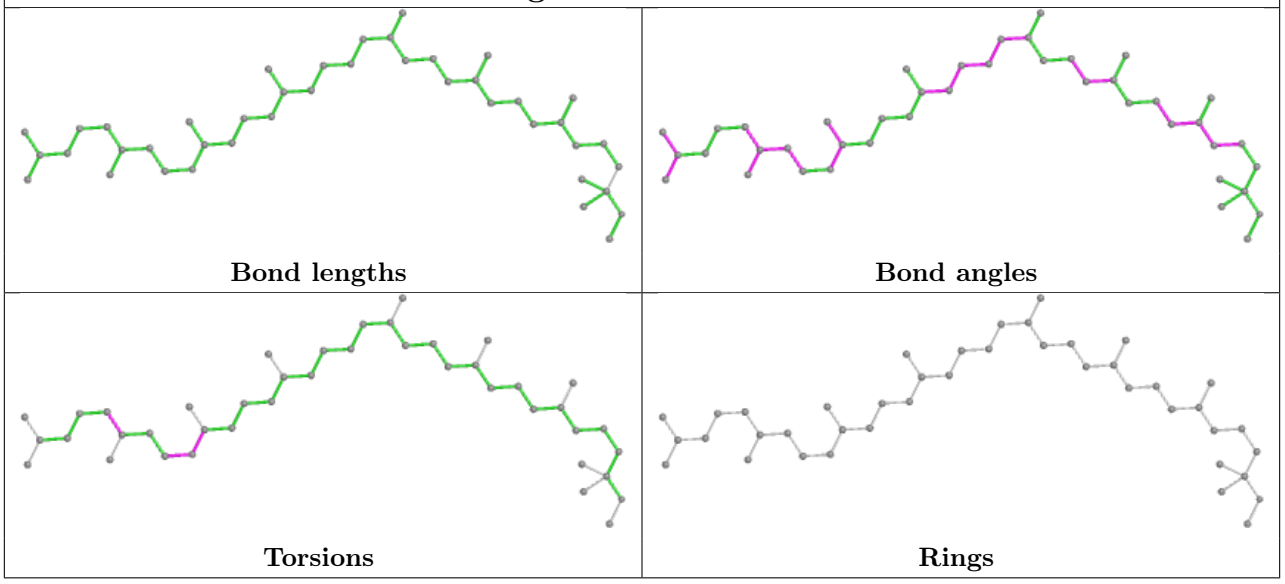

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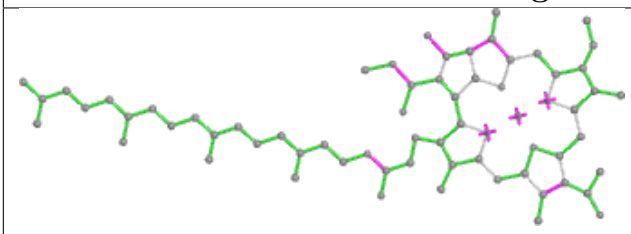
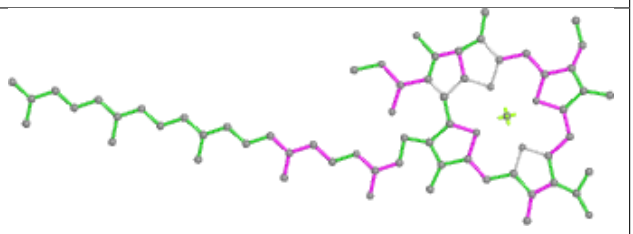
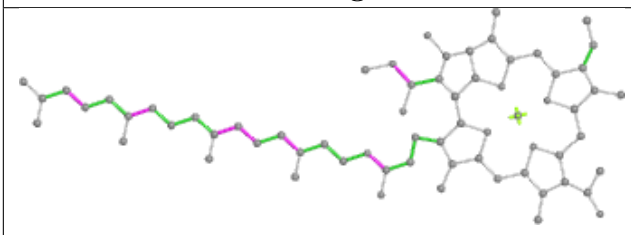


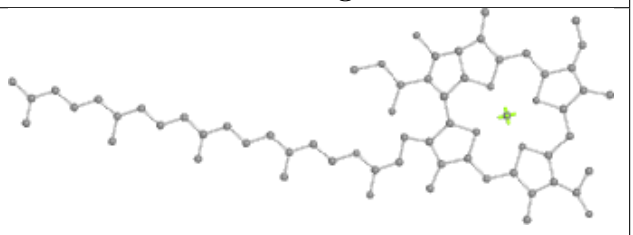
Bond lengths



Bond angles

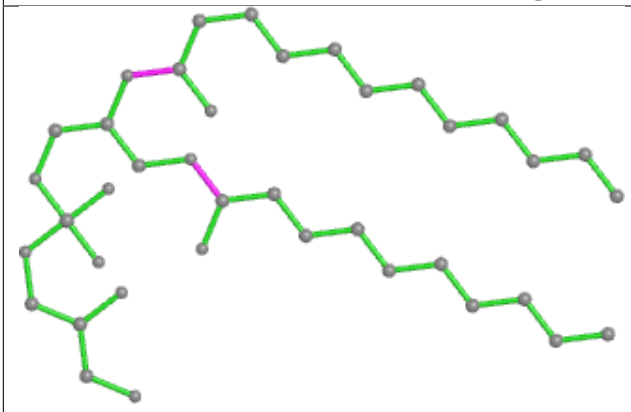


Torsions



Rings

Ligand PGV l 305



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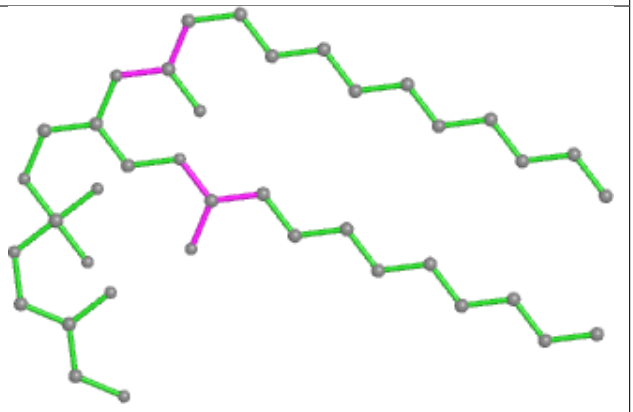
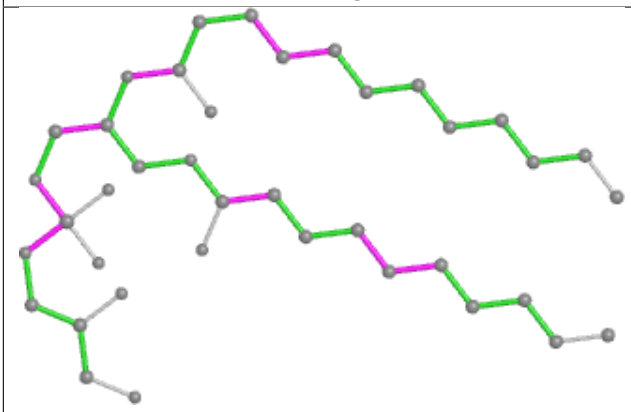


Bond angles



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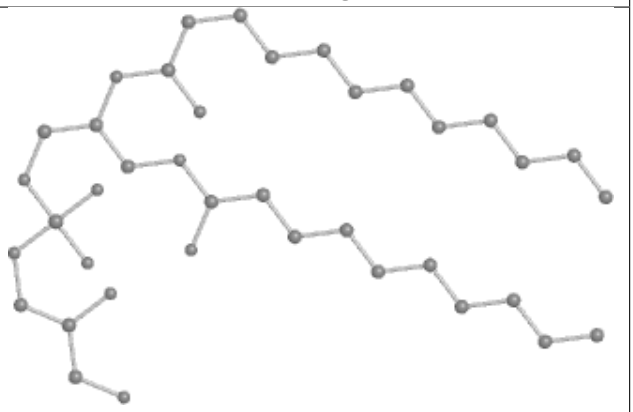
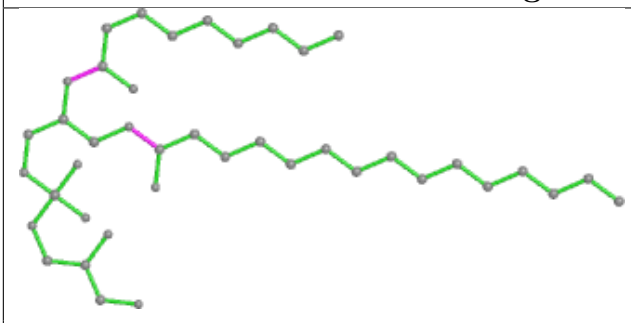


