Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 09:38 PM JST

PDB ID	:	7F0L
EMDB ID	:	EMD-31400
Title	:	STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF RHODOBACTER SPHAEROIDES MONOMER
Authors	:	Tani, K.; Nagashima, V.P.; Kanno, R.; Kawamura, S.; Kikuchi, R.; Ji, X.-C.; Hall, M.; Yu, L.-J.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on	:	2021-06-05
Resolution	:	2.94 Å(reported)
Based on initial model	:	5Y5S

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 ⓘ 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:

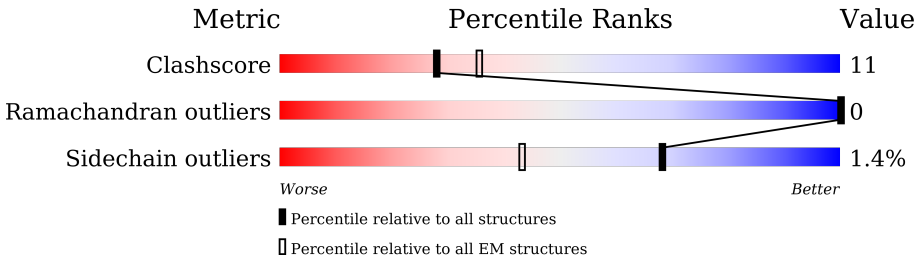
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.94 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	282	79% 20%
2	M	308	77% 22%
3	H	260	82% 12% 5%
4	1	54	87% 13%
4	3	54	7% 93% 6%
4	A	54	59% 24% 17%
4	D	54	76% 24%

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Mol	Chain	Length	Quality of chain
4	F	54	87% 11%
4	I	54	80% 20%
4	K	54	80% 20%
4	O	54	74% 24%
4	Q	54	7% 69% 31%
4	S	54	6% 80% 20%
4	V	54	76% 24%
4	Y	54	76% 22%
5	2	49	6% 84% 14%
5	4	49	8% 73% 14% 12%
5	6	49	10% 73% 12% 14%
5	8	49	27% 61% 16% 22%
5	B	49	82% 8% 10%
5	E	49	71% 16% 12%
5	G	49	6% 84% 8% 8%
5	J	49	76% 12% 12%
5	N	49	73% 14% 12%
5	P	49	8% 76% 12% 12%
5	R	49	78% 10% 12%
5	T	49	76% 12% 12%
5	W	49	10% 61% 27% 12%
5	Z	49	12% 78% 8% 12%
6	5	54	6% 78% 20%
6	7	54	26% 81% 13% 6%
7	X	82	54% 11% 35%

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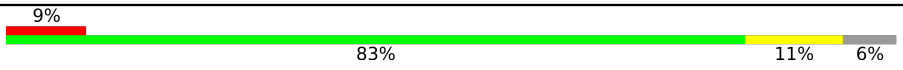
Mol	Chain	Length	Quality of chain
8	U	53	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 23458 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		

- 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		

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	246	Total	C	N	O	S	0	0
			1864	1197	314	343	10		

- Molecule 4 is a protein called Light-harvesting protein B-875 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		
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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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
			457	311	73	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		

- 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		

- Molecule 6 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
6	7	51	Total	C	N	O	S	0	0
			415	281	68	64	2		

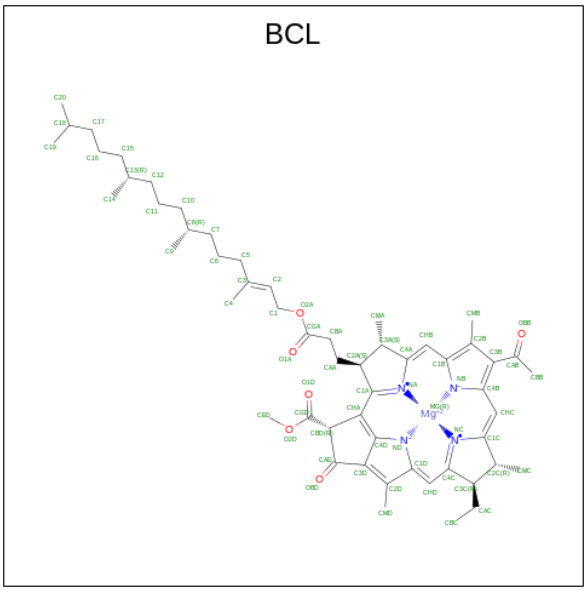
- Molecule 7 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	53	Total	C	N	O	S	0	0
			405	269	69	64	3		

- Molecule 8 is a protein called protein-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	50	Total	C	N	O	S	0	0
			369	252	57	57	3		

- Molecule 9 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
9	L	1	Total	C	Mg	N	O	0
			198	165	3	12	18	
9	L	1	Total	C	Mg	N	O	0
			198	165	3	12	18	

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Mol	Chain	Residues	Atoms					AltConf
9	L	1	Total	C	Mg	N	O	0
			198	165	3	12	18	
9	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
9	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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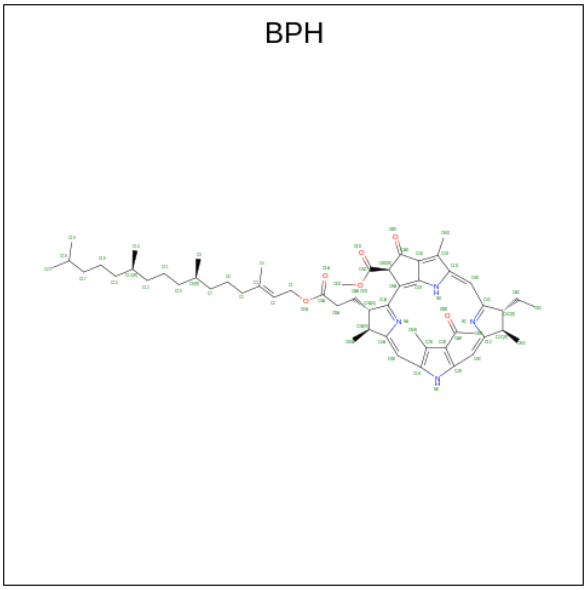
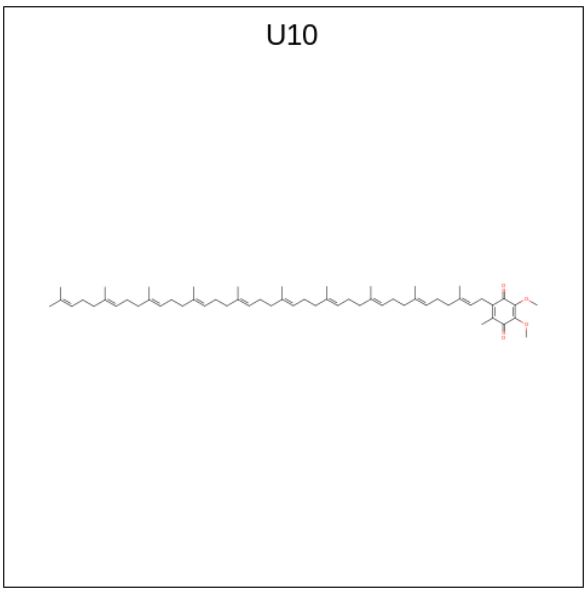
Mol	Chain	Residues	Atoms					AltConf
9	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



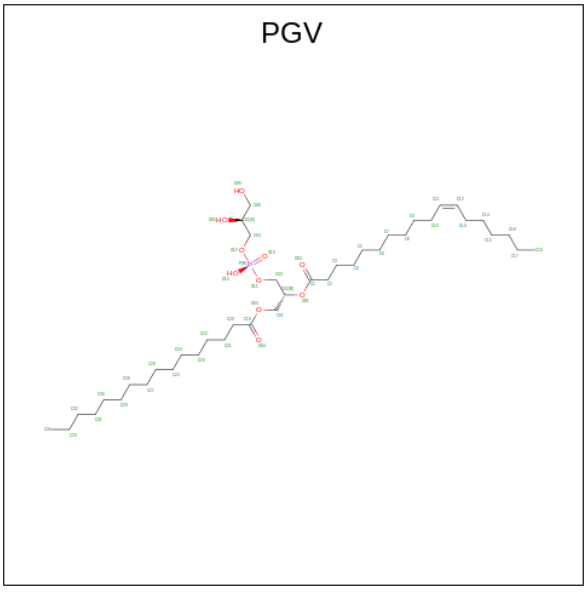
Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	N	O	0
			65	55	4	6	
10	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



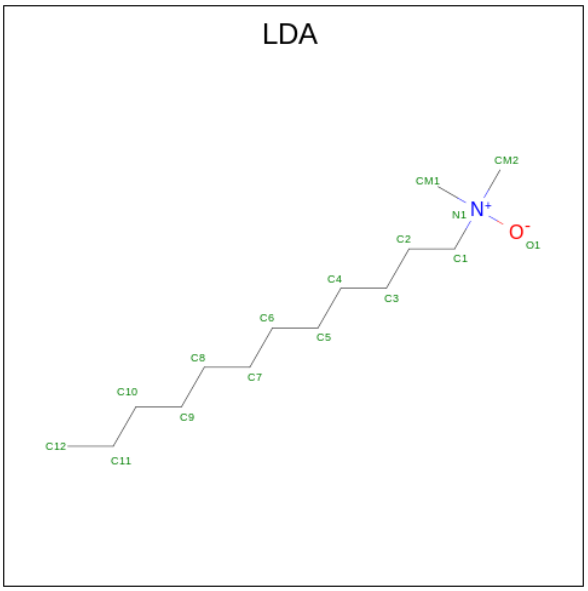
Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total	C	O	0
			70	62	8	
11	L	1	Total	C	O	0
			70	62	8	
11	M	1	Total	C	O	0
			48	44	4	

- 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	C	O	P	0
			117	86	28	3	
12	L	1	Total	C	O	P	0
			117	86	28	3	
12	L	1	Total	C	O	P	0
			117	86	28	3	
12	M	1	Total	C	O	P	0
			85	63	20	2	
12	M	1	Total	C	O	P	0
			85	63	20	2	
12	H	1	Total	C	O	P	0
			121	90	28	3	
12	H	1	Total	C	O	P	0
			121	90	28	3	
12	H	1	Total	C	O	P	0
			121	90	28	3	
12	K	1	Total	C	O	P	0
			41	34	6	1	
12	Q	1	Total	C	O	P	0
			39	28	10	1	
12	Y	1	Total	C	O	P	0
			43	32	10	1	
12	3	1	Total	C	O	P	0
			51	40	10	1	
12	X	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

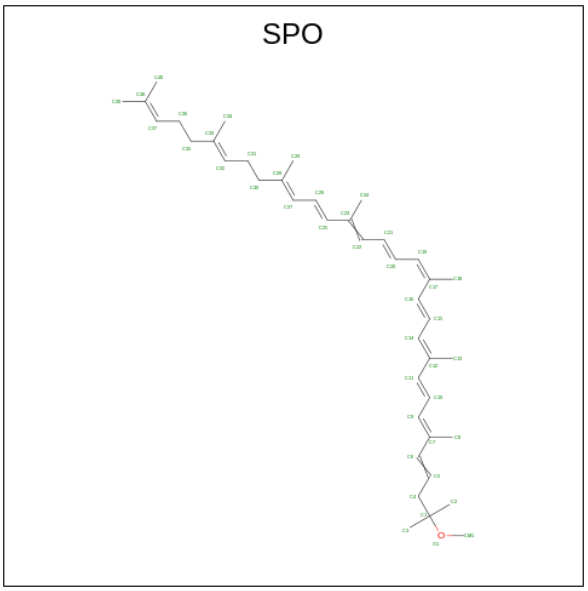


Mol	Chain	Residues	Atoms	AltConf
13	L	1	Total C N O 32 28 2 2	0
13	L	1	Total C N O 32 28 2 2	0
13	M	1	Total C N O 16 14 1 1	0
13	Y	1	Total C N O 12 10 1 1	0
13	X	1	Total C N O 29 25 2 2	0
13	X	1	Total C N O 29 25 2 2	0

- Molecule 14 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
14	M	1	Total Fe 1 1	0

- Molecule 15 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total 42	C 41	O 1	0
15	D	1	Total 42	C 41	O 1	0
15	E	1	Total 42	C 41	O 1	0
15	F	1	Total 84	C 82	O 2	0
15	F	1	Total 84	C 82	O 2	0
15	G	1	Total 84	C 82	O 2	0
15	G	1	Total 84	C 82	O 2	0
15	K	1	Total 42	C 41	O 1	0
15	N	1	Total 42	C 41	O 1	0
15	O	1	Total 84	C 82	O 2	0
15	O	1	Total 84	C 82	O 2	0
15	P	1	Total 42	C 41	O 1	0
15	R	1	Total 42	C 41	O 1	0
15	S	1	Total 84	C 82	O 2	0

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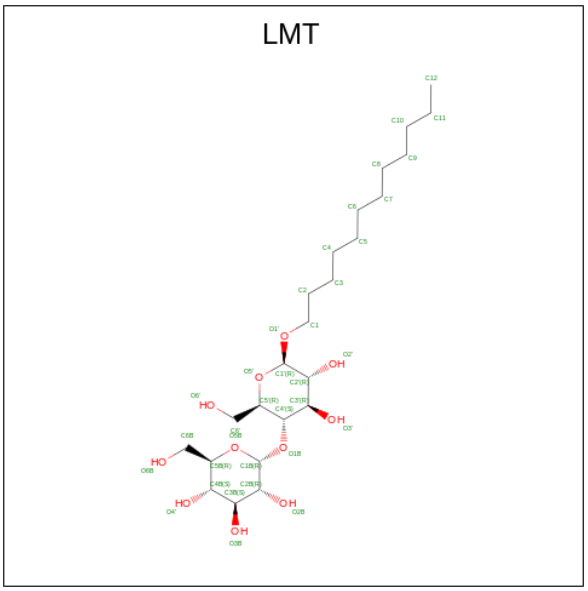
Mol	Chain	Residues	Atoms			AltConf
15	S	1	Total	C	O	0
			84	82	2	
15	T	1	Total	C	O	0
			42	41	1	
15	V	1	Total	C	O	0
			84	82	2	
15	V	1	Total	C	O	0
			84	82	2	
15	W	1	Total	C	O	0
			42	41	1	
15	1	1	Total	C	O	0
			126	123	3	
15	1	1	Total	C	O	0
			126	123	3	
15	1	1	Total	C	O	0
			126	123	3	
15	3	1	Total	C	O	0
			42	41	1	
15	5	1	Total	C	O	0
			84	82	2	
15	5	1	Total	C	O	0
			84	82	2	
15	8	1	Total	C	O	0
			42	41	1	
15	X	1	Total	C	O	0
			42	41	1	