Rings

Ligand PGV F 503



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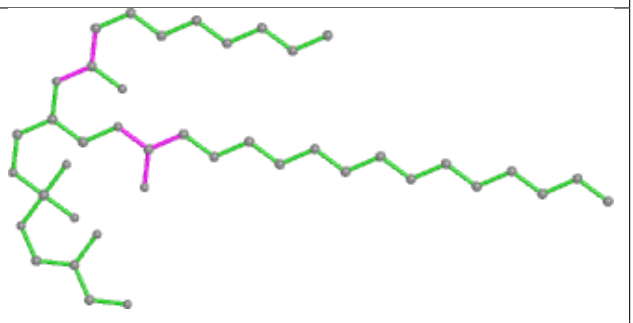
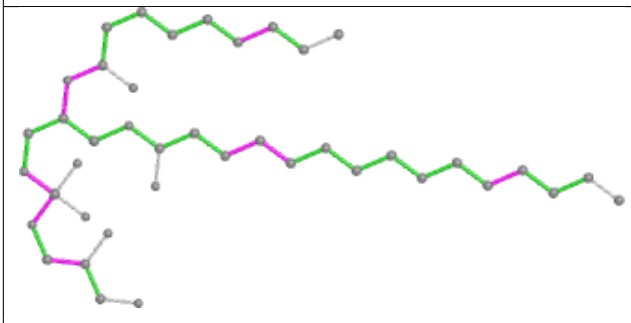


Bond angles



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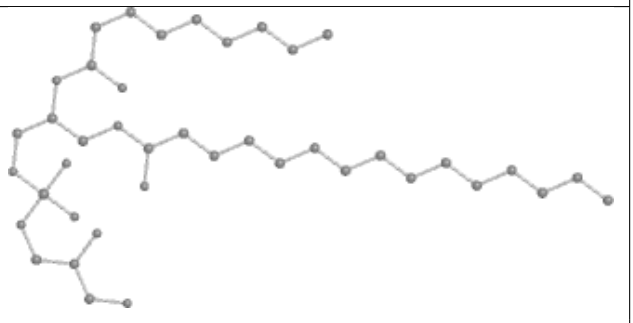
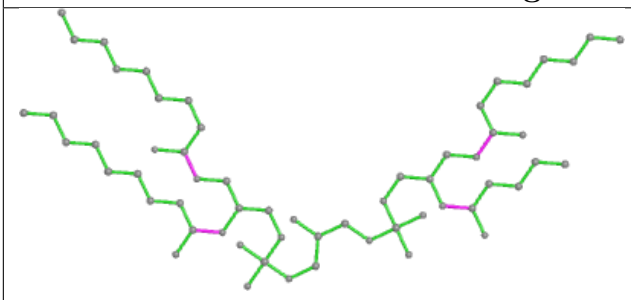


Rings

Ligand CDL X 103



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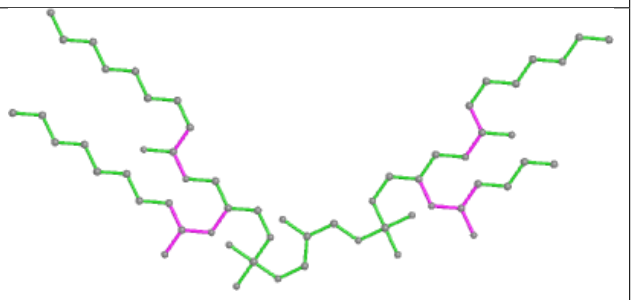

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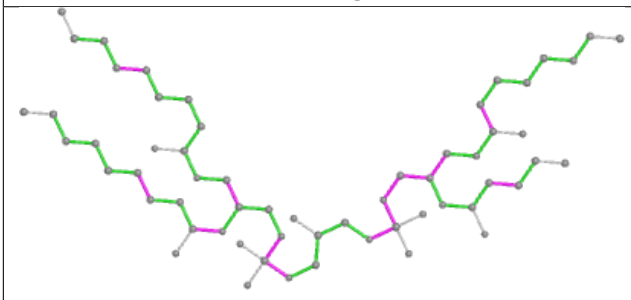

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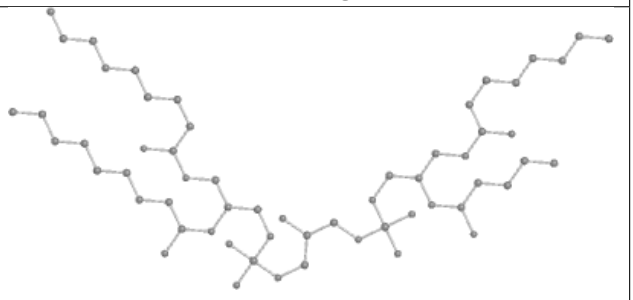
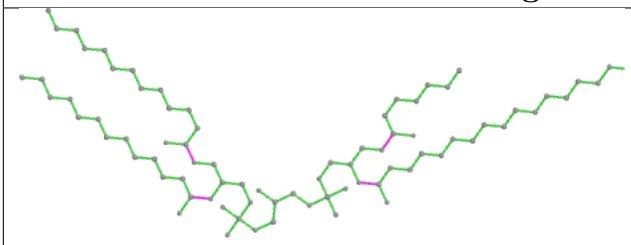


Rings

Ligand CDL m 410



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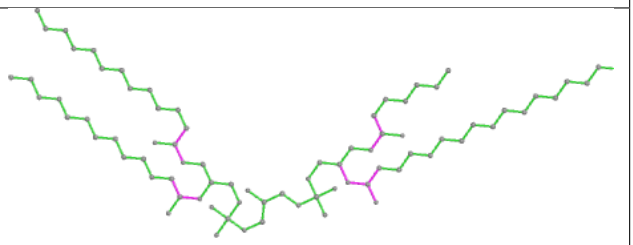
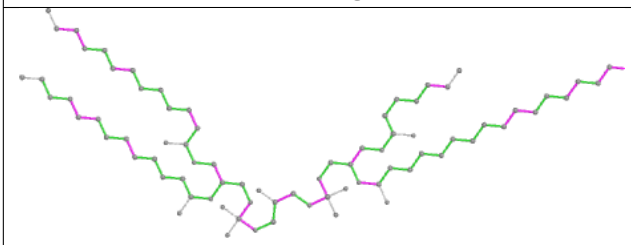


Bond angles



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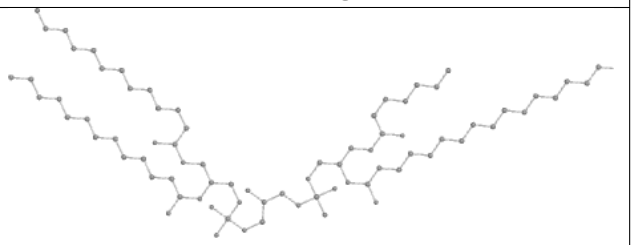
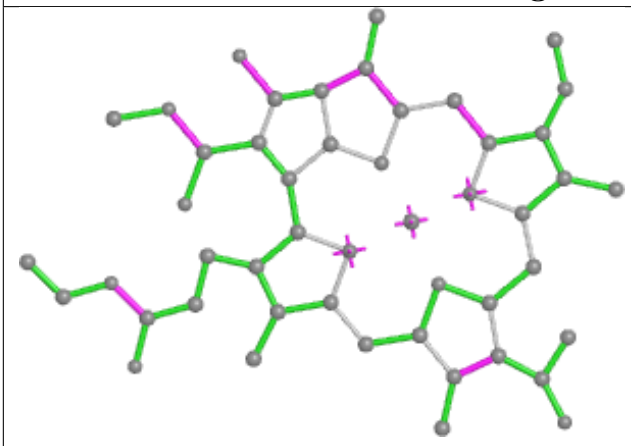


Rings

Ligand BCL a 101



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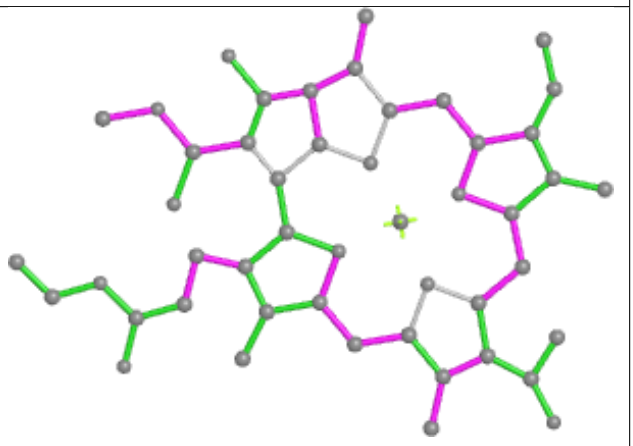
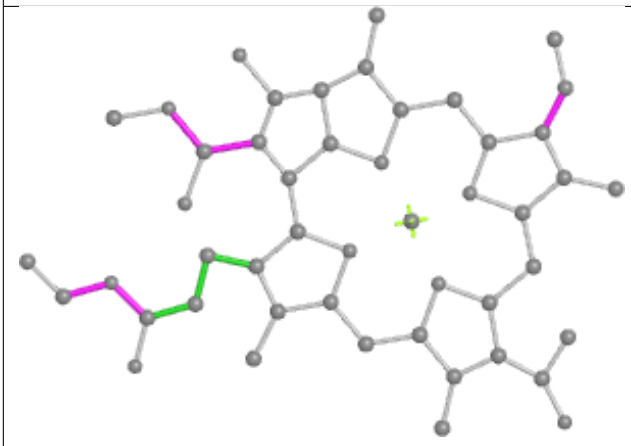


Bond angles



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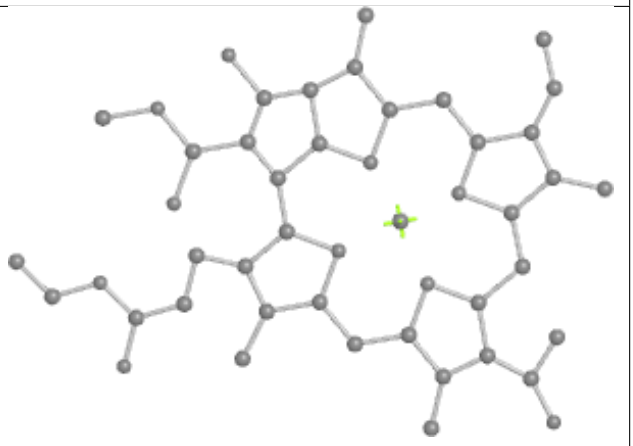
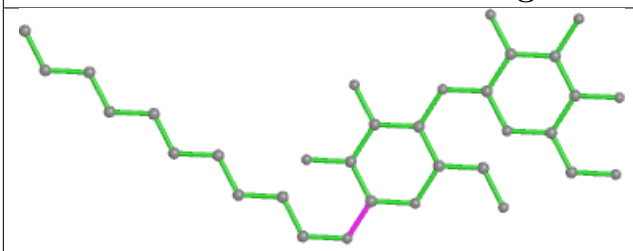


Rings

Ligand LMT M 409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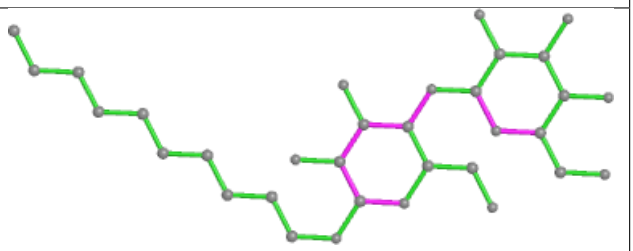
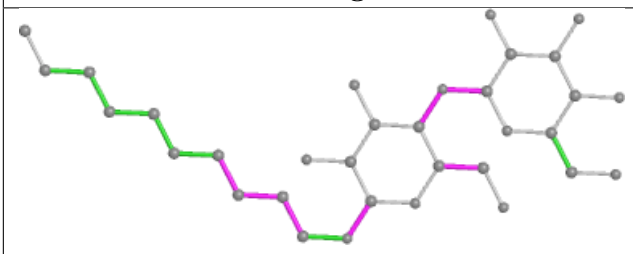

Bond angles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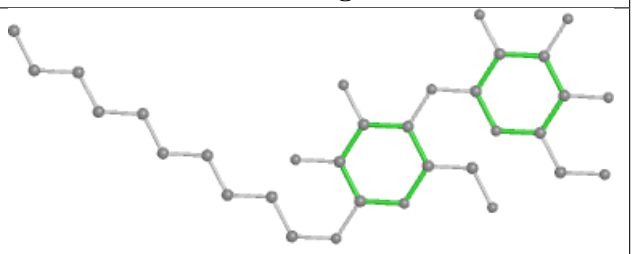
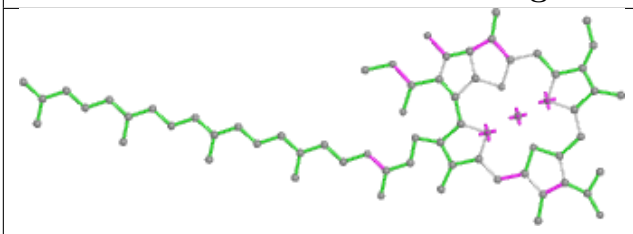

Rings

Ligand BCL z 102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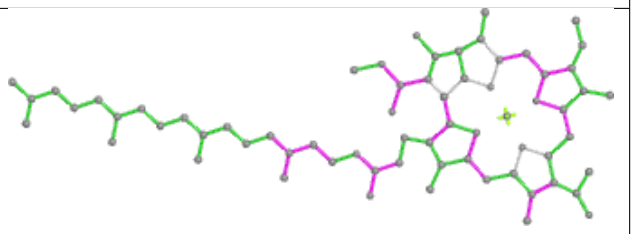
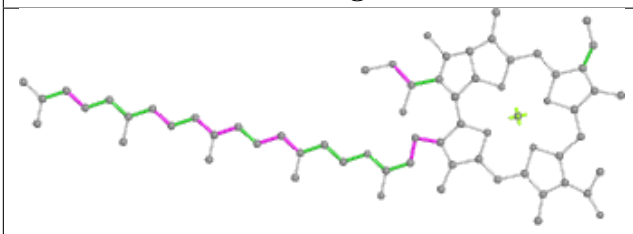

Bond angles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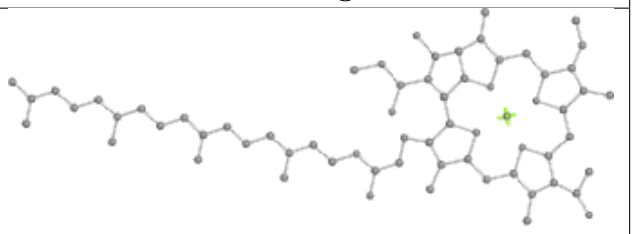
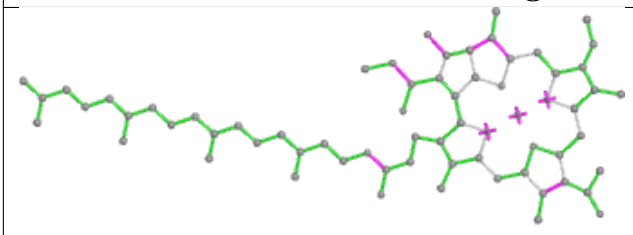

Rings

Ligand BCL V 101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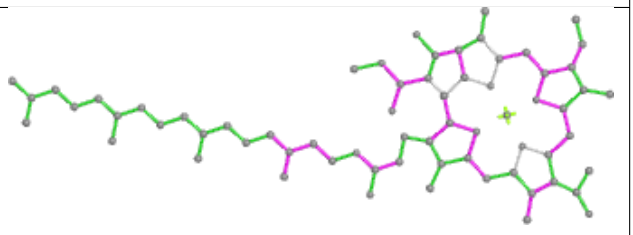
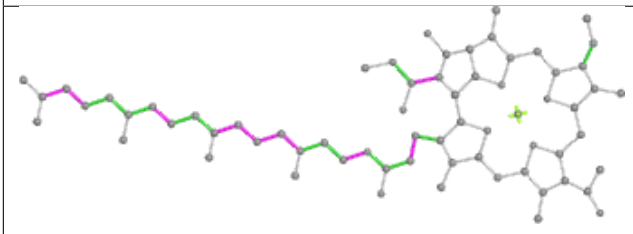