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			95	66	29	
16	M	1	Total	C	O	0
			95	66	29	
16	M	1	Total	C	O	0
			95	66	29	
16	H	1	Total	C	O	0
			65	43	22	
16	H	1	Total	C	O	0
			65	43	22	
16	A	1	Total	C	O	0
			97	64	33	
16	A	1	Total	C	O	0
			97	64	33	
16	A	1	Total	C	O	0
			97	64	33	
16	D	1	Total	C	O	0
			27	16	11	
16	F	1	Total	C	O	0
			43	27	16	
16	F	1	Total	C	O	0
			43	27	16	
16	I	1	Total	C	O	0
			27	16	11	
16	K	1	Total	C	O	0
			35	24	11	
16	Q	1	Total	C	O	0
			43	31	12	

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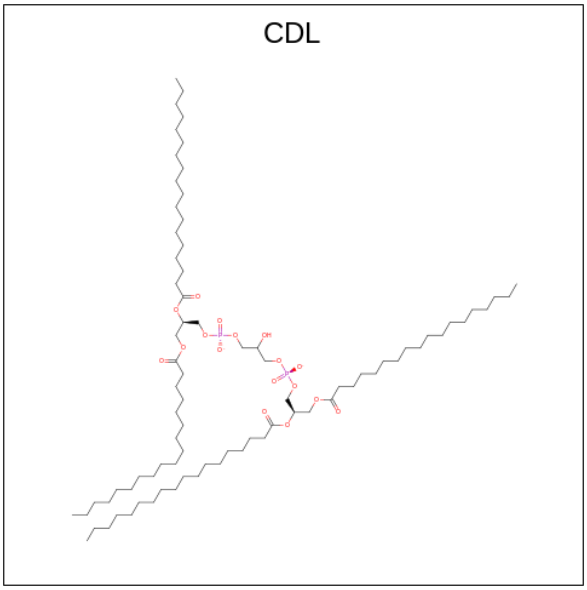
Mol	Chain	Residues	Atoms	AltConf
16	Q	1	Total C O 43 31 12	0
16	S	1	Total C O 55 38 17	0
16	S	1	Total C O 55 38 17	0
16	1	1	Total C O 24 15 9	0
16	3	1	Total C O 35 24 11	0
16	4	1	Total C O 27 16 11	0
16	5	1	Total C O 33 22 11	0
16	X	1	Total C O 31 20 11	0
16	U	1	Total C O 67 45 22	0
16	U	1	Total C O 67 45 22	0

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



Mol	Chain	Residues	Atoms	AltConf
17	M	1	Total C O P 79 60 17 2	0

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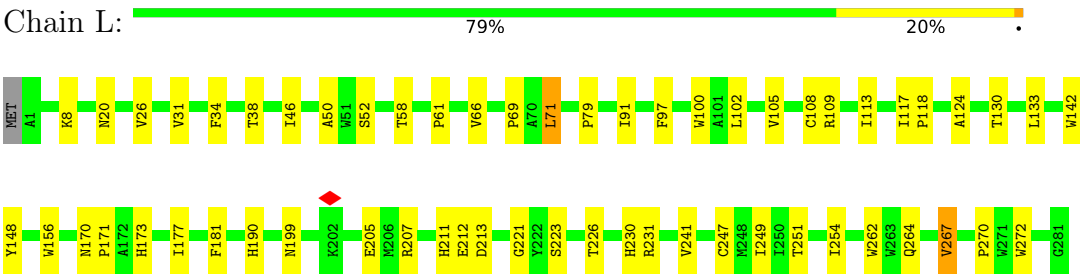
Mol	Chain	Residues	Atoms				AltConf
17	H	1	Total	C	O	P	0
			98	62	32	4	
17	H	1	Total	C	O	P	0
			98	62	32	4	
17	Y	1	Total	C	O	P	0
			48	30	16	2	

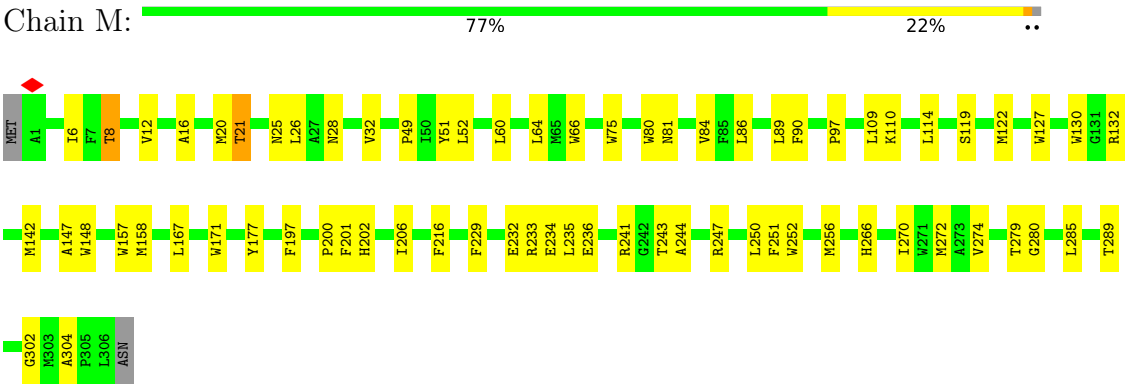
3 Residue-property plots (i)

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.

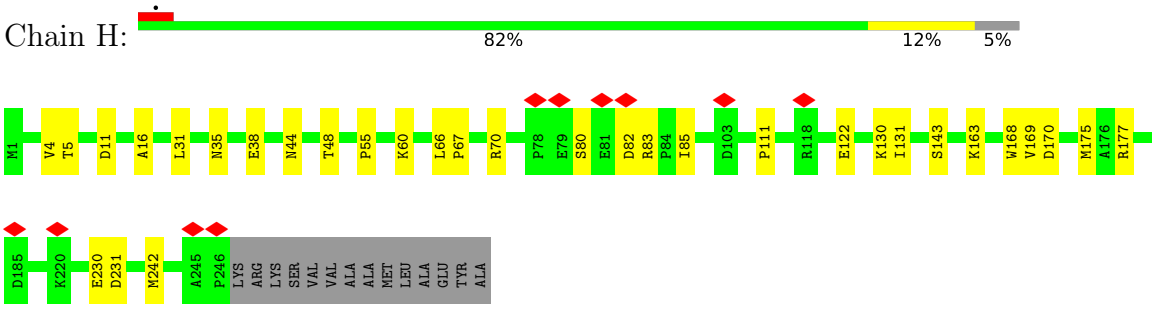
• Molecule 1: Photosynthetic reaction center L subunit



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain

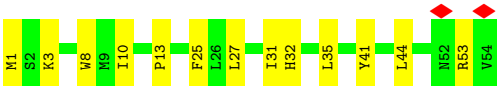


• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain A:

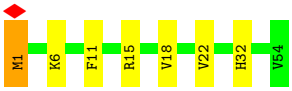
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain D:



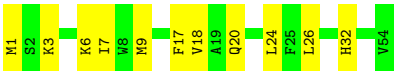
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain F:



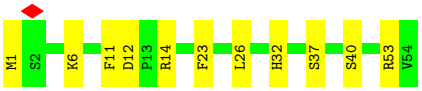
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain I:



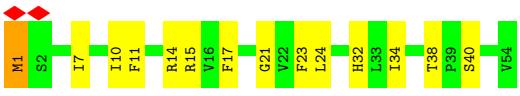
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain K:



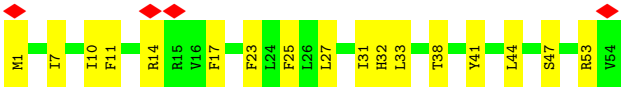
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain O:



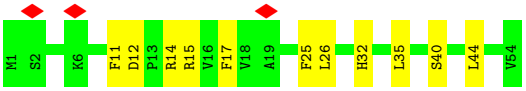
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain Q:



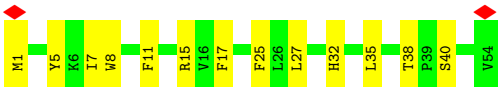
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain S:



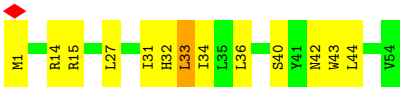
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain V:



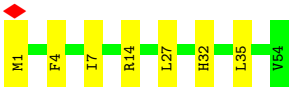
• Molecule 4: Light-harvesting protein B-875 alpha chain

Chain Y:



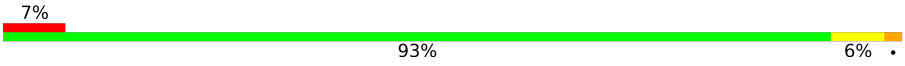
• Molecule 4: Light-harvesting protein B-875 alpha chain

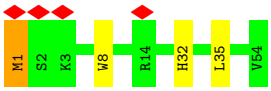
Chain 1:



• Molecule 4: Light-harvesting protein B-875 alpha chain

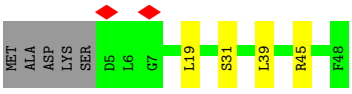
Chain 3:





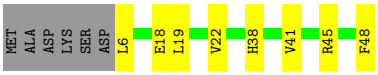
• Molecule 5: Antenna pigment protein beta chain

Chain B:



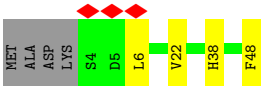
• Molecule 5: Antenna pigment protein beta chain

Chain E:



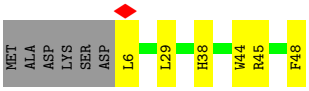
• Molecule 5: Antenna pigment protein beta chain

Chain G:



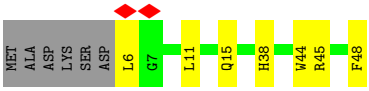
• Molecule 5: Antenna pigment protein beta chain

Chain J:



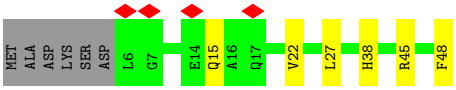
• Molecule 5: Antenna pigment protein beta chain

Chain N:



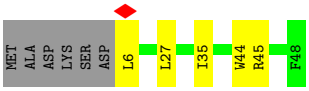
• Molecule 5: Antenna pigment protein beta chain

Chain P:



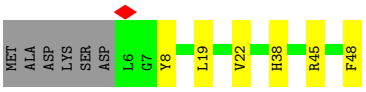
• Molecule 5: Antenna pigment protein beta chain

Chain R:



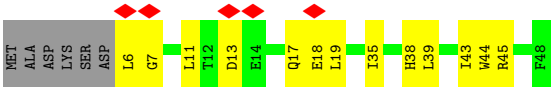
• Molecule 5: Antenna pigment protein beta chain

Chain T:



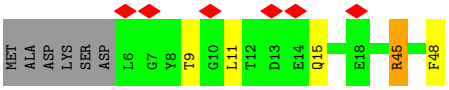
• Molecule 5: Antenna pigment protein beta chain

Chain W:



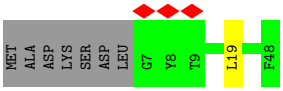
• Molecule 5: Antenna pigment protein beta chain

Chain Z:



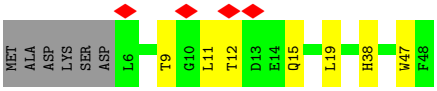
• Molecule 5: Antenna pigment protein beta chain

Chain 2:



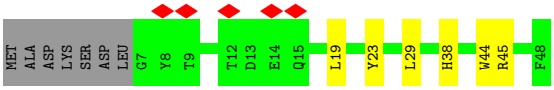
• Molecule 5: Antenna pigment protein beta chain

Chain 4:



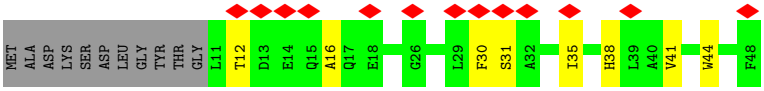
• Molecule 5: Antenna pigment protein beta chain

Chain 6:



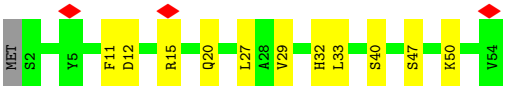
• Molecule 5: Antenna pigment protein beta chain

Chain 8:



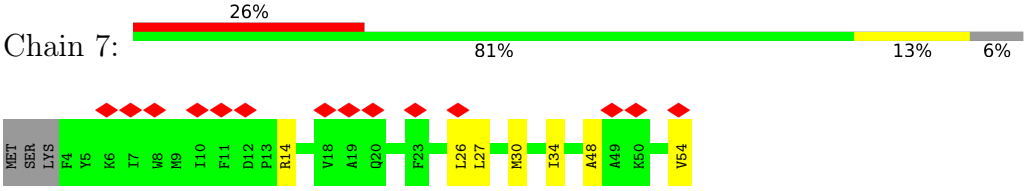
• Molecule 6: Light-harvesting protein B-875 alpha chain

Chain 5:



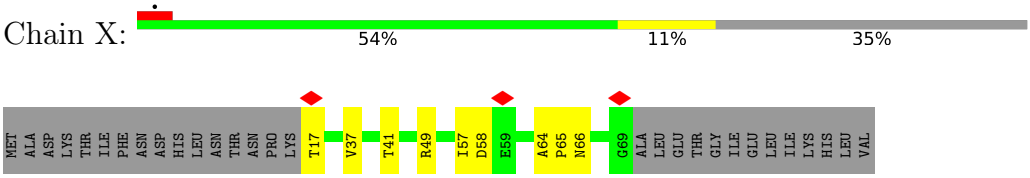
• Molecule 6: Light-harvesting protein B-875 alpha chain

Chain 7:



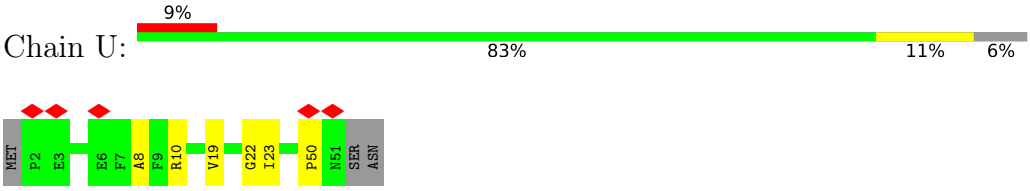
• Molecule 7: PufX

Chain X:



• Molecule 8: protein-U

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160448	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.466	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.064	Depositor
Map size (Å)	306.32, 306.32, 306.32	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.094, 1.094, 1.094	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, SPO, FME, U10, LDA, FE, PGV, BPH, BCL, LMT

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	0.34	0/2321	0.44	0/3177
2	M	0.33	0/2530	0.44	0/3455
3	H	0.30	0/1914	0.48	0/2607
4	1	0.31	0/461	0.41	0/625
4	3	0.29	0/461	0.42	0/625
4	A	0.31	0/389	0.41	0/528
4	D	0.31	0/459	0.42	0/622
4	F	0.32	0/461	0.42	0/625
4	I	0.32	0/461	0.42	0/625
4	K	0.32	0/461	0.43	0/625
4	O	0.32	0/457	0.43	0/621
4	Q	0.32	0/461	0.44	0/625
4	S	0.32	0/461	0.42	0/625
4	V	0.32	0/461	0.43	0/625
4	Y	0.33	0/461	0.43	0/625
5	2	0.28	0/356	0.40	0/488
5	4	0.28	0/364	0.42	0/499
5	6	0.25	0/344	0.37	0/472
5	8	0.25	0/308	0.33	0/424
5	B	0.28	0/372	0.38	0/510
5	E	0.32	0/364	0.40	0/499
5	G	0.30	0/378	0.41	0/518
5	J	0.28	0/364	0.40	0/499
5	N	0.28	0/364	0.38	0/499
5	P	0.29	0/364	0.40	0/499
5	R	0.30	0/360	0.43	0/494
5	T	0.28	0/364	0.40	0/499
5	W	0.29	0/360	0.38	0/494
5	Z	0.29	0/364	0.38	0/499
6	5	0.28	0/461	0.42	0/625
6	7	0.25	0/427	0.43	0/582
7	X	0.27	0/417	0.45	0/566

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
8	U	0.28	0/381	0.40	0/516
All	All	0.31	0/18931	0.43	0/25817