Bond angles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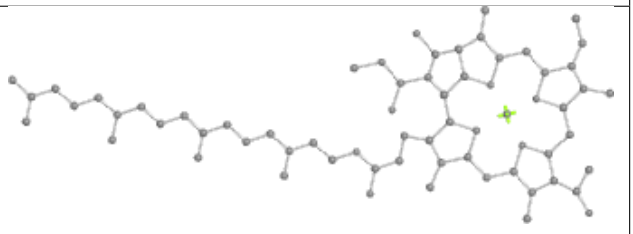
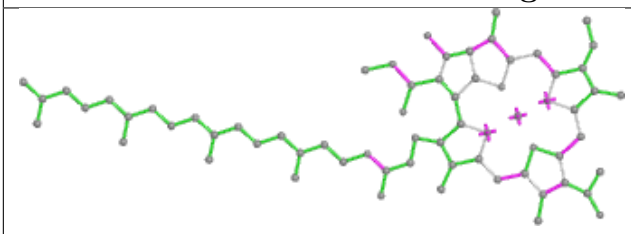
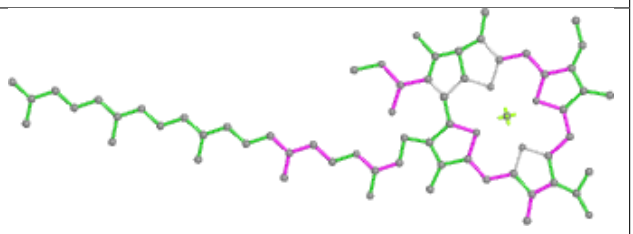

Rings

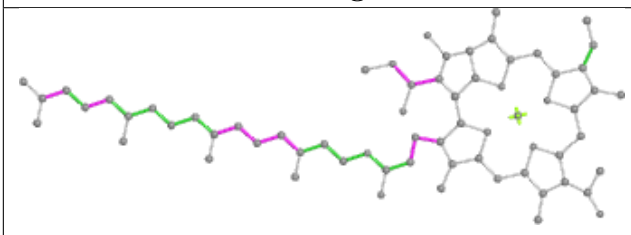
Ligand BCL 06 101



Bond lengths



Bond angles



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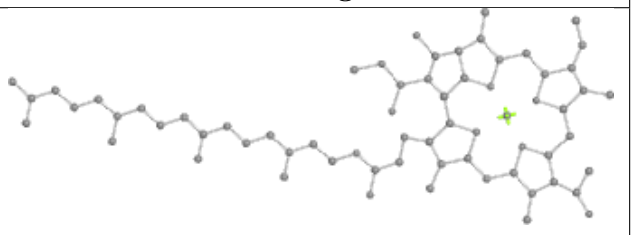
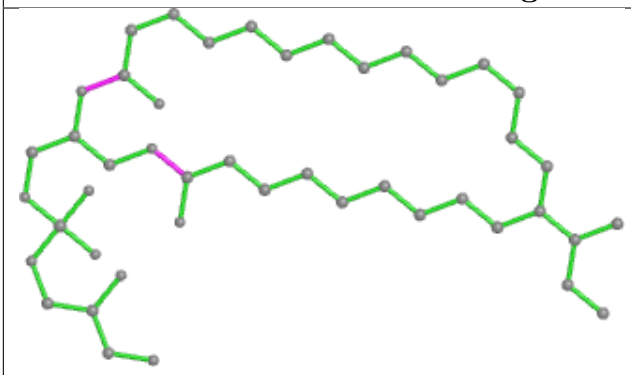
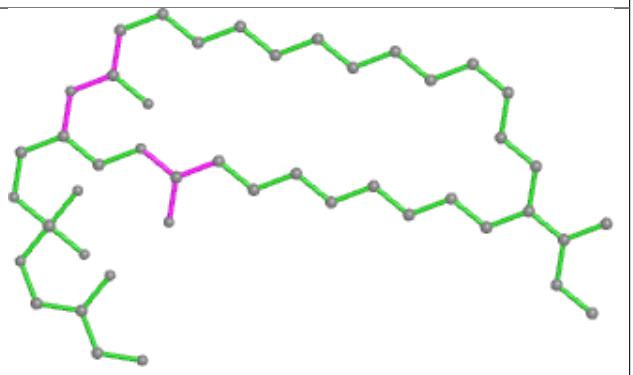


Rings

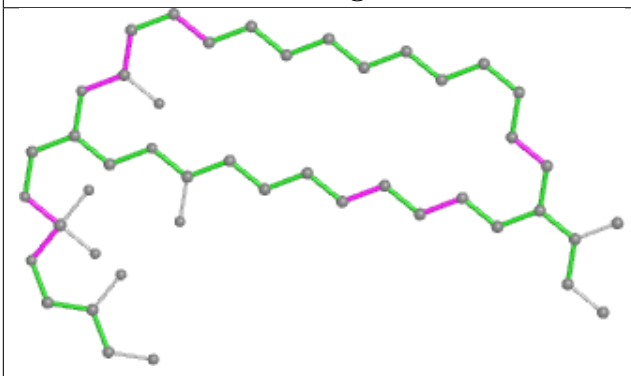
Ligand PGV H 801



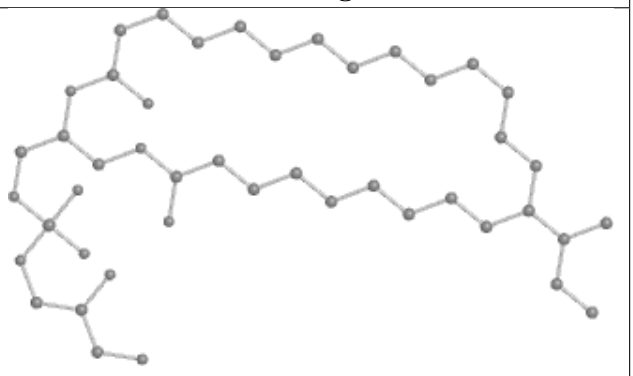
Bond lengths



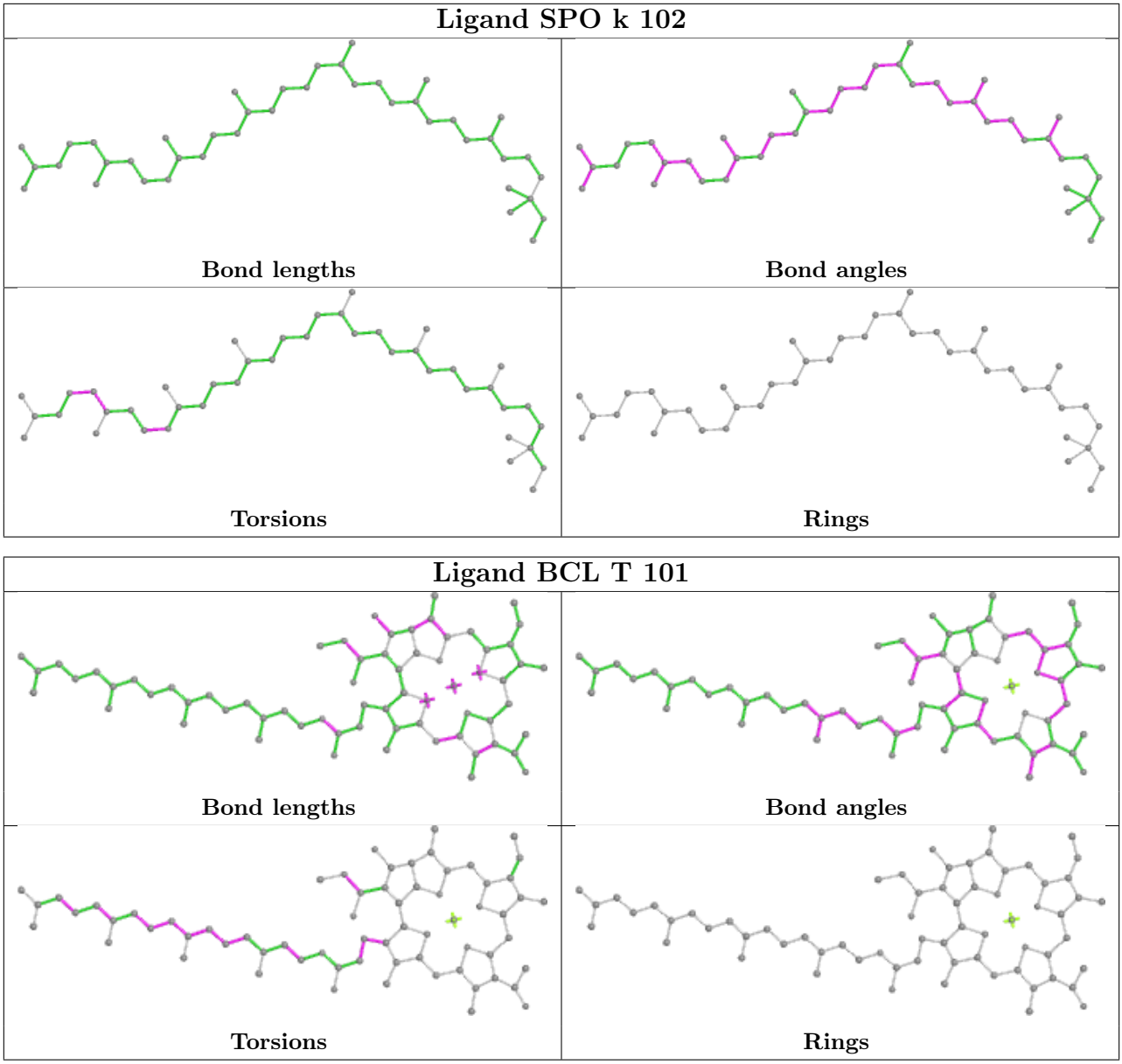
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