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)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2233	0	2189	49	0
2	M	2437	0	2355	55	0
3	H	1864	0	1862	22	0
4	1	457	0	476	7	0
4	3	457	0	476	4	0
4	A	386	0	400	15	0
4	D	455	0	469	11	0
4	F	457	0	476	7	0
4	I	457	0	476	11	0
4	K	457	0	476	9	0
4	O	453	0	465	15	0
4	Q	457	0	476	16	0
4	S	454	0	469	12	0
4	V	457	0	476	16	0
4	Y	457	0	476	14	0
5	2	343	0	325	1	0
5	4	351	0	336	6	0
5	6	332	0	314	6	0
5	8	296	0	273	7	0
5	B	359	0	340	4	0
5	E	351	0	336	9	0
5	G	365	0	345	4	0
5	J	351	0	336	10	0
5	N	351	0	336	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	351	0	336	6	0
5	R	347	0	332	5	0
5	T	351	0	336	6	0
5	W	347	0	332	11	0
5	Z	351	0	336	4	0
6	5	447	0	465	12	0
6	7	415	0	422	5	0
7	X	405	0	412	6	0
8	U	369	0	366	6	0
9	1	66	0	74	6	0
9	2	66	0	74	5	0
9	3	66	0	74	4	0
9	4	66	0	74	5	0
9	5	66	0	74	6	0
9	6	66	0	74	5	0
9	7	66	0	74	6	0
9	8	60	0	58	7	0
9	A	61	0	61	2	0
9	B	66	0	74	9	0
9	D	66	0	74	6	0
9	E	66	0	74	8	0
9	F	66	0	74	4	0
9	G	66	0	74	4	0
9	I	66	0	74	9	0
9	J	66	0	74	4	0
9	K	66	0	74	7	0
9	L	198	0	222	16	0
9	M	66	0	74	3	0
9	N	66	0	74	2	0
9	O	66	0	74	6	0
9	P	66	0	74	4	0
9	Q	66	0	74	1	0
9	R	66	0	74	4	0
9	S	66	0	74	6	0
9	T	66	0	74	5	0
9	V	66	0	74	9	0
9	W	66	0	74	8	0
9	Y	66	0	74	7	0
9	Z	66	0	74	4	0
10	L	65	0	76	5	0
10	M	65	0	76	6	0
11	L	70	0	86	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	48	0	63	1	0
12	3	51	0	76	1	0
12	H	121	0	149	6	0
12	K	41	0	60	3	0
12	L	117	0	147	8	0
12	M	85	0	110	6	0
12	Q	39	0	48	1	0
12	X	39	0	48	3	0
12	Y	43	0	54	7	0
13	L	32	0	62	2	0
13	M	16	0	31	0	0
13	X	29	0	53	2	0
13	Y	12	0	20	5	0
14	M	1	0	0	0	0
15	1	126	0	180	13	0
15	3	42	0	60	2	0
15	5	84	0	120	10	0
15	8	42	0	60	5	0
15	D	42	0	60	4	0
15	E	42	0	60	3	0
15	F	84	0	120	7	0
15	G	84	0	120	16	0
15	K	42	0	60	7	0
15	M	42	0	60	4	0
15	N	42	0	60	8	0
15	O	84	0	120	13	0
15	P	42	0	60	2	0
15	R	42	0	60	5	0
15	S	84	0	120	11	0
15	T	42	0	60	10	0
15	V	84	0	120	9	0
15	W	42	0	60	4	0
15	X	42	0	60	5	0
16	1	24	0	21	0	0
16	3	35	0	46	3	0
16	4	27	0	27	0	0
16	5	33	0	39	2	0
16	A	97	0	119	7	0
16	D	27	0	27	0	0
16	F	43	0	40	0	0
16	H	65	0	79	5	0
16	I	27	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	35	0	46	2	0
16	M	95	0	121	6	0
16	Q	43	0	55	4	0
16	S	55	0	68	2	0
16	U	67	0	83	2	0
16	X	31	0	35	0	0
17	H	98	0	92	6	0
17	M	79	0	105	6	0
17	Y	48	0	46	2	0
All	All	23458	0	24489	507	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (507) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:105:SPO:H6	9:5:102:BCL:HMB2	1.59	0.83
1:L:231:ARG:HH12	2:M:8:THR:HG22	1.49	0.77
15:5:103:SPO:H6	9:7:101:BCL:HMB2	1.67	0.77
16:H:302:LMT:H5'	4:O:38:THR:HG22	1.65	0.76
2:M:75:TRP:HE1	15:M:807:SPO:HM12	1.50	0.76
2:M:247:ARG:NH2	3:H:111:PRO:O	2.20	0.74
4:A:40:SER:O	5:B:45:ARG:NH1	2.21	0.74
5:R:35:ILE:HG12	9:R:102:BCL:H92	1.69	0.73
4:Q:7:ILE:HB	15:S:103:SPO:H343	1.69	0.73
5:N:6:LEU:HD13	5:P:15:GLN:HB3	1.71	0.73
3:H:31:LEU:O	3:H:35:ASN:ND2	2.23	0.71
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.56	0.69
1:L:31:VAL:HG22	11:M:806:U10:H362	1.74	0.69
5:G:48:PHE:HB3	15:G:103:SPO:H82	1.73	0.69
4:A:18:VAL:HG11	13:X:103:LDA:HM12	1.74	0.68
5:T:48:PHE:HB3	15:T:102:SPO:H82	1.75	0.68
1:L:26:VAL:HG13	12:H:307:PGV:H011	1.75	0.68
1:L:199:ASN:HB3	17:M:811:CDL:HA22	1.76	0.68
15:1:102:SPO:H6	9:3:103:BCL:HMB2	1.76	0.68
4:A:32:HIS:CE1	9:B:101:BCL:HMD1	2.29	0.68
12:H:307:PGV:H02	4:F:18:VAL:HG21	1.77	0.66
5:P:48:PHE:HB3	15:R:101:SPO:H82	1.76	0.66
6:5:15:ARG:HH12	8:U:10:ARG:HH21	1.41	0.66
1:L:264:GLN:HB2	12:L:306:PGV:H061	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:104:PGV:H251	4:O:21:GLY:HA3	1.77	0.66
15:W:102:SPO:H25	9:Y:103:BCL:HED3	1.78	0.66
6:5:40:SER:O	5:6:45:ARG:NH1	2.29	0.66
4:V:38:THR:HG21	4:Y:44:LEU:HD13	1.79	0.65
2:M:6:ILE:HD12	16:M:810:LMT:H11	1.79	0.65
15:1:105:SPO:H392	5:4:19:LEU:HA	1.78	0.65
4:O:40:SER:O	5:P:45:ARG:NH1	2.29	0.64
2:M:110:LYS:HG3	13:Y:101:LDA:H12	1.80	0.64
9:L:301:BCL:H2	10:L:302:BPH:HBB3	1.78	0.64
4:O:1:FME:SD	4:O:1:FME:N	2.70	0.63
15:F:103:SPO:H6	9:I:101:BCL:HMB2	1.81	0.63
9:K:102:BCL:HED3	15:N:101:SPO:H25	1.81	0.63
15:5:103:SPO:H32A	9:7:101:BCL:HBB2	1.81	0.63
4:S:32:HIS:CE1	9:T:101:BCL:HMD1	2.33	0.63
2:M:21:THR:HB	2:M:26:LEU:HD21	1.79	0.62
15:G:102:SPO:H6	9:K:102:BCL:HMB2	1.79	0.62
8:U:10:ARG:HG3	8:U:50:PRO:HB3	1.82	0.62
3:H:130:LYS:NZ	3:H:170:ASP:OD2	2.25	0.62
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.81	0.62
10:M:804:BPH:HHC	10:M:804:BPH:HBB3	1.82	0.62
16:H:301:LMT:O6'	16:H:301:LMT:O1B	2.17	0.62
4:1:7:ILE:HB	15:1:105:SPO:H343	1.80	0.62
5:N:44:TRP:CD1	15:N:101:SPO:H83	2.35	0.61
4:F:32:HIS:CE1	9:G:101:BCL:HMD1	2.35	0.61
4:V:11:PHE:HE1	4:Y:14:ARG:HA	1.66	0.61
9:8:102:BCL:HBA2	9:8:102:BCL:HBD	1.83	0.61
2:M:12:VAL:HG11	3:H:169:VAL:HG11	1.81	0.61
1:L:170:ASN:HB3	1:L:173:HIS:HB2	1.83	0.60
4:Y:36:LEU:O	4:Y:42:ASN:ND2	2.34	0.60
4:1:32:HIS:CE1	9:2:101:BCL:HMD1	2.36	0.60
5:J:48:PHE:HB3	15:N:101:SPO:H82	1.83	0.60
5:E:48:PHE:HB3	15:F:104:SPO:H82	1.83	0.60
4:V:40:SER:O	5:W:45:ARG:NH1	2.34	0.60
4:Q:10:ILE:HG23	4:S:14:ARG:HG2	1.84	0.59
12:L:306:PGV:H222	16:U:102:LMT:H101	1.83	0.59
10:M:804:BPH:HBC3	10:M:804:BPH:HHD	1.83	0.59
9:L:301:BCL:H111	9:L:308:BCL:HBB2	1.84	0.59
13:L:311:LDA:H12	13:X:103:LDA:HM22	1.84	0.59
2:M:119:SER:HB3	15:M:807:SPO:H311	1.85	0.59
15:G:103:SPO:H83	5:J:44:TRP:CD1	2.37	0.59
11:L:304:U10:H1M3	2:M:89:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:49:ARG:HH11	7:X:49:ARG:HA	1.69	0.58
9:D:101:BCL:HBB2	15:X:102:SPO:H31	1.85	0.58
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.39	0.58
4:I:7:ILE:HB	15:K:103:SPO:H343	1.85	0.58
4:I:32:HIS:CE1	9:J:101:BCL:HMD1	2.38	0.58
9:J:101:BCL:H61	15:N:101:SPO:H243	1.85	0.58
15:D:102:SPO:H182	9:F:102:BCL:H91	1.86	0.57
4:K:32:HIS:CE1	9:N:102:BCL:HMD1	2.39	0.57
1:L:247:CYS:O	1:L:251:THR:OG1	2.22	0.57
4:Q:32:HIS:CE1	9:R:102:BCL:HMD1	2.39	0.57
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.86	0.57
2:M:233:ARG:NH2	3:H:230:GLU:OE1	2.37	0.57
3:H:5:THR:HG22	3:H:11:ASP:HB3	1.87	0.57
5:R:44:TRP:CD1	15:R:101:SPO:H83	2.39	0.57
6:7:27:LEU:HD23	9:8:102:BCL:HED2	1.86	0.57
16:H:302:LMT:H21	4:O:34:ILE:HG12	1.86	0.57
4:D:3:LYS:HD3	5:G:22:VAL:HG22	1.86	0.57
5:W:6:LEU:N	5:Z:15:GLN:OE1	2.38	0.57
4:S:35:LEU:HD11	9:T:101:BCL:HHD	1.87	0.57
15:K:103:SPO:H6	9:O:101:BCL:HMB2	1.87	0.56
4:K:40:SER:O	5:N:45:ARG:NH1	2.37	0.56
2:M:201:PHE:HD2	2:M:279:THR:HG23	1.70	0.56
4:V:32:HIS:CE1	9:W:101:BCL:HMD1	2.41	0.56
2:M:52:LEU:O	4:V:15:ARG:NH2	2.33	0.56
15:D:102:SPO:H6	9:F:102:BCL:HMB2	1.88	0.56
4:K:37:SER:HA	16:K:101:LMT:H6'1	1.88	0.56
4:Y:32:HIS:CE1	9:Z:101:BCL:HMD1	2.41	0.56
9:1:101:BCL:HED3	15:1:103:SPO:H25	1.88	0.55
15:T:102:SPO:H351	9:V:101:BCL:H122	1.87	0.55
2:M:60:LEU:HD12	10:M:804:BPH:H121	1.88	0.55
5:Z:9:THR:HG23	5:Z:11:LEU:H	1.71	0.55
15:5:104:SPO:H83	5:6:44:TRP:CD1	2.42	0.54
1:L:147:PRO:HD3	7:X:66:ASN:HD22	1.73	0.54
5:8:31:SER:HB3	9:8:102:BCL:H51	1.90	0.54
4:I:6:LYS:HB3	15:K:103:SPO:H392	1.89	0.54
15:F:103:SPO:H293	15:F:104:SPO:H402	1.88	0.54
5:Z:48:PHE:HB3	15:1:103:SPO:H82	1.90	0.54
1:L:58:THR:HA	12:L:305:PGV:H062	1.90	0.53
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.89	0.53
16:M:808:LMT:H122	3:H:16:ALA:HB2	1.89	0.53
5:G:48:PHE:HD2	9:G:101:BCL:H202	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:101:BCL:HMD1	5:P:38:HIS:CE1	2.44	0.53
9:S:102:BCL:HED3	15:S:104:SPO:H25	1.90	0.53
12:Y:104:PGV:H72	9:1:101:BCL:H102	1.89	0.53
9:B:101:BCL:H193	15:E:101:SPO:H14	1.89	0.53
5:8:44:TRP:CG	15:8:101:SPO:H133	2.44	0.53
2:M:81:ASN:HB3	2:M:84:VAL:HB	1.90	0.53
9:B:101:BCL:H193	15:E:101:SPO:H11	1.91	0.53
4:Q:47:SER:OG	4:Q:53:ARG:NH1	2.42	0.53
16:3:101:LMT:H2'	16:5:101:LMT:H5'	1.90	0.53
2:M:243:THR:OG1	2:M:247:ARG:NH1	2.40	0.52
1:L:156:TRP:CD1	7:X:65:PRO:HB2	2.45	0.52
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.45	0.52
8:U:22:GLY:HA3	16:U:102:LMT:H112	1.91	0.52
1:L:133:LEU:HD13	16:A:701:LMT:H112	1.90	0.52
17:H:304:CDL:H1	4:K:14:ARG:HB3	1.90	0.52
10:L:302:BPH:HBB3	10:L:302:BPH:HHC	1.91	0.52
5:J:6:LEU:HD12	5:N:15:GLN:HE22	1.75	0.52
4:Y:15:ARG:HG2	17:Y:102:CDL:H711	1.92	0.52
15:T:102:SPO:H83	5:W:44:TRP:CD1	2.45	0.51
4:Y:40:SER:O	5:Z:45:ARG:NH1	2.43	0.51
1:L:205:GLU:O	1:L:207:ARG:NH1	2.43	0.51
4:A:30:MET:HG3	16:A:702:LMT:H102	1.92	0.51
4:O:32:HIS:CE1	9:P:102:BCL:HMD1	2.45	0.51
4:Y:42:ASN:HD21	13:Y:101:LDA:H22	1.74	0.51
12:K:104:PGV:H72	4:O:15:ARG:HG2	1.93	0.51
16:S:105:LMT:H5B	16:S:105:LMT:H6D	1.92	0.51
4:V:25:PHE:HB2	9:V:101:BCL:H52	1.93	0.51
6:5:15:ARG:HH12	8:U:10:ARG:NH2	2.08	0.51
8:U:19:VAL:O	8:U:23:ILE:HG12	2.11	0.51
15:T:102:SPO:H351	9:V:101:BCL:H8	1.93	0.51
4:S:12:ASP:HB3	4:S:15:ARG:HG3	1.92	0.51
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.93	0.50
5:J:48:PHE:HD2	9:J:101:BCL:H202	1.75	0.50
15:1:105:SPO:HM11	6:5:29:VAL:HG13	1.93	0.50
4:I:3:LYS:HB3	4:I:6:LYS:HE2	1.92	0.50
5:8:35:ILE:HD13	9:8:102:BCL:H93	1.92	0.50
17:M:811:CDL:H212	17:H:304:CDL:H151	1.92	0.50
4:A:27:LEU:HD23	9:B:101:BCL:HED3	1.92	0.50
4:D:13:PRO:HG3	5:E:19:LEU:HD21	1.93	0.50
4:I:26:LEU:HD22	16:K:101:LMT:H101	1.93	0.50
1:L:8:LYS:HB3	3:H:85:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:130:TRP:NE1	2:M:147:ALA:O	2.43	0.50
2:M:232:GLU:OE2	3:H:177:ARG:NH1	2.45	0.50
2:M:280:GLY:HA2	9:M:803:BCL:HED2	1.93	0.50
4:F:11:PHE:HZ	4:I:17:PHE:HB2	1.76	0.50
15:O:103:SPO:H31	9:S:102:BCL:HBB2	1.94	0.50
4:V:35:LEU:HD11	9:W:101:BCL:HHD	1.93	0.50
5:W:35:ILE:HG12	9:W:101:BCL:H71	1.93	0.50
4:3:35:LEU:HD11	9:4:101:BCL:HHD	1.94	0.50
5:J:6:LEU:HD12	5:N:15:GLN:NE2	2.27	0.50
4:A:37:SER:HG	16:A:702:LMT:H2O2	1.47	0.50
1:L:91:ILE:HD13	16:A:702:LMT:H112	1.94	0.49
3:H:55:PRO:HB2	17:H:304:CDL:H541	1.94	0.49
2:M:285:LEU:O	2:M:289:THR:OG1	2.27	0.49
4:A:37:SER:OG	16:A:702:LMT:O2'	2.20	0.49
15:G:103:SPO:H25	9:I:101:BCL:H2A	1.94	0.49
15:O:102:SPO:H352	5:P:22:VAL:HB	1.95	0.49
9:T:101:BCL:H42	15:T:102:SPO:H293	1.95	0.49
1:L:213:ASP:OD1	1:L:223:SER:OG	2.20	0.49
9:F:102:BCL:HMD1	5:G:38:HIS:CE1	2.47	0.49
16:M:809:LMT:H6D	16:M:809:LMT:H51	1.94	0.49
1:L:181:PHE:HB3	10:M:804:BPH:HBB2	1.94	0.49
4:A:6:LYS:HD3	15:D:102:SPO:H393	1.94	0.49
5:8:41:VAL:HG11	9:8:102:BCL:HBC1	1.95	0.49
4:O:7:ILE:HB	15:O:103:SPO:H343	1.95	0.49
2:M:233:ARG:NH1	3:H:122:GLU:OE1	2.46	0.49
9:A:703:BCL:H101	15:X:102:SPO:H292	1.94	0.49
15:T:102:SPO:H25	9:V:101:BCL:HED3	1.95	0.49
9:5:102:BCL:HMD1	5:6:38:HIS:CE1	2.48	0.49
5:J:6:LEU:HB2	5:N:11:LEU:HD11	1.95	0.49
15:S:103:SPO:H41	4:V:32:HIS:CG	2.47	0.49
9:8:102:BCL:HAA1	9:8:102:BCL:H72	1.95	0.49
9:K:102:BCL:HMD1	5:N:38:HIS:CE1	2.48	0.48
4:Q:27:LEU:HD23	9:R:102:BCL:HED3	1.95	0.48
15:5:103:SPO:H402	5:6:19:LEU:HA	1.95	0.48
15:O:102:SPO:H32	5:P:22:VAL:HG12	1.96	0.48
4:Q:33:LEU:HB3	16:Q:101:LMT:H42	1.94	0.48
4:1:4:PHE:CE1	15:1:105:SPO:H302	2.48	0.48
15:G:102:SPO:H6	9:K:102:BCL:HHB	1.95	0.48
1:L:79:PRO:HG3	16:A:702:LMT:H1B	1.95	0.48
10:L:302:BPH:HHC	10:L:302:BPH:CBB	2.43	0.48
2:M:64:LEU:HD13	10:M:804:BPH:H111	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:10:ILE:HG23	4:Q:14:ARG:HG2	1.95	0.48
15:W:102:SPO:H22	9:Y:103:BCL:O1D	2.12	0.48
6:5:20:GLN:NE2	5:6:23:TYR:OH	2.43	0.48
4:F:1:FME:HE3	5:J:29:LEU:HD13	1.95	0.48
4:A:38:THR:HG21	4:D:44:LEU:HD13	1.94	0.48
4:3:32:HIS:CE1	9:4:101:BCL:HMD1	2.49	0.48
15:V:102:SPO:HM11	4:Y:33:LEU:HD13	1.95	0.48
15:K:103:SPO:C13	9:O:101:BCL:H2	2.44	0.48
1:L:20:ASN:N	1:L:20:ASN:OD1	2.47	0.47
1:L:262:TRP:HE1	12:L:306:PGV:H22	1.78	0.47
12:L:305:PGV:H012	12:M:801:PGV:H061	1.94	0.47
4:I:20:GLN:HG3	9:K:102:BCL:H91	1.96	0.47
5:N:6:LEU:HD21	15:O:102:SPO:H401	1.95	0.47
15:S:103:SPO:H361	15:S:103:SPO:H341	1.37	0.47
4:Y:33:LEU:HG	13:Y:101:LDA:H71	1.95	0.47
4:D:41:TYR:OH	5:E:45:ARG:O	2.19	0.47
9:7:101:BCL:H18	9:7:101:BCL:H152	1.52	0.47
1:L:46:ILE:HD11	9:L:308:BCL:H201	1.97	0.47
4:A:35:LEU:HD21	9:B:101:BCL:HHD	1.97	0.47
2:M:148:TRP:HD1	17:M:811:CDL:HB32	1.79	0.47
15:O:102:SPO:H41	4:Q:32:HIS:CG	2.50	0.47
4:3:8:TRP:HB3	5:4:19:LEU:HD23	1.96	0.47
9:7:101:BCL:H41	9:7:101:BCL:H61	1.59	0.47
16:A:702:LMT:O3'	16:A:702:LMT:O2B	2.25	0.47
4:K:11:PHE:HZ	4:O:17:PHE:HB2	1.77	0.47
15:W:102:SPO:H392	9:Y:103:BCL:H41	1.95	0.47
1:L:171:PRO:HG2	12:X:101:PGV:H91	1.96	0.47
2:M:167:LEU:HD21	16:Q:101:LMT:H71	1.96	0.47
9:O:101:BCL:H2A	15:P:101:SPO:H25	1.96	0.47
6:5:33:LEU:HD11	16:5:101:LMT:H51	1.97	0.47
9:5:102:BCL:H62	9:5:102:BCL:H41	1.68	0.47
9:7:101:BCL:H2A	15:8:101:SPO:H25	1.96	0.47
1:L:50:ALA:HA	12:L:305:PGV:H101	1.96	0.47
1:L:105:VAL:O	1:L:109:ARG:HG3	2.15	0.47
4:A:40:SER:HB2	4:D:53:ARG:HD2	1.97	0.47
9:E:102:BCL:H42	15:F:104:SPO:H293	1.96	0.47
5:W:39:LEU:O	5:W:43:ILE:HG12	2.15	0.47
4:D:8:TRP:HB3	5:E:19:LEU:HD23	1.97	0.47
15:D:102:SPO:H342	5:E:22:VAL:HG11	1.97	0.47
12:Y:104:PGV:H042	4:1:14:ARG:HD2	1.96	0.47
15:5:103:SPO:H293	15:5:104:SPO:H352	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:30:MET:O	6:7:34:ILE:HG12	2.15	0.47
4:D:32:HIS:CE1	9:E:102:BCL:HMD1	2.49	0.47
4:O:11:PHE:HZ	4:Q:17:PHE:HB2	1.80	0.47
4:O:24:LEU:HG	9:P:102:BCL:HED1	1.98	0.46
9:5:102:BCL:H141	9:5:102:BCL:H171	1.97	0.46
15:8:101:SPO:H20	15:8:101:SPO:H181	1.84	0.46
1:L:124:ALA:HB1	9:L:301:BCL:H71	1.95	0.46
1:L:205:GLU:HB3	3:H:67:PRO:HA	1.97	0.46
10:M:804:BPH:H201	12:Y:104:PGV:H211	1.96	0.46
3:H:175:MET:SD	3:H:177:ARG:NH1	2.89	0.46
4:D:25:PHE:HD1	9:D:101:BCL:H2	1.80	0.46
9:T:101:BCL:H203	9:T:101:BCL:H162	1.73	0.46
16:3:101:LMT:H52	16:3:101:LMT:H81	1.70	0.46
5:8:30:PHE:CE2	15:8:101:SPO:H302	2.51	0.46
1:L:130:THR:HG23	1:L:249:ILE:HD13	1.97	0.46
4:A:35:LEU:HD21	9:B:101:BCL:HAC1	1.96	0.46
15:O:102:SPO:H20	15:O:102:SPO:H181	1.72	0.46
12:Y:104:PGV:H41	9:1:101:BCL:H111	1.96	0.46
2:M:109:LEU:HB2	13:Y:101:LDA:H32	1.98	0.46
9:N:102:BCL:H93	9:N:102:BCL:H61	1.75	0.46
4:V:27:LEU:HD23	9:W:101:BCL:HED3	1.98	0.46
15:V:103:SPO:H292	15:W:102:SPO:H351	1.97	0.46
5:N:48:PHE:HB3	15:P:101:SPO:H82	1.96	0.46
15:N:101:SPO:H10	15:N:101:SPO:H81	1.64	0.46
6:5:12:ASP:HB3	6:5:15:ARG:HD2	1.97	0.46
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.98	0.46
2:M:177:TYR:HE1	15:M:807:SPO:H22	1.79	0.46
4:A:13:PRO:HB3	5:B:19:LEU:HD21	1.96	0.46
9:S:102:BCL:HMD1	5:T:38:HIS:CE1	2.51	0.46
1:L:97:PHE:CZ	9:L:301:BCL:H112	2.49	0.46
4:Q:11:PHE:HZ	4:S:17:PHE:HB2	1.81	0.46
1:L:254:ILE:HG23	12:X:101:PGV:H011	1.98	0.46
1:L:270:PRO:HB2	16:3:101:LMT:H3'	1.97	0.46