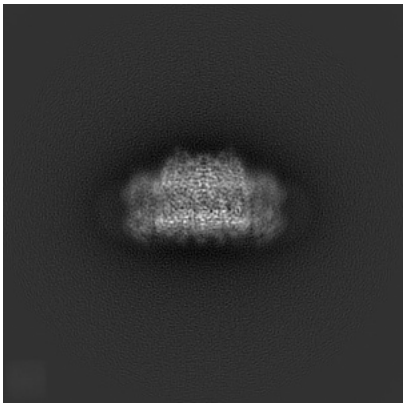
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32192. These allow visual inspection of the internal detail of the map and identification of artifacts.

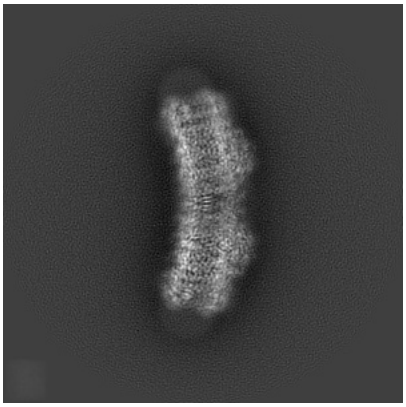
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

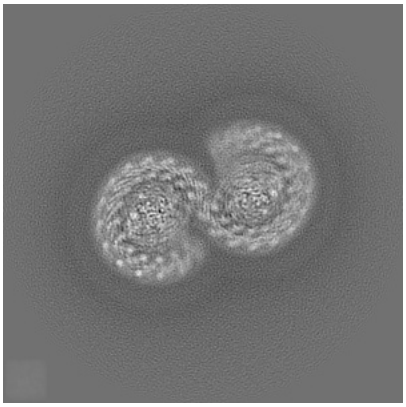
6.1.1 Primary map



X



Y

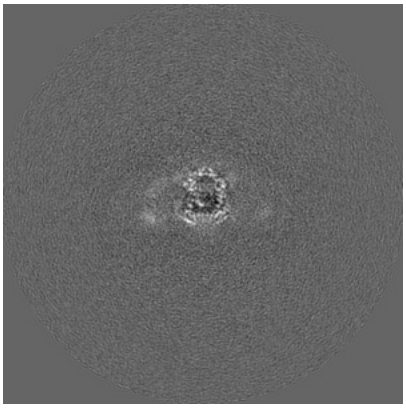


Z

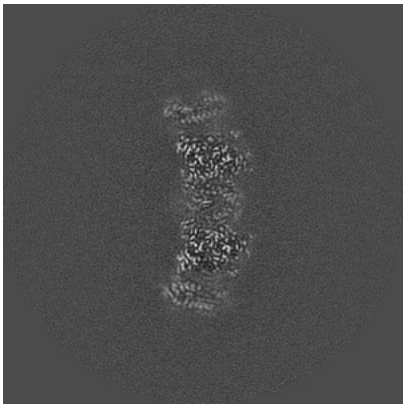
The images above show the map projected in three orthogonal directions.

6.2 Central slices

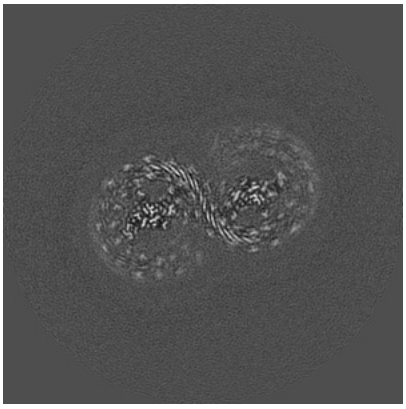
6.2.1 Primary map



X Index: 225



Y Index: 225

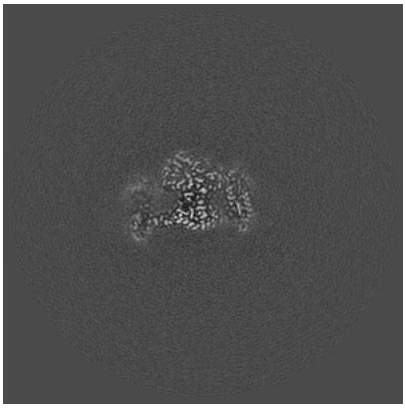


Z Index: 225

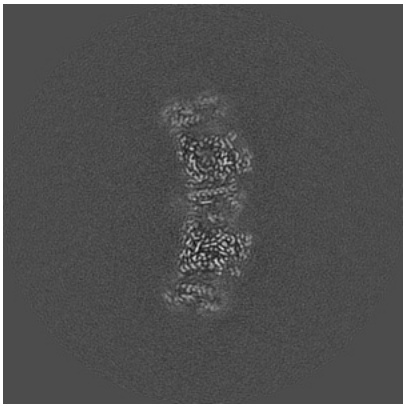
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

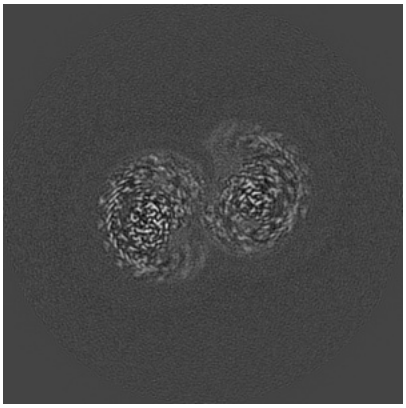
6.3.1 Primary map



X Index: 163



Y Index: 221

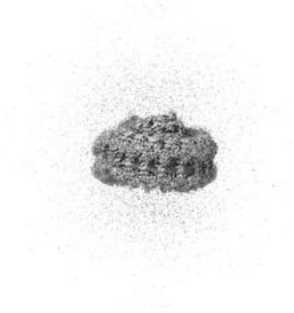


Z Index: 209

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

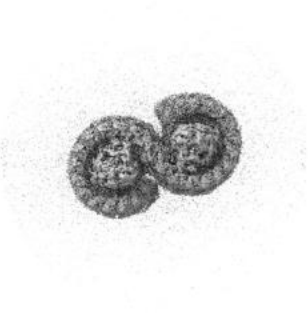
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

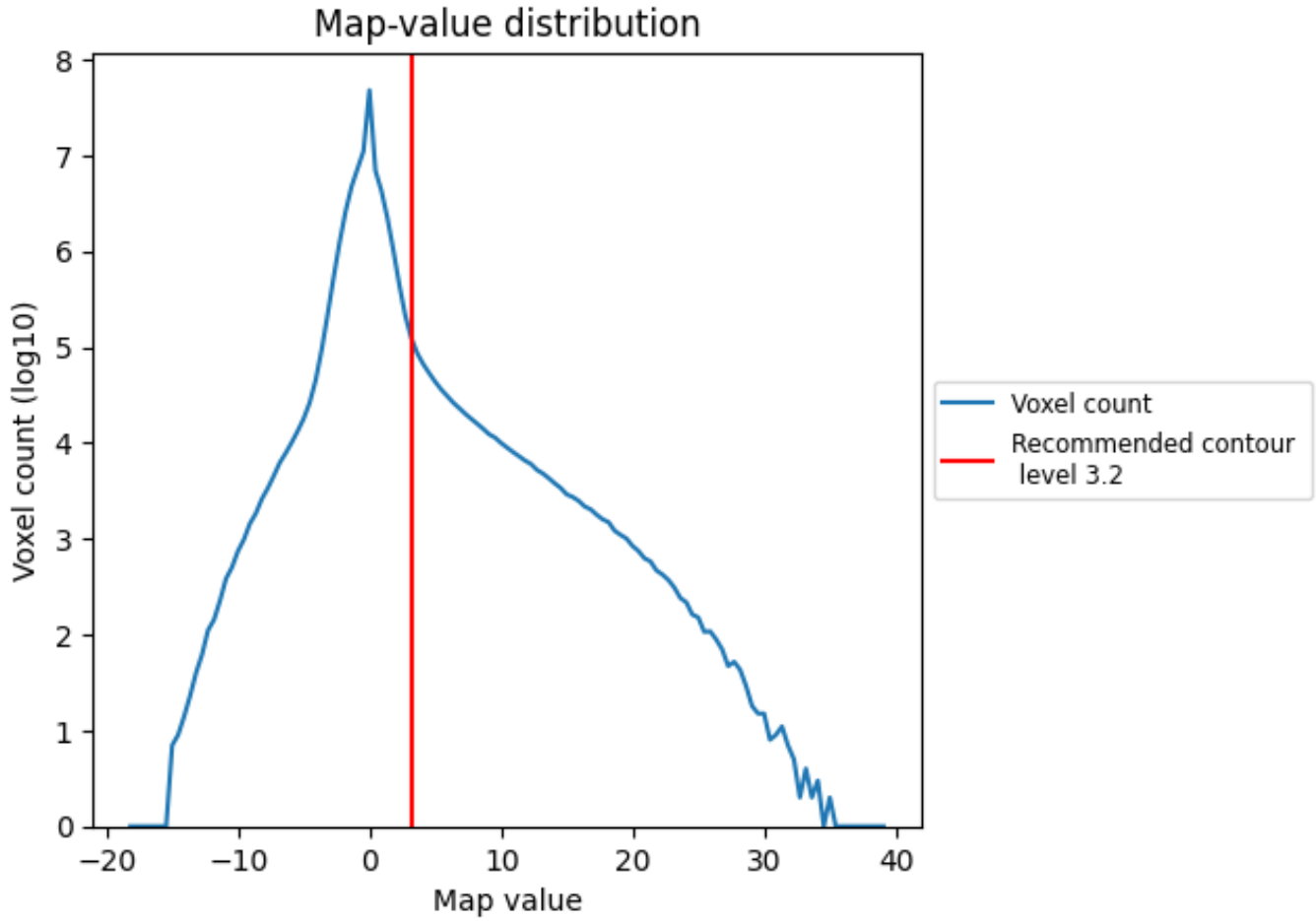
6.5 Mask visualisation (i)

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

7 Map analysis

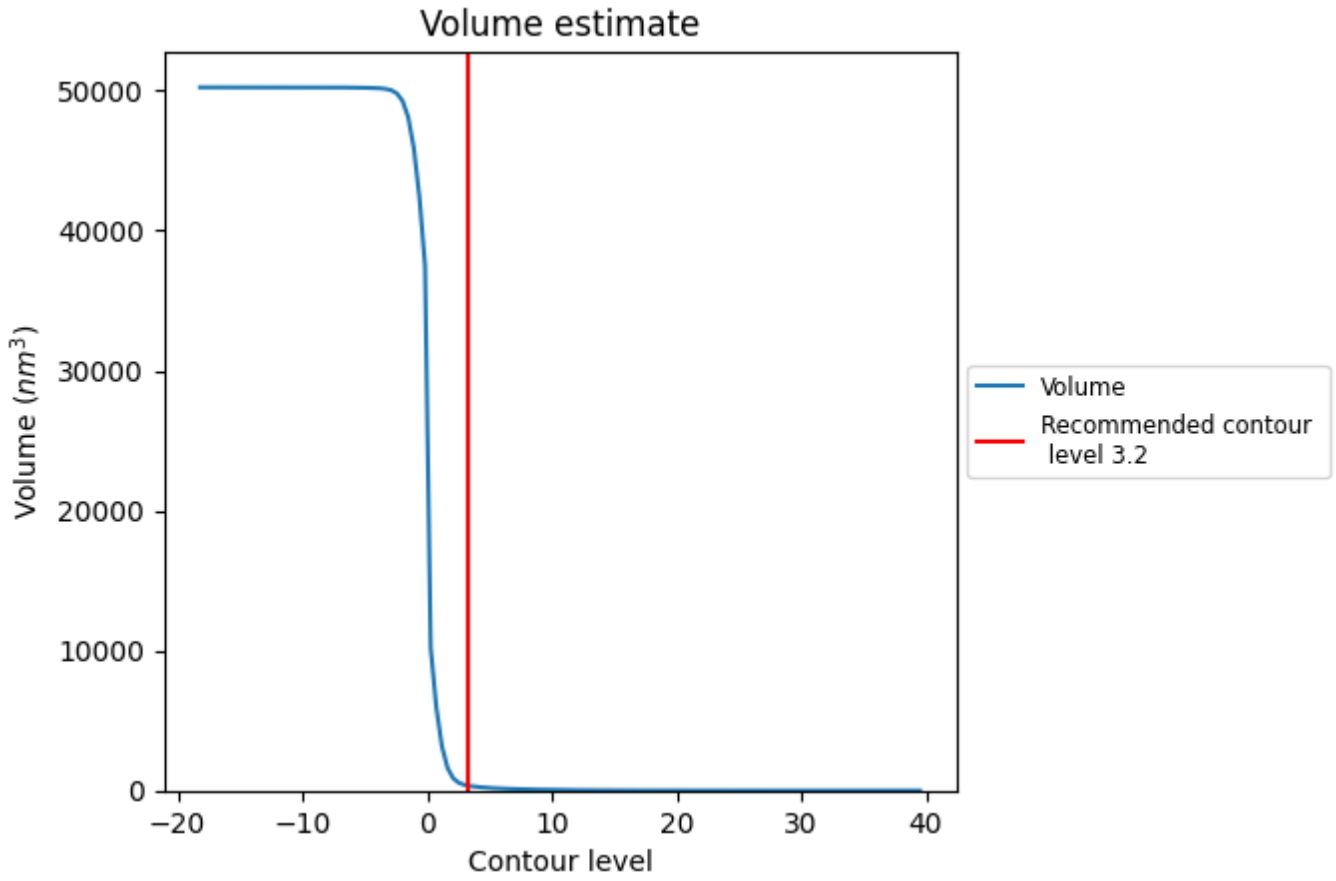
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