2:M:302:GLY:O	2:M:304:ALA:N	2.49	0.46
4:A:14:ARG:HA	4:A:14:ARG:HD3	1.77	0.46
5:J:45:ARG:NH1	4:K:53:ARG:HD2	2.31	0.46
9:W:101:BCL:H112	9:W:101:BCL:H72	1.42	0.46
9:V:101:BCL:HMD1	5:W:38:HIS:CE1	2.51	0.46
9:L:301:BCL:H192	9:L:301:BCL:H162	1.69	0.46
5:E:6:LEU:HD12	15:F:103:SPO:H401	1.97	0.46
9:I:101:BCL:H192	9:I:101:BCL:H162	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:BCL:HMB1	9:I:101:BCL:HBB2	1.98	0.46
15:N:101:SPO:H361	15:N:101:SPO:H341	1.65	0.46
9:1:101:BCL:H141	9:1:101:BCL:H161	1.73	0.46
9:2:101:BCL:HBB3	9:2:101:BCL:HMB1	1.98	0.46
4:I:24:LEU:HB2	9:I:101:BCL:H42	1.98	0.45
15:O:103:SPO:H22	5:R:27:LEU:HD12	1.98	0.45
12:3:102:PGV:H102	12:3:102:PGV:H131	1.71	0.45
1:L:71:LEU:HD22	7:X:64:ALA:HB2	1.98	0.45
2:M:289:THR:HB	16:M:808:LMT:H41	1.97	0.45
12:M:812:PGV:H222	4:S:26:LEU:HD11	1.98	0.45
4:D:35:LEU:HD11	9:E:102:BCL:HHD	1.97	0.45
5:J:48:PHE:CD2	9:J:101:BCL:H202	2.50	0.45
15:V:102:SPO:H361	15:V:102:SPO:H341	1.46	0.45
9:W:101:BCL:H62	9:W:101:BCL:H41	1.63	0.45
12:Y:104:PGV:H52	12:Y:104:PGV:H21	1.66	0.45
9:L:309:BCL:H61	9:L:309:BCL:H41	1.65	0.45
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.99	0.45
16:M:809:LMT:H12	16:M:809:LMT:H42	1.70	0.45
16:M:810:LMT:H4B	8:U:8:ALA:HB2	1.98	0.45
3:H:60:LYS:HA	3:H:60:LYS:HD3	1.67	0.45
9:V:101:BCL:HMB1	9:V:101:BCL:HBB2	1.99	0.45
15:1:105:SPO:H20	15:1:105:SPO:H181	1.75	0.45
5:4:9:THR:HG23	5:4:11:LEU:H	1.81	0.45
5:R:6:LEU:HD21	5:T:19:LEU:HD12	1.98	0.45
9:Y:103:BCL:H142	9:Y:103:BCL:H111	1.74	0.45
2:M:28:ASN:HA	4:V:15:ARG:HH21	1.82	0.45
17:M:811:CDL:HB62	17:M:811:CDL:HA61	1.98	0.45
5:T:8:TYR:HE1	5:W:11:LEU:HD11	1.82	0.45
15:5:104:SPO:H20	15:5:104:SPO:H181	1.75	0.45
10:L:302:BPH:H112	9:L:308:BCL:H202	1.99	0.45
4:A:24:LEU:HB2	9:A:703:BCL:H43	1.98	0.45
9:Y:103:BCL:H141	9:Y:103:BCL:H161	1.75	0.45
5:8:12:THR:O	5:8:16:ALA:N	2.43	0.45
9:8:102:BCL:HMB1	9:8:102:BCL:HBB2	1.98	0.45
2:M:25:ASN:HB3	2:M:28:ASN:HD22	1.82	0.45
2:M:80:TRP:CH2	4:Y:34:ILE:HG12	2.51	0.45
12:M:812:PGV:H91	12:M:812:PGV:H201	1.99	0.45
12:M:812:PGV:O14	12:Q:103:PGV:H222	2.17	0.45
4:F:6:LYS:HB3	15:G:102:SPO:H402	1.98	0.45
9:1:101:BCL:HMB1	9:1:101:BCL:HBB3	1.99	0.45
9:5:102:BCL:H192	9:5:102:BCL:H162	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:102:SPO:H20	15:1:102:SPO:H181	1.73	0.45
5:4:47:TRP:O	6:5:47:SER:OG	2.35	0.45
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.99	0.44
9:L:308:BCL:HMD1	2:M:206:ILE:HD13	1.98	0.44
6:5:32:HIS:CE1	9:6:101:BCL:HMD1	2.52	0.44
15:5:104:SPO:H311	15:5:104:SPO:H291	1.42	0.44
9:W:101:BCL:HMB1	9:W:101:BCL:HBB2	1.99	0.44
9:4:101:BCL:HBB3	9:4:101:BCL:HMB1	2.00	0.44
1:L:34:PHE:O	1:L:38:THR:OG1	2.23	0.44
1:L:221:GLY:HA3	17:Y:102:CDL:H342	1.98	0.44
9:D:101:BCL:HHD	5:E:41:VAL:HG21	1.98	0.44
9:F:102:BCL:H193	9:F:102:BCL:H162	1.86	0.44
4:Q:27:LEU:O	4:Q:31:ILE:HG13	2.18	0.44
15:T:102:SPO:H25	9:V:101:BCL:H2A	1.99	0.44
15:1:102:SPO:H392	5:2:19:LEU:HA	1.99	0.44
9:D:101:BCL:HMB2	15:X:102:SPO:H6	2.00	0.44
9:R:102:BCL:HMB1	9:R:102:BCL:HBB2	1.99	0.44
9:L:309:BCL:H161	9:L:309:BCL:H122	1.69	0.44
2:M:200:PRO:HB3	12:M:801:PGV:O04	2.18	0.44
15:K:103:SPO:H181	15:K:103:SPO:H20	1.81	0.44
4:O:23:PHE:HE1	4:Q:25:PHE:CE1	2.36	0.44
12:H:306:PGV:O13	4:F:15:ARG:NH1	2.51	0.44
4:Q:38:THR:HG21	4:S:44:LEU:HD13	2.00	0.44
9:T:101:BCL:H52	15:T:102:SPO:H243	1.99	0.44
15:V:102:SPO:H26	15:V:102:SPO:H241	1.84	0.44
9:5:102:BCL:H111	9:5:102:BCL:H143	1.73	0.44
17:H:304:CDL:H352	4:K:26:LEU:HD12	2.00	0.44
5:E:48:PHE:HE2	9:E:102:BCL:H161	1.83	0.44
3:H:131:ILE:HG22	3:H:168:TRP:HE3	1.83	0.44
4:K:6:LYS:HB3	15:O:102:SPO:H392	2.00	0.43
9:P:102:BCL:HMB1	9:P:102:BCL:HBB2	1.99	0.43
1:L:61:PRO:HG3	12:L:305:PGV:H62	2.01	0.43
1:L:108:CYS:HG	2:M:251:PHE:HE1	1.63	0.43
15:S:103:SPO:H37	5:T:22:VAL:HG21	2.00	0.43
4:Y:27:LEU:O	4:Y:31:ILE:HG13	2.19	0.43
15:X:102:SPO:H26	15:X:102:SPO:H241	1.80	0.43
3:H:44:ASN:N	3:H:48:THR:O	2.41	0.43
9:Z:101:BCL:H93	9:Z:101:BCL:H112	1.75	0.43
1:L:241:VAL:HG21	10:L:302:BPH:HBC3	2.01	0.43
15:G:102:SPO:H291	9:I:101:BCL:H193	1.99	0.43
9:P:102:BCL:H102	9:P:102:BCL:H61	1.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:103:SPO:H20	15:S:103:SPO:H181	1.68	0.43
15:T:102:SPO:C25	9:V:101:BCL:HED3	2.47	0.43
9:W:101:BCL:H141	9:W:101:BCL:H162	1.78	0.43
9:Y:103:BCL:HBB3	9:Y:103:BCL:HMB1	2.00	0.43
12:H:307:PGV:H292	4:F:22:VAL:HG22	2.00	0.43
15:G:103:SPO:H10	15:G:103:SPO:H81	1.59	0.43
5:W:6:LEU:HB3	5:W:7:GLY:H	1.62	0.43
9:3:103:BCL:HHD	9:3:103:BCL:HAC1	1.88	0.43
9:6:101:BCL:H202	9:6:101:BCL:H162	1.82	0.43
6:7:26:LEU:O	6:7:30:MET:HG2	2.18	0.43
9:L:308:BCL:H18	9:L:308:BCL:H151	1.59	0.43
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.54	0.43
9:E:102:BCL:H91	9:E:102:BCL:H112	1.68	0.43
15:V:103:SPO:H361	15:V:103:SPO:H341	1.77	0.43
9:Z:101:BCL:H141	9:Z:101:BCL:H162	1.77	0.43
9:7:101:BCL:HMD1	5:8:38:HIS:CE1	2.54	0.43
1:L:66:VAL:HB	1:L:148:TYR:HB2	2.01	0.43
9:L:309:BCL:HHC	9:M:803:BCL:H42	2.00	0.43
16:H:302:LMT:H22	16:Q:102:LMT:H31	2.00	0.43
15:5:104:SPO:H10	15:5:104:SPO:H81	1.79	0.43
9:M:803:BCL:HAA2	9:M:803:BCL:HBD	2.01	0.43
9:B:101:BCL:HMB1	9:B:101:BCL:HBB2	2.00	0.43
15:F:103:SPO:H15	15:F:103:SPO:H131	1.93	0.43
4:O:34:ILE:O	4:O:38:THR:HG23	2.19	0.43
12:Y:104:PGV:H042	4:1:14:ARG:HH11	1.84	0.43
12:Y:104:PGV:H241	12:Y:104:PGV:H212	1.92	0.43
6:5:27:LEU:HD23	9:6:101:BCL:HED2	1.99	0.43
15:O:102:SPO:H26	15:O:102:SPO:H241	1.82	0.43
1:L:207:ARG:HD2	1:L:211:HIS:CD2	2.53	0.43
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.53	0.43
2:M:148:TRP:CD1	17:M:811:CDL:HB32	2.53	0.43
15:G:103:SPO:H20	15:G:103:SPO:H181	1.85	0.43
5:N:6:LEU:HD11	15:O:102:SPO:H401	2.01	0.43
9:3:103:BCL:HMD1	5:4:38:HIS:CE1	2.54	0.43
9:6:101:BCL:HMB1	9:6:101:BCL:HBB2	2.00	0.43
7:X:57:ILE:O	7:X:58:ASP:HB2	2.19	0.43
12:H:306:PGV:H62	12:H:306:PGV:H31	1.81	0.42
15:R:101:SPO:H15	15:R:101:SPO:H131	1.91	0.42
15:S:104:SPO:H15	15:S:104:SPO:H131	1.90	0.42
2:M:241:ARG:NH1	3:H:38:GLU:OE1	2.53	0.42
9:G:101:BCL:H42	15:G:103:SPO:H293	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:7:ILE:HA	4:V:7:ILE:HD12	1.73	0.42
9:3:103:BCL:H141	9:3:103:BCL:H162	1.89	0.42
5:4:12:THR:H	5:4:15:GLN:HB2	1.84	0.42
7:X:37:VAL:O	7:X:41:THR:HG23	2.18	0.42
2:M:114:LEU:HD23	2:M:114:LEU:HA	1.87	0.42
17:H:304:CDL:H351	4:K:23:PHE:HA	2.01	0.42
9:O:101:BCL:HHD	9:O:101:BCL:HAC1	1.88	0.42
15:R:101:SPO:H10	15:R:101:SPO:H81	1.60	0.42
4:S:17:PHE:HD2	15:S:104:SPO:H401	1.83	0.42
15:S:104:SPO:H82	15:S:104:SPO:H42	2.00	0.42
6:5:11:PHE:HE1	6:7:14:ARG:HG3	1.85	0.42
6:5:50:LYS:NZ	15:5:104:SPO:HM12	2.34	0.42
15:8:101:SPO:H81	15:8:101:SPO:H10	1.76	0.42
1:L:113:ILE:HG22	2:M:229:PHE:HE2	1.85	0.42
1:L:207:ARG:HG3	2:M:142:MET:HG2	2.00	0.42
1:L:212:GLU:HB3	11:L:303:U10:H4M3	2.01	0.42
12:H:306:PGV:H042	4:I:18:VAL:HG21	2.02	0.42
15:G:102:SPO:H20	15:G:102:SPO:H181	1.81	0.42
15:O:103:SPO:H341	15:O:103:SPO:H361	1.41	0.42
17:M:811:CDL:HB62	17:M:811:CDL:OA9	2.19	0.42
4:V:7:ILE:HB	15:V:103:SPO:H343	2.01	0.42
15:5:104:SPO:H15	15:5:104:SPO:H131	1.83	0.42
9:E:102:BCL:H61	9:E:102:BCL:H101	1.71	0.42
9:S:102:BCL:HHD	9:S:102:BCL:HAC1	1.79	0.42
15:V:103:SPO:H6	9:1:101:BCL:HMB2	2.01	0.42
11:L:304:U10:H13	2:M:90:PHE:HZ	1.84	0.42
2:M:127:TRP:CB	12:M:812:PGV:H212	2.50	0.42
3:H:163:LYS:HB2	3:H:163:LYS:HE3	1.81	0.42
5:B:31:SER:HB3	9:B:101:BCL:H72	2.01	0.42
4:1:27:LEU:HD23	9:2:101:BCL:HED3	2.02	0.42
9:L:309:BCL:HMB1	9:L:309:BCL:HBB2	2.01	0.42
9:G:101:BCL:HMB1	9:G:101:BCL:HBB2	2.01	0.42
15:G:102:SPO:H26	15:G:102:SPO:H241	1.87	0.42
9:K:102:BCL:H61	9:K:102:BCL:H41	1.84	0.42
12:K:104:PGV:H301	12:K:104:PGV:H272	1.86	0.42
4:S:11:PHE:HZ	4:V:17:PHE:HB2	1.85	0.42
15:V:102:SPO:H20	15:V:102:SPO:H181	1.81	0.42
2:M:252:TRP:HB3	2:M:256:MET:HE2	2.02	0.42
4:O:38:THR:HG21	4:Q:44:LEU:HD13	2.01	0.42
9:S:102:BCL:O1D	15:S:104:SPO:H22	2.19	0.42
9:6:101:BCL:H162	9:6:101:BCL:H141	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:226:THR:HA	11:L:303:U10:H3M2	2.02	0.42
15:M:807:SPO:H15	15:M:807:SPO:H131	1.88	0.42
4:D:10:ILE:HD11	15:F:103:SPO:H37	2.02	0.42
15:K:103:SPO:H361	15:K:103:SPO:H341	1.55	0.42
15:3:104:SPO:H20	15:3:104:SPO:H181	1.89	0.42
1:L:230:HIS:CE1	2:M:234:GLU:OE1	2.73	0.41
11:L:304:U10:H121	11:L:304:U10:H101	1.64	0.41
9:B:101:BCL:H141	9:B:101:BCL:H162	1.77	0.41
9:V:101:BCL:H62	9:V:101:BCL:H41	1.71	0.41
12:X:101:PGV:H252	12:X:101:PGV:H281	1.86	0.41
9:I:101:BCL:HMD1	5:J:38:HIS:CE1	2.55	0.41
4:Q:41:TYR:OH	5:R:45:ARG:O	2.26	0.41
4:V:8:TRP:HB3	5:W:19:LEU:HD23	2.01	0.41
9:O:101:BCL:H141	9:O:101:BCL:H161	1.74	0.41
9:2:101:BCL:H192	9:2:101:BCL:H162	1.82	0.41
2:M:51:TYR:O	2:M:132:ARG:NH1	2.42	0.41
3:H:111:PRO:HG3	3:H:242:MET:SD	2.61	0.41
9:E:102:BCL:HBB2	9:E:102:BCL:HMB1	2.02	0.41
15:K:103:SPO:H293	15:N:101:SPO:H37	2.02	0.41
4:S:40:SER:O	5:T:45:ARG:NH1	2.54	0.41
15:3:104:SPO:H10	15:3:104:SPO:H81	1.74	0.41
3:H:66:LEU:HB3	3:H:70:ARG:HB2	2.02	0.41
9:D:101:BCL:H102	15:E:101:SPO:H343	2.03	0.41
9:K:102:BCL:H151	9:K:102:BCL:H111	1.60	0.41
15:O:103:SPO:H6	9:S:102:BCL:HMB2	2.02	0.41
4:Y:36:LEU:HD13	4:Y:43:TRP:CH2	2.56	0.41
9:Z:101:BCL:HMB1	9:Z:101:BCL:HBB2	2.02	0.41
2:M:270:ILE:O	2:M:274:VAL:HG13	2.19	0.41
3:H:80:SER:OG	3:H:82:ASP:OD1	2.26	0.41
9:D:101:BCL:HMD1	5:E:38:HIS:CE1	2.56	0.41
15:G:102:SPO:H361	15:G:102:SPO:H341	1.58	0.41
15:T:102:SPO:H15	15:T:102:SPO:H131	1.86	0.41
4:1:35:LEU:HD11	9:2:101:BCL:HHD	2.03	0.41
15:N:101:SPO:H20	15:N:101:SPO:H181	1.82	0.41
4:Y:42:ASN:ND2	13:Y:101:LDA:H22	2.35	0.41
15:1:103:SPO:H10	15:1:103:SPO:H81	1.74	0.41
6:7:48:ALA:HB1	6:7:54:VAL:HB	2.03	0.41
15:G:103:SPO:H27	9:I:101:BCL:HBA1	2.02	0.41
15:R:101:SPO:H20	15:R:101:SPO:H181	1.81	0.41
4:3:1:FME:HE1	5:6:29:LEU:HD13	2.02	0.41
9:4:101:BCL:HBB2	9:4:101:BCL:H122	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:HIS:HA	11:L:303:U10:O2	2.20	0.41
2:M:234:GLU:OE2	2:M:266:HIS:CE1	2.74	0.41
2:M:250:LEU:HD23	2:M:250:LEU:HA	1.84	0.41
5:B:39:LEU:HD12	5:B:39:LEU:HA	1.91	0.41
9:I:101:BCL:H141	9:I:101:BCL:H161	1.83	0.41
9:Q:104:BCL:HBB3	9:Q:104:BCL:HMB1	2.02	0.41
9:4:101:BCL:H162	9:4:101:BCL:H141	1.78	0.41
15:X:102:SPO:H15	15:X:102:SPO:H131	1.95	0.41
13:L:311:LDA:H21	13:L:311:LDA:HM23	1.79	0.41
15:G:103:SPO:H393	4:I:20:GLN:HE21	1.84	0.41
16:S:101:LMT:H62	16:S:101:LMT:H32	1.93	0.41
15:V:103:SPO:H391	5:W:6:LEU:HD21	2.03	0.41
12:L:310:PGV:H291	12:L:310:PGV:H322	1.79	0.40
2:M:202:HIS:O	2:M:206:ILE:HG13	2.21	0.40
4:I:6:LYS:HG2	4:I:9:MET:SD	2.61	0.40
15:1:103:SPO:H15	15:1:103:SPO:H131	1.83	0.40
1:L:177:ILE:HD13	9:L:309:BCL:HMD1	2.03	0.40
17:H:304:CDL:H172	17:H:304:CDL:H141	1.76	0.40
15:G:102:SPO:H10	15:G:102:SPO:H81	1.97	0.40
16:Q:101:LMT:H82	16:Q:101:LMT:H111	1.92	0.40
4:V:5:TYR:CD2	5:W:17:GLN:HG2	2.56	0.40
9:Y:103:BCL:H192	9:Y:103:BCL:H162	1.74	0.40
3:H:4:VAL:HG11	16:H:302:LMT:O2'	2.22	0.40
4:V:7:ILE:HG13	4:V:11:PHE:CD2	2.56	0.40
4:Y:33:LEU:HD12	4:Y:33:LEU:HA	1.88	0.40
11:L:304:U10:H13	2:M:90:PHE:CZ	2.57	0.40
9:L:308:BCL:H121	9:L:308:BCL:H162	1.96	0.40
4:D:27:LEU:O	4:D:31:ILE:HG13	2.21	0.40
9:E:102:BCL:H162	9:E:102:BCL:H141	1.74	0.40
4:S:17:PHE:CZ	15:S:103:SPO:H32	2.57	0.40
9:L:301:BCL:H143	9:L:301:BCL:H161	1.79	0.40
4:Q:23:PHE:HE1	4:S:25:PHE:CE1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/282 (99%)	267 (96%)	12 (4%)	0	100	100
2	M	304/308 (99%)	293 (96%)	11 (4%)	0	100	100
3	H	244/260 (94%)	231 (95%)	13 (5%)	0	100	100
4	1	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
4	3	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	A	43/54 (80%)	43 (100%)	0	0	100	100
4	D	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	F	52/54 (96%)	52 (100%)	0	0	100	100
4	I	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	K	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	O	52/54 (96%)	52 (100%)	0	0	100	100
4	Q	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	S	52/54 (96%)	52 (100%)	0	0	100	100
4	V	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
4	Y	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
5	2	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
5	4	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	6	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
5	8	36/49 (74%)	36 (100%)	0	0	100	100
5	B	42/49 (86%)	42 (100%)	0	0	100	100
5	E	41/49 (84%)	41 (100%)	0	0	100	100
5	G	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
5	J	41/49 (84%)	41 (100%)	0	0	100	100
5	N	41/49 (84%)	41 (100%)	0	0	100	100
5	P	41/49 (84%)	37 (90%)	4 (10%)	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	41/49 (84%)	41 (100%)	0	0	100	100
5	W	41/49 (84%)	41 (100%)	0	0	100	100
5	Z	41/49 (84%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	5	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
6	7	49/54 (91%)	49 (100%)	0	0	100	100
7	X	51/82 (62%)	48 (94%)	3 (6%)	0	100	100
8	U	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	2211/2427 (91%)	2144 (97%)	67 (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	220/221 (100%)	215 (98%)	5 (2%)	50	78
2	M	239/241 (99%)	230 (96%)	9 (4%)	33	64
3	H	197/208 (95%)	194 (98%)	3 (2%)	65	85
4	1	48/48 (100%)	48 (100%)	0	100	100
4	3	48/48 (100%)	48 (100%)	0	100	100
4	A	41/48 (85%)	41 (100%)	0	100	100
4	D	47/48 (98%)	47 (100%)	0	100	100
4	F	48/48 (100%)	48 (100%)	0	100	100
4	I	48/48 (100%)	48 (100%)	0	100	100
4	K	48/48 (100%)	47 (98%)	1 (2%)	53	79
4	O	47/48 (98%)	46 (98%)	1 (2%)	53	79
4	Q	48/48 (100%)	48 (100%)	0	100	100
4	S	48/48 (100%)	48 (100%)	0	100	100
4	V	48/48 (100%)	48 (100%)	0	100	100
4	Y	48/48 (100%)	47 (98%)	1 (2%)	53	79
5	2	34/40 (85%)	34 (100%)	0	100	100
5	4	35/40 (88%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	6	32/40 (80%)	32 (100%)	0	100 100
5	8	26/40 (65%)	26 (100%)	0	100 100
5	B	36/40 (90%)	36 (100%)	0	100 100
5	E	35/40 (88%)	34 (97%)	1 (3%)	42 73
5	G	37/40 (92%)	36 (97%)	1 (3%)	44 74
5	J	35/40 (88%)	35 (100%)	0	100 100
5	N	35/40 (88%)	35 (100%)	0	100 100
5	P	35/40 (88%)	34 (97%)	1 (3%)	42 73
5	R	34/40 (85%)	34 (100%)	0	100 100
5	T	35/40 (88%)	35 (100%)	0	100 100
5	W	34/40 (85%)	32 (94%)	2 (6%)	19 47
5	Z	35/40 (88%)	34 (97%)	1 (3%)	42 73
6	5	48/49 (98%)	48 (100%)	0	100 100
6	7	43/49 (88%)	43 (100%)	0	100 100
7	X	40/66 (61%)	39 (98%)	1 (2%)	47 76
8	U	34/37 (92%)	34 (100%)	0	100 100
All	All	1866/2007 (93%)	1839 (99%)	27 (1%)	68 86