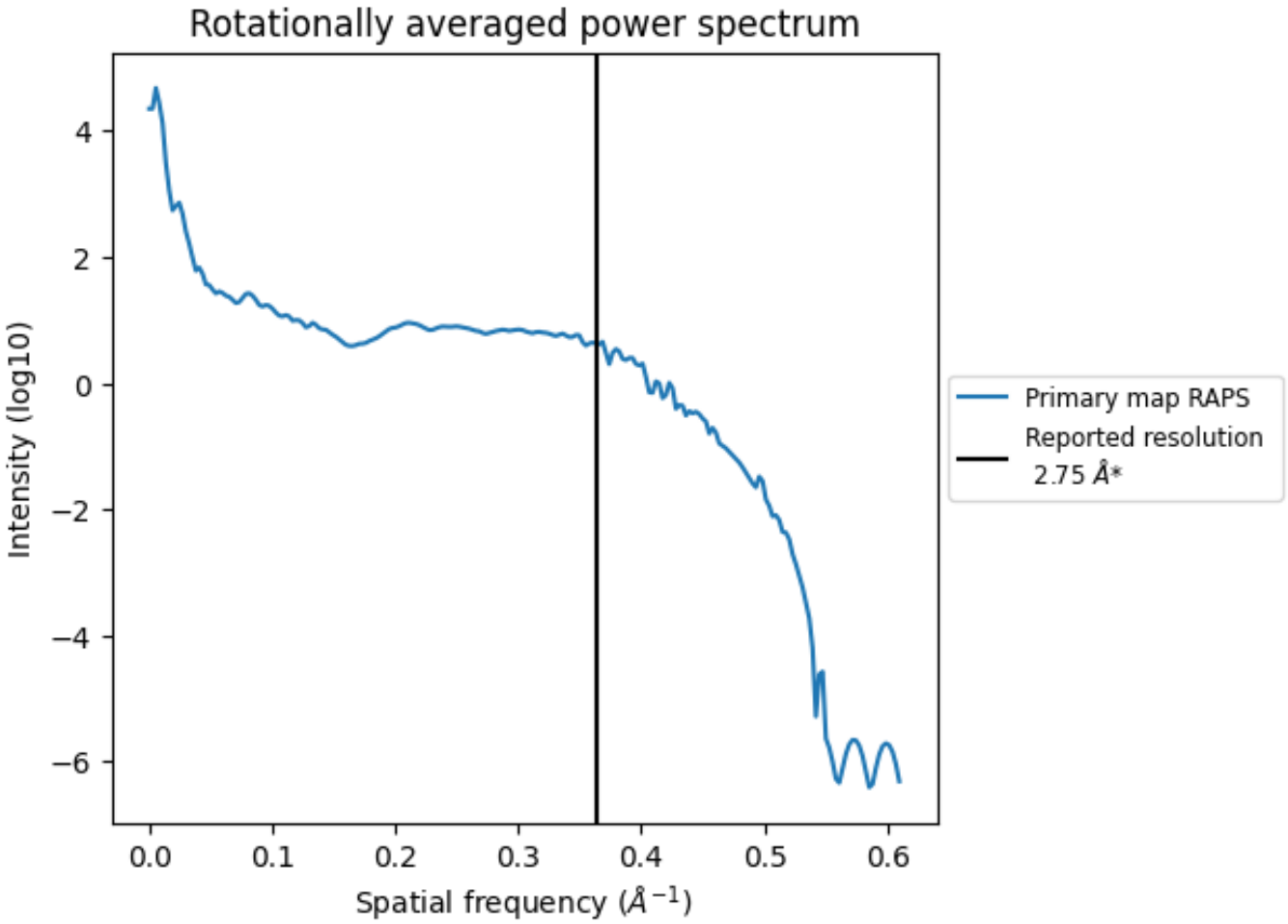
7.2 Volume estimate



The volume at the recommended contour level is 369 nm^3; this corresponds to an approximate mass of 334 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)

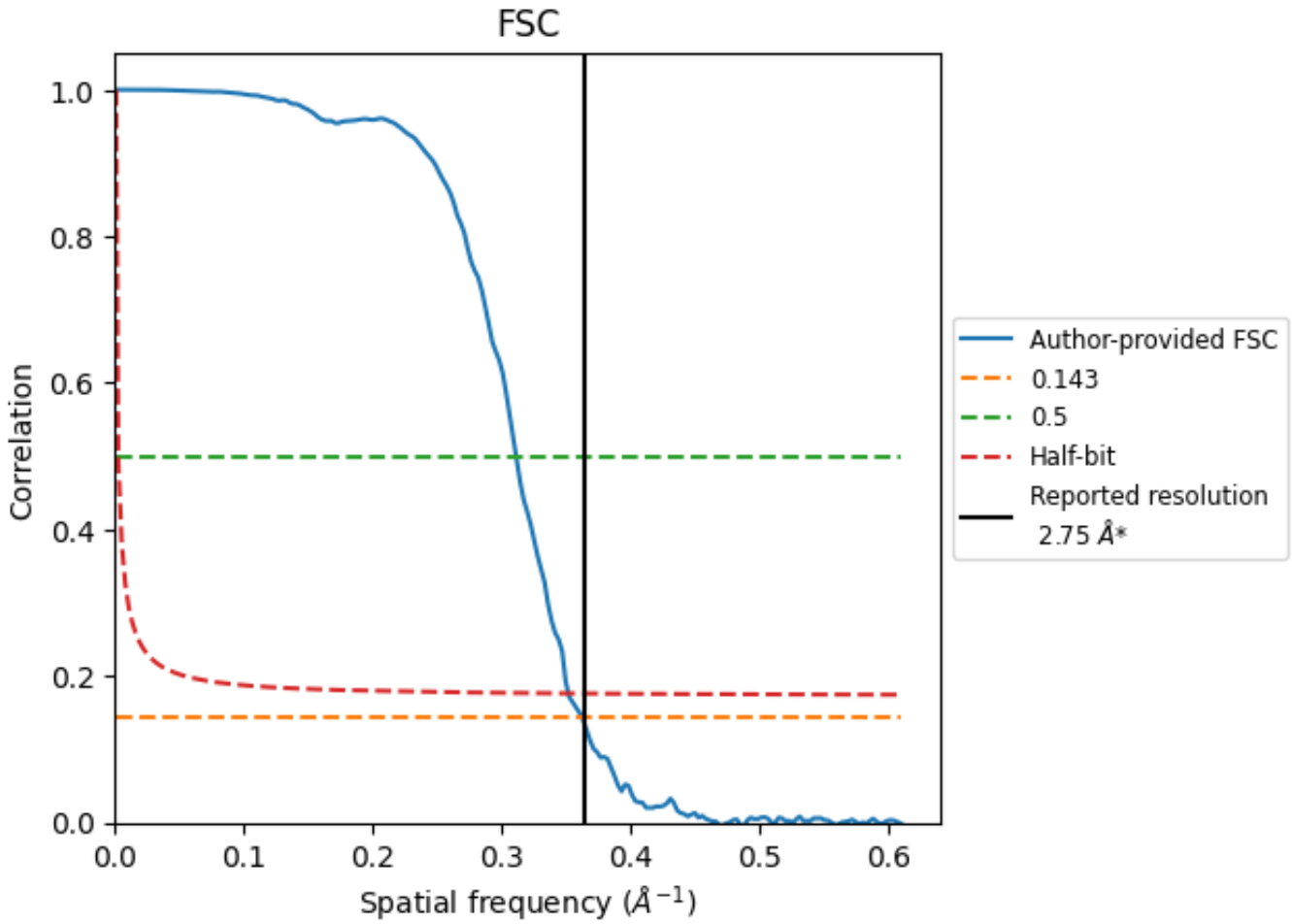


*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

8.2 Resolution estimates (i)

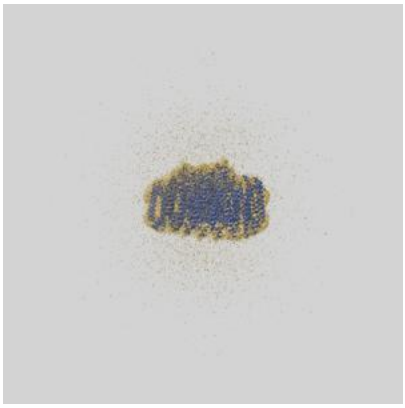
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.76	3.22	2.84
Unmasked-calculated*	-	-	-

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

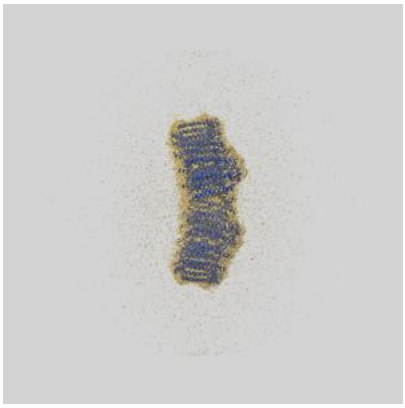
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32192 and PDB model 7VY2. Per-residue inclusion information can be found in section 3 on page 25.

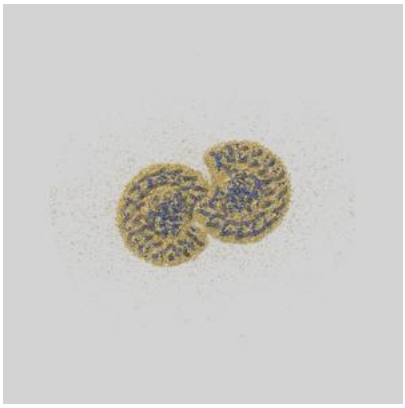
9.1 Map-model overlay



X



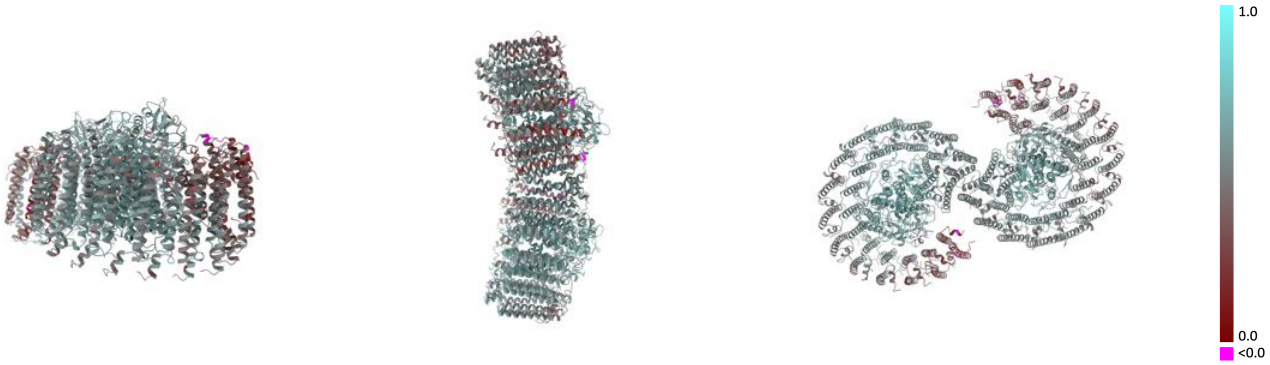
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.2 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.

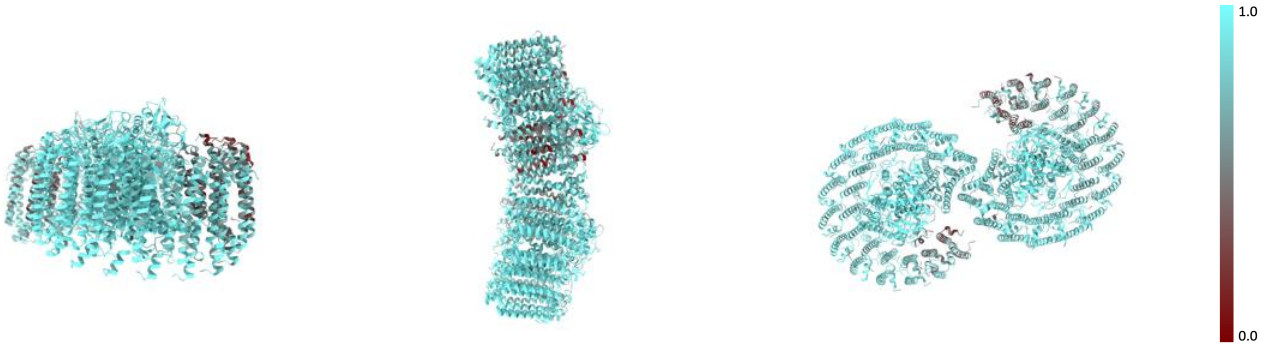
9.2 Q-score mapped to coordinate model (i)



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.

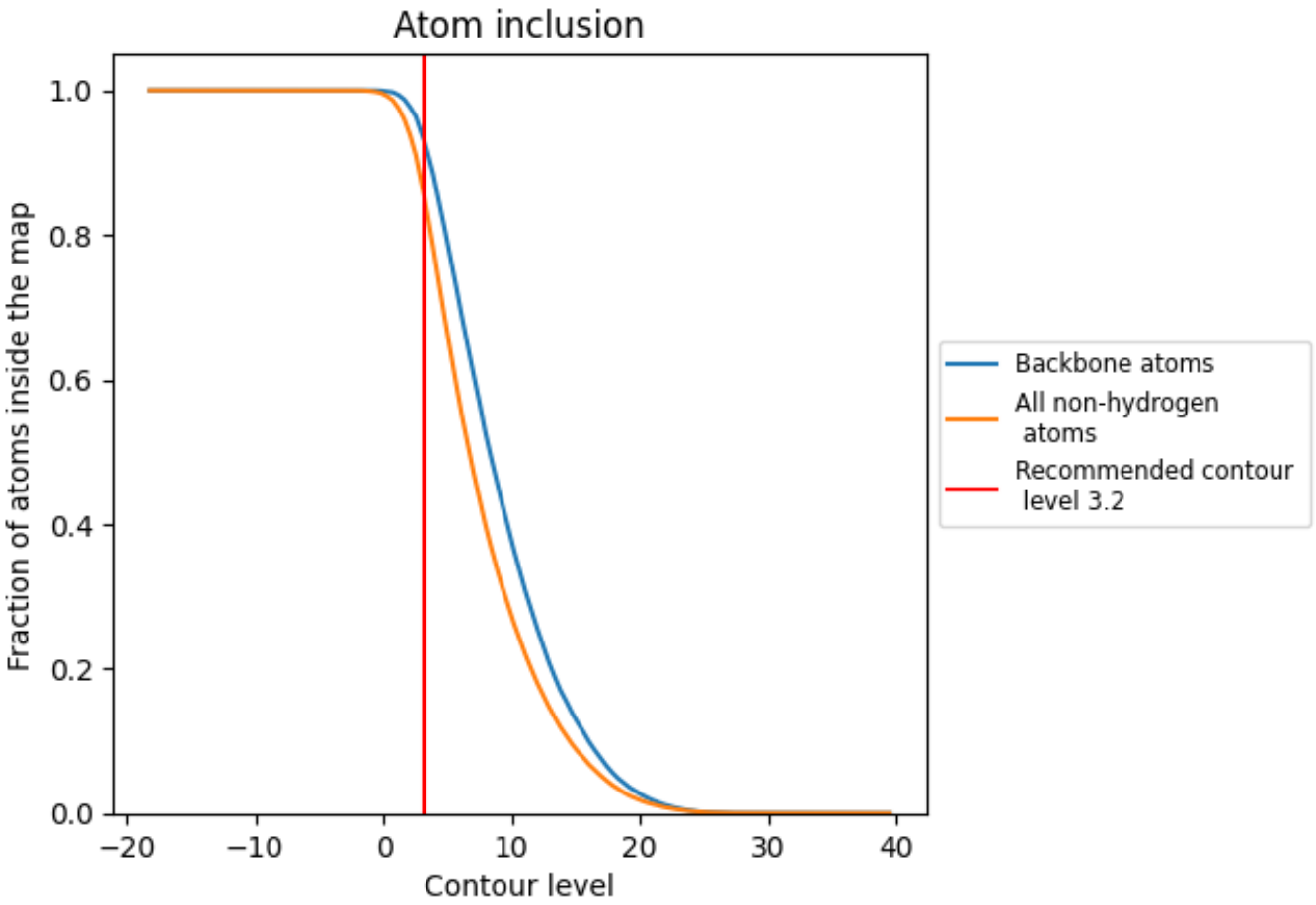
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.2).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8524	0.5340
01	0.8581	0.5400
02	0.8497	0.5040
03	0.7877	0.4750
04	0.7407	0.3920
05	0.6289	0.3950
06	0.6848	0.3400
07	0.5332	0.2820
08	0.5090	0.2570
1	0.7768	0.4610
2	0.6864	0.4350
3	0.6225	0.3840
4	0.6174	0.3640
5	0.5951	0.3770
6	0.4848	0.2950
7	0.5418	0.3420
8	0.4841	0.3260
A	0.9082	0.5620
B	0.8652	0.5340
D	0.9275	0.5610
E	0.8546	0.5180
F	0.9034	0.5560
G	0.8270	0.5140
H	0.9313	0.5860
I	0.8906	0.5410
J	0.8635	0.5020
K	0.8466	0.5330
L	0.9372	0.6060
M	0.9212	0.6020
N	0.8523	0.5060
O	0.8590	0.5110
P	0.8143	0.4950
Q	0.8093	0.5000
R	0.8172	0.4950
S	0.8010	0.5010

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Chain	Atom inclusion	Q-score
T	0.8054	0.4800
U	0.5022	0.4050
V	0.8095	0.4950
W	0.8030	0.4440
X	0.8422	0.5170
Y	0.7504	0.4640
Z	0.7951	0.4490
a	0.9353	0.5570
b	0.9111	0.5610
d	0.9366	0.5730
e	0.9217	0.5580
f	0.9092	0.5780
g	0.8867	0.5620
h	0.9453	0.6110
i	0.8981	0.5510
j	0.8837	0.5490
k	0.9019	0.5630
l	0.9541	0.6310
m	0.9624	0.6480
n	0.8569	0.5310
o	0.9206	0.5640
p	0.8725	0.5250
q	0.9178	0.5630
r	0.8557	0.5010
s	0.8960	0.5680
t	0.8889	0.5250
u	0.4085	0.3190
v	0.9211	0.5720
w	0.8668	0.5080
x	0.8660	0.5180
y	0.8596	0.5560
z	0.8568	0.5040