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	52	SER
1	L	71	LEU
1	L	102	LEU
1	L	267	VAL
1	L	272	TRP
2	M	8	THR
2	M	20	MET
2	M	21	THR
2	M	86	LEU
2	M	197	PHE
2	M	216	PHE
2	M	235	LEU
2	M	236	GLU
2	M	272	MET
3	H	83	ARG

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Mol	Chain	Res	Type
3	H	143	SER
3	H	231	ASP
5	E	18	GLU
5	G	6	LEU
4	K	12	ASP
4	O	14	ARG
5	P	27	LEU
5	W	13	ASP
5	W	18	GLU
4	Y	33	LEU
5	Z	45	ARG
7	X	17	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
5	G	17	GLN
7	X	66	ASN
8	U	51	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	Y	1	4	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
4	FME	F	1	4	8,9,10	0.53	0	7,9,11	0.91	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FME	S	1	4	5,6,10	0.79	0	3,6,11	0.67	0
4	FME	A	1	4	8,9,10	0.50	0	7,9,11	0.88	1 (14%)
4	FME	K	1	4	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
4	FME	O	1	4	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
4	FME	3	1	4	8,9,10	0.49	0	7,9,11	0.95	1 (14%)
4	FME	1	1	4	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
4	FME	Q	1	4	8,9,10	0.51	0	7,9,11	0.97	1 (14%)
4	FME	I	1	4	8,9,10	0.51	0	7,9,11	0.96	1 (14%)
4	FME	V	1	4	8,9,10	0.52	0	7,9,11	1.03	1 (14%)
4	FME	D	1	4	8,9,10	0.49	0	7,9,11	1.05	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	Y	1	4	-	1/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	S	1	4	-	1/2/5/11	-
4	FME	A	1	4	-	3/7/9/11	-
4	FME	K	1	4	-	1/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	3	1	4	-	0/7/9/11	-
4	FME	1	1	4	-	0/7/9/11	-
4	FME	Q	1	4	-	0/7/9/11	-
4	FME	I	1	4	-	1/7/9/11	-
4	FME	V	1	4	-	1/7/9/11	-
4	FME	D	1	4	-	0/7/9/11	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	1	FME	O-C-CA	-2.53	118.14	124.78
4	D	1	FME	O-C-CA	-2.53	118.14	124.78
4	I	1	FME	O-C-CA	-2.49	118.26	124.78
4	Y	1	FME	O-C-CA	-2.48	118.28	124.78
4	1	1	FME	O-C-CA	-2.47	118.31	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	1	FME	O-C-CA	-2.45	118.36	124.78
4	V	1	FME	O-C-CA	-2.41	118.45	124.78
4	3	1	FME	O-C-CA	-2.41	118.47	124.78
4	Q	1	FME	O-C-CA	-2.39	118.51	124.78
4	F	1	FME	O-C-CA	-2.33	118.67	124.78
4	A	1	FME	O-C-CA	-2.27	118.83	124.78

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	A	1	FME	N-CA-CB-CG
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	V	1	FME	CB-CA-N-CN
4	Y	1	FME	O1-CN-N-CA
4	I	1	FME	CA-CB-CG-SD
4	A	1	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	FME	1	0
4	O	1	FME	1	0
4	3	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 112 ligands modelled in this entry, 1 is monoatomic - leaving 111 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	SPO	3	104	-	40,41,41	0.64	0	47,50,50	2.02	16 (34%)
15	SPO	V	102	-	40,41,41	0.65	0	47,50,50	1.71	12 (25%)
9	BCL	S	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.88	15 (21%)
12	PGV	L	310	-	44,44,50	1.00	2 (4%)	48,49,56	1.13	4 (8%)
15	SPO	X	102	-	40,41,41	0.66	0	47,50,50	1.81	11 (23%)
15	SPO	1	102	-	40,41,41	0.65	0	47,50,50	2.02	14 (29%)
9	BCL	4	101	-	58,74,74	1.67	10 (17%)	69,115,115	1.64	13 (18%)
16	LMT	4	102	-	28,28,36	0.46	0	39,39,47	0.77	1 (2%)
17	CDL	H	305	-	35,35,99	1.38	3 (8%)	42,44,111	1.31	6 (14%)
9	BCL	F	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.70	16 (23%)
16	LMT	F	101	-	27,27,36	0.48	0	38,38,47	0.88	2 (5%)
9	BCL	K	102	-	58,74,74	1.65	8 (13%)	69,115,115	1.70	12 (17%)
9	BCL	O	101	-	58,74,74	1.61	8 (13%)	69,115,115	1.72	11 (15%)
17	CDL	Y	102	-	47,47,99	1.16	3 (6%)	52,58,111	1.07	3 (5%)
13	LDA	X	104	-	12,15,15	2.13	1 (8%)	14,17,17	0.50	0
15	SPO	5	103	-	40,41,41	0.66	0	47,50,50	1.97	15 (31%)
17	CDL	M	811	-	78,78,99	1.03	4 (5%)	84,90,111	1.20	6 (7%)
13	LDA	L	311	-	12,15,15	2.09	1 (8%)	14,17,17	0.53	0
15	SPO	E	101	-	40,41,41	0.63	0	47,50,50	1.71	12 (25%)
16	LMT	A	702	-	36,36,36	0.39	0	47,47,47	0.74	1 (2%)
11	U10	L	304	-	35,35,63	0.77	2 (5%)	42,45,79	0.67	0
9	BCL	T	101	-	58,74,74	1.65	10 (17%)	69,115,115	1.65	12 (17%)
12	PGV	M	801	-	46,46,50	0.94	2 (4%)	49,52,56	1.17	4 (8%)
9	BCL	M	803	-	58,74,74	1.66	11 (18%)	69,115,115	1.74	14 (20%)
10	BPH	M	804	-	51,70,70	0.57	1 (1%)	52,101,101	0.76	1 (1%)
15	SPO	R	101	-	40,41,41	0.68	0	47,50,50	2.32	15 (31%)
9	BCL	L	308	-	58,74,74	1.61	9 (15%)	69,115,115	1.82	15 (21%)
12	PGV	H	303	-	33,33,50	1.14	2 (6%)	36,38,56	1.15	4 (11%)
15	SPO	S	104	-	40,41,41	0.66	0	47,50,50	1.66	16 (34%)
12	PGV	L	306	-	32,32,50	1.10	2 (6%)	35,38,56	1.18	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	PGV	Q	103	-	38,38,50	1.05	2 (5%)	41,44,56	1.04	2 (4%)
15	SPO	K	103	-	40,41,41	0.66	0	47,50,50	1.81	10 (21%)
12	PGV	H	307	-	46,46,50	0.95	2 (4%)	49,52,56	1.02	3 (6%)
15	SPO	F	104	-	40,41,41	0.64	0	47,50,50	1.86	13 (27%)
9	BCL	3	103	-	58,74,74	1.67	9 (15%)	69,115,115	1.69	12 (17%)
15	SPO	V	103	-	40,41,41	0.68	0	47,50,50	1.82	14 (29%)
16	LMT	H	302	-	31,31,36	0.45	0	42,42,47	1.09	3 (7%)
9	BCL	D	101	-	58,74,74	1.62	10 (17%)	69,115,115	1.76	17 (24%)
13	LDA	L	307	-	12,15,15	2.08	1 (8%)	14,17,17	0.50	0
9	BCL	8	102	-	52,68,74	1.80	11 (21%)	61,107,115	1.66	11 (18%)
9	BCL	Z	101	-	58,74,74	1.64	10 (17%)	69,115,115	1.70	14 (20%)
9	BCL	W	101	-	58,74,74	1.63	11 (18%)	69,115,115	1.68	13 (18%)
12	PGV	X	101	-	38,38,50	1.04	2 (5%)	41,44,56	1.10	3 (7%)
15	SPO	T	102	-	40,41,41	0.69	0	47,50,50	1.84	13 (27%)
15	SPO	G	102	-	40,41,41	0.64	0	47,50,50	1.80	12 (25%)
9	BCL	1	101	-	58,74,74	1.63	8 (13%)	69,115,115	1.90	18 (26%)
9	BCL	E	102	-	58,74,74	1.65	11 (18%)	69,115,115	1.63	18 (26%)
16	LMT	M	810	-	34,34,36	0.42	0	45,45,47	1.15	4 (8%)
16	LMT	U	102	-	36,36,36	0.35	0	47,47,47	0.73	1 (2%)
11	U10	M	806	-	48,48,63	0.71	2 (4%)	58,61,79	0.58	0
12	PGV	Y	104	-	42,42,50	0.98	2 (4%)	44,48,56	1.09	3 (6%)
15	SPO	1	105	-	40,41,41	0.66	0	47,50,50	1.77	13 (27%)
9	BCL	7	101	-	58,74,74	1.63	9 (15%)	69,115,115	1.69	12 (17%)
15	SPO	O	103	-	40,41,41	0.67	0	47,50,50	1.83	14 (29%)
16	LMT	I	102	-	28,28,36	0.43	0	39,39,47	0.71	1 (2%)
16	LMT	F	105	-	17,17,36	0.45	0	22,22,47	0.57	0
9	BCL	P	102	-	58,74,74	1.62	10 (17%)	69,115,115	1.69	14 (20%)
9	BCL	B	101	-	58,74,74	1.65	10 (17%)	69,115,115	1.65	14 (20%)
17	CDL	H	304	-	60,60,99	1.18	4 (6%)	66,72,111	1.17	4 (6%)
15	SPO	S	103	-	40,41,41	0.67	0	47,50,50	1.98	15 (31%)
9	BCL	J	101	-	58,74,74	1.67	10 (17%)	69,115,115	1.69	13 (18%)
15	SPO	N	101	-	40,41,41	0.65	0	47,50,50	2.11	16 (34%)
16	LMT	1	104	-	24,25,36	0.61	1 (4%)	31,34,47	0.82	1 (3%)
9	BCL	L	309	-	58,74,74	1.65	10 (17%)	69,115,115	1.60	13 (18%)
15	SPO	1	103	-	40,41,41	0.66	0	47,50,50	1.97	17 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	LMT	A	701	-	36,36,36	0.34	0	47,47,47	0.71	0
16	LMT	K	101	-	36,36,36	0.41	0	47,47,47	0.96	2 (4%)
16	LMT	Q	101	-	24,24,36	0.44	0	29,29,47	0.97	1 (3%)
15	SPO	F	103	-	40,41,41	0.64	0	47,50,50	1.66	12 (25%)
9	BCL	R	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.69	15 (21%)
13	LDA	Y	101	-	8,11,15	2.55	1 (12%)	10,13,17	0.45	0
12	PGV	L	305	-	38,38,50	1.05	2 (5%)	41,44,56	1.07	3 (7%)
16	LMT	U	101	-	33,33,36	0.38	0	44,44,47	0.78	1 (2%)
16	LMT	3	101	-	36,36,36	0.42	0	47,47,47	0.91	3 (6%)
12	PGV	K	104	-	38,40,50	1.02	2 (5%)	40,42,56	1.16	3 (7%)
9	BCL	Q	104	-	58,74,74	1.60	8 (13%)	69,115,115	1.73	14 (20%)
10	BPH	L	302	-	51,70,70	0.60	2 (3%)	52,101,101	0.69	1 (1%)
9	BCL	G	101	-	58,74,74	1.66	10 (17%)	69,115,115	1.66	13 (18%)
16	LMT	5	101	-	34,34,36	0.39	0	45,45,47	0.73	0
15	SPO	8	101	-	40,41,41	0.65	0	47,50,50	2.13	13 (27%)
15	SPO	G	103	-	40,41,41	0.64	0	47,50,50	2.14	14 (29%)
9	BCL	I	101	-	58,74,74	1.63	9 (15%)	69,115,115	1.74	15 (21%)
9	BCL	N	102	-	58,74,74	1.63	11 (18%)	69,115,115	1.74	13 (18%)
13	LDA	M	802	-	12,15,15	2.08	1 (8%)	14,17,17	0.57	0
16	LMT	S	105	-	31,31,36	0.45	0	42,42,47	0.67	0
16	LMT	D	103	-	28,28,36	0.43	0	39,39,47	0.67	1 (2%)
15	SPO	D	102	-	40,41,41	0.65	0	47,50,50	1.84	15 (31%)
9	BCL	V	101	-	58,74,74	1.62	8 (13%)	69,115,115	1.67	12 (17%)
9	BCL	Y	103	-	58,74,74	1.60	9 (15%)	69,115,115	1.77	14 (20%)
16	LMT	X	105	-	32,32,36	0.40	0	43,43,47	0.80	1 (2%)
12	PGV	H	306	-	39,39,50	1.07	2 (5%)	42,45,56	1.22	3 (7%)
12	PGV	M	812	-	37,37,50	1.05	2 (5%)	40,43,56	1.18	4 (10%)
15	SPO	O	102	-	40,41,41	0.66	0	47,50,50	1.82	12 (25%)
9	BCL	5	102	-	58,74,74	1.64	8 (13%)	69,115,115	1.71	13 (18%)
9	BCL	L	301	-	58,74,74	1.64	10 (17%)	69,115,115	1.66	16 (23%)
16	LMT	Q	102	-	19,19,36	0.49	0	24,24,47	0.55	0
15	SPO	M	807	-	40,41,41	0.63	0	47,50,50	1.67	10 (21%)
9	BCL	A	703	-	53,69,74	1.71	10 (18%)	63,109,115	1.70	13 (20%)
15	SPO	P	101	-	40,41,41	0.64	0	47,50,50	1.76	12 (25%)
16	LMT	S	101	-	25,25,36	0.46	0	30,30,47	0.81	0
16	LMT	A	704	-	28,28,36	0.45	0	39,39,47	0.75	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	LMT	M	809	-	36,36,36	0.37	0	47,47,47	0.69	1 (2%)
16	LMT	M	808	-	27,27,36	0.46	0	32,33,47	0.64	1 (3%)
9	BCL	2	101	-	58,74,74	1.64	10 (17%)	69,115,115	1.72	13 (18%)
12	PGV	3	102	-	50,50,50	0.90	2 (4%)	53,56,56	1.05	3 (5%)
13	LDA	X	103	-	9,12,15	2.43	1 (11%)	11,14,17	0.49	0
16	LMT	H	301	-	36,36,36	0.37	0	47,47,47	0.92	2 (4%)
9	BCL	6	101	-	58,74,74	1.65	10 (17%)	69,115,115	1.61	11 (15%)
11	U10	L	303	-	35,35,63	0.81	2 (5%)	42,45,79	0.67	0
15	SPO	W	102	-	40,41,41	0.67	0	47,50,50	1.72	14 (29%)
15	SPO	5	104	-	40,41,41	0.63	0	47,50,50	1.93	11 (23%)

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	SPO	3	104	-	-	4/47/47/47	-
15	SPO	V	102	-	-	3/47/47/47	-
9	BCL	S	102	-	-	15/37/137/137	-
12	PGV	L	310	-	-	7/46/46/55	-
15	SPO	X	102	-	-	4/47/47/47	-
15	SPO	1	102	-	-	5/47/47/47	-
9	BCL	4	101	-	-	9/37/137/137	-
16	LMT	4	102	-	-	2/13/53/61	0/2/2/2
17	CDL	H	305	-	-	8/37/37/110	-
9	BCL	F	102	-	-	9/37/137/137	-
16	LMT	F	101	-	-	5/11/51/61	0/2/2/2
9	BCL	K	102	-	-	11/37/137/137	-
9	BCL	O	101	-	-	12/37/137/137	-
17	CDL	Y	102	-	-	16/56/56/110	-
13	LDA	X	104	-	-	0/13/13/13	-
15	SPO	5	103	-	-	5/47/47/47	-
17	CDL	M	811	-	-	30/89/89/110	-
13	LDA	L	311	-	-	2/13/13/13	-
15	SPO	E	101	-	-	6/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LMT	A	702	-	-	6/21/61/61	0/2/2/2
11	U10	L	304	-	-	5/30/54/87	0/1/1/1
9	BCL	T	101	-	-	13/37/137/137	-
12	PGV	M	801	-	-	14/51/51/55	-
9	BCL	M	803	-	-	10/37/137/137	-
10	BPH	M	804	-	-	6/37/105/105	0/5/6/6
15	SPO	R	101	-	-	7/47/47/47	-
9	BCL	L	308	-	-	7/37/137/137	-
12	PGV	H	303	-	-	3/35/35/55	-
15	SPO	S	104	-	-	10/47/47/47	-
12	PGV	L	306	-	-	13/37/37/55	-
12	PGV	Q	103	-	-	9/43/43/55	-
15	SPO	K	103	-	-	4/47/47/47	-
12	PGV	H	307	-	-	13/51/51/55	-
15	SPO	F	104	-	-	1/47/47/47	-
9	BCL	3	103	-	-	11/37/137/137	-
15	SPO	V	103	-	-	5/47/47/47	-
16	LMT	H	302	-	-	6/16/56/61	0/2/2/2
9	BCL	D	101	-	-	9/37/137/137	-
13	LDA	L	307	-	-	4/13/13/13	-
9	BCL	8	102	-	-	14/29/129/137	-
9	BCL	Z	101	-	-	12/37/137/137	-
9	BCL	W	101	-	-	19/37/137/137	-
12	PGV	X	101	-	-	8/43/43/55	-
15	SPO	T	102	-	-	7/47/47/47	-
15	SPO	G	102	-	-	7/47/47/47	-
9	BCL	1	101	-	-	12/37/137/137	-
9	BCL	E	102	-	-	13/37/137/137	-
16	LMT	M	810	-	-	7/19/59/61	0/2/2/2
16	LMT	U	102	-	-	3/21/61/61	0/2/2/2
11	U10	M	806	-	-	1/45/69/87	0/1/1/1
12	PGV	Y	104	-	-	13/47/47/55	-
15	SPO	1	105	-	-	6/47/47/47	-
9	BCL	7	101	-	-	15/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SPO	O	103	-	-	10/47/47/47	-
16	LMT	I	102	-	-	3/13/53/61	0/2/2/2
16	LMT	F	105	-	-	1/9/29/61	0/1/1/2
9	BCL	P	102	-	-	15/37/137/137	-
9	BCL	B	101	-	-	7/37/137/137	-
17	CDL	H	304	-	-	23/71/71/110	-
15	SPO	S	103	-	-	6/47/47/47	-
9	BCL	J	101	-	-	14/37/137/137	-
15	SPO	N	101	-	-	9/47/47/47	-
16	LMT	1	104	-	-	2/11/44/61	0/2/2/2
9	BCL	L	309	-	-	12/37/137/137	-
15	SPO	1	103	-	-	4/47/47/47	-
16	LMT	A	701	-	-	5/21/61/61	0/2/2/2
16	LMT	K	101	-	-	2/21/61/61	0/2/2/2
16	LMT	Q	101	-	-	2/15/35/61	0/1/1/2
15	SPO	F	103	-	-	4/47/47/47	-
9	BCL	R	102	-	-	13/37/137/137	-
13	LDA	Y	101	-	-	1/9/9/13	-
12	PGV	L	305	-	-	13/43/43/55	-
16	LMT	U	101	-	-	1/18/58/61	0/2/2/2
16	LMT	3	101	-	-	7/21/61/61	0/2/2/2
12	PGV	K	104	-	-	14/40/42/55	-
9	BCL	Q	104	-	-	17/37/137/137	-
10	BPH	L	302	-	-	3/37/105/105	0/5/6/6
9	BCL	G	101	-	-	15/37/137/137	-
16	LMT	5	101	-	-	5/19/59/61	0/2/2/2
15	SPO	8	101	-	-	2/47/47/47	-
15	SPO	G	103	-	-	6/47/47/47	-
9	BCL	I	101	-	-	10/37/137/137	-
9	BCL	N	102	-	-	14/37/137/137	-
13	LDA	M	802	-	-	2/13/13/13	-
16	LMT	S	105	-	-	5/16/56/61	0/2/2/2
16	LMT	D	103	-	-	2/13/53/61	0/2/2/2
15	SPO	D	102	-	-	2/47/47/47	-
9	BCL	V	101	-	-	15/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	Y	103	-	-	15/37/137/137	-
16	LMT	X	105	-	-	4/17/57/61	0/2/2/2
12	PGV	H	306	-	-	14/44/44/55	-
12	PGV	M	812	-	-	19/42/42/55	-
15	SPO	O	102	-	-	5/47/47/47	-
9	BCL	5	102	-	-	12/37/137/137	-
9	BCL	L	301	-	-	20/37/137/137	-
16	LMT	Q	102	-	-	2/11/31/61	0/1/1/2
15	SPO	M	807	-	-	8/47/47/47	-
9	BCL	A	703	-	-	9/31/131/137	-
15	SPO	P	101	-	-	8/47/47/47	-
16	LMT	S	101	-	-	4/17/37/61	0/1/1/2
16	LMT	A	704	-	-	0/13/53/61	0/2/2/2
16	LMT	M	809	-	-	8/21/61/61	0/2/2/2
16	LMT	M	808	-	-	2/19/39/61	0/1/1/2
9	BCL	2	101	-	-	15/37/137/137	-
12	PGV	3	102	-	-	10/55/55/55	-
13	LDA	X	103	-	-	1/10/10/13	-
16	LMT	H	301	-	-	4/21/61/61	0/2/2/2
9	BCL	6	101	-	-	16/37/137/137	-
11	U10	L	303	-	-	9/30/54/87	0/1/1/1
15	SPO	W	102	-	-	10/47/47/47	-
15	SPO	5	104	-	-	8/47/47/47	-

All (362) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	104	LDA	O1-N1	-7.33	1.25	1.42
13	X	103	LDA	O1-N1	-7.27	1.25	1.42
13	L	311	LDA	O1-N1	-7.19	1.25	1.42
13	L	307	LDA	O1-N1	-7.19	1.25	1.42
13	Y	101	LDA	O1-N1	-7.18	1.25	1.42
13	M	802	LDA	O1-N1	-7.17	1.25	1.42
9	F	102	BCL	O2D-CGD	5.13	1.45	1.33
9	6	101	BCL	O2D-CGD	5.11	1.45	1.33
9	8	102	BCL	O2D-CGD	5.08	1.45	1.33
9	5	102	BCL	O2D-CGD	5.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	703	BCL	O2D-CGD	5.05	1.45	1.33
9	3	103	BCL	O2D-CGD	5.02	1.45	1.33
9	I	101	BCL	O2D-CGD	5.02	1.45	1.33
9	P	102	BCL	O2D-CGD	5.02	1.45	1.33
9	T	101	BCL	O2D-CGD	5.01	1.45	1.33
9	N	102	BCL	O2D-CGD	5.00	1.45	1.33
9	W	101	BCL	O2D-CGD	4.99	1.45	1.33
9	E	102	BCL	O2D-CGD	4.99	1.45	1.33
9	J	101	BCL	O2D-CGD	4.99	1.45	1.33
9	4	101	BCL	O2D-CGD	4.99	1.45	1.33
9	O	101	BCL	O2D-CGD	4.98	1.45	1.33
9	G	101	BCL	O2D-CGD	4.98	1.45	1.33
9	D	101	BCL	O2D-CGD	4.97	1.45	1.33
9	V	101	BCL	O2D-CGD	4.97	1.45	1.33
9	J	101	BCL	C3B-C2B	4.96	1.48	1.39
9	B	101	BCL	O2D-CGD	4.96	1.45	1.33
9	2	101	BCL	O2D-CGD	4.96	1.45	1.33
9	K	102	BCL	O2D-CGD	4.95	1.45	1.33
9	Q	104	BCL	O2D-CGD	4.94	1.45	1.33
9	Z	101	BCL	O2D-CGD	4.93	1.45	1.33
9	7	101	BCL	O2D-CGD	4.93	1.45	1.33
9	Y	103	BCL	O2D-CGD	4.92	1.45	1.33
9	8	102	BCL	C3B-C2B	4.90	1.48	1.39
9	6	101	BCL	C3B-C2B	4.89	1.48	1.39
9	M	803	BCL	O2D-CGD	4.89	1.45	1.33
9	1	101	BCL	O2D-CGD	4.88	1.45	1.33
9	L	301	BCL	O2D-CGD	4.88	1.45	1.33
9	L	309	BCL	O2D-CGD	4.87	1.45	1.33
9	S	102	BCL	O2D-CGD	4.86	1.45	1.33
9	L	308	BCL	C3B-C2B	4.86	1.48	1.39
9	3	103	BCL	C3B-C2B	4.82	1.48	1.39
9	R	102	BCL	O2D-CGD	4.79	1.44	1.33
9	N	102	BCL	C3B-C2B	4.78	1.48	1.39
9	K	102	BCL	C3B-C2B	4.78	1.48	1.39
9	G	101	BCL	C3B-C2B	4.78	1.48	1.39
9	M	803	BCL	C3B-C2B	4.77	1.48	1.39
9	T	101	BCL	C3B-C2B	4.76	1.48	1.39
9	B	101	BCL	C3B-C2B	4.75	1.48	1.39
9	O	101	BCL	C3B-C2B	4.75	1.47	1.39
9	E	102	BCL	C3B-C2B	4.74	1.47	1.39
9	L	301	BCL	C3B-C2B	4.74	1.47	1.39
9	4	101	BCL	C3B-C2B	4.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	309	BCL	C3B-C2B	4.74	1.47	1.39
9	7	101	BCL	C3B-C2B	4.70	1.47	1.39
9	L	308	BCL	O2D-CGD	4.69	1.44	1.33
9	F	102	BCL	C3B-C2B	4.67	1.47	1.39
9	D	101	BCL	C3B-C2B	4.65	1.47	1.39
9	Z	101	BCL	C3B-C2B	4.64	1.47	1.39
9	S	102	BCL	C3B-C2B	4.64	1.47	1.39
9	5	102	BCL	C3B-C2B	4.63	1.47	1.39
9	2	101	BCL	C3B-C2B	4.63	1.47	1.39
9	8	102	BCL	OBD-CAD	4.60	1.28	1.22
9	R	102	BCL	C3B-C2B	4.60	1.47	1.39
9	1	101	BCL	C3B-C2B	4.58	1.47	1.39
9	J	101	BCL	OBD-CAD	4.58	1.28	1.22
9	W	101	BCL	C3B-C2B	4.55	1.47	1.39
9	P	102	BCL	C3B-C2B	4.53	1.47	1.39
9	4	101	BCL	OBD-CAD	4.52	1.28	1.22
9	F	102	BCL	OBD-CAD	4.49	1.28	1.22
9	Y	103	BCL	C3B-C2B	4.49	1.47	1.39
9	Q	104	BCL	C3B-C2B	4.48	1.47	1.39
9	3	103	BCL	OBD-CAD	4.48	1.28	1.22
9	V	101	BCL	C3B-C2B	4.47	1.47	1.39
9	L	301	BCL	OBD-CAD	4.46	1.28	1.22
9	I	101	BCL	C3B-C2B	4.45	1.47	1.39
9	B	101	BCL	OBD-CAD	4.44	1.28	1.22
9	B	101	BCL	C3D-C2D	4.44	1.47	1.39
9	7	101	BCL	OBD-CAD	4.43	1.28	1.22
9	E	102	BCL	OBD-CAD	4.42	1.28	1.22
9	L	309	BCL	C3D-C2D	4.41	1.47	1.39
9	E	102	BCL	O2A-CGA	4.41	1.46	1.33
9	Q	104	BCL	OBD-CAD	4.40	1.28	1.22
12	H	306	PGV	O03-C19	4.40	1.46	1.33
9	R	102	BCL	OBD-CAD	4.40	1.28	1.22
9	5	102	BCL	OBD-CAD	4.40	1.28	1.22
9	G	101	BCL	OBD-CAD	4.39	1.28	1.22
9	W	101	BCL	OBD-CAD	4.38	1.28	1.22
9	G	101	BCL	C3D-C2D	4.38	1.47	1.39
9	I	101	BCL	OBD-CAD	4.38	1.28	1.22
9	K	102	BCL	C3D-C2D	4.38	1.47	1.39
9	Z	101	BCL	OBD-CAD	4.37	1.28	1.22
9	A	703	BCL	C3B-C2B	4.37	1.47	1.39
9	P	102	BCL	C3D-C2D	4.37	1.47	1.39
9	D	101	BCL	OBD-CAD	4.36	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	703	BCL	OBD-CAD	4.36	1.28	1.22
9	V	101	BCL	OBD-CAD	4.36	1.28	1.22
9	A	703	BCL	O2A-CGA	4.35	1.46	1.33
9	S	102	BCL	OBD-CAD	4.34	1.28	1.22
9	6	101	BCL	OBD-CAD	4.34	1.28	1.22
9	T	101	BCL	OBD-CAD	4.34	1.28	1.22
9	K	102	BCL	OBD-CAD	4.33	1.28	1.22
9	P	102	BCL	OBD-CAD	4.32	1.28	1.22
9	M	803	BCL	OBD-CAD	4.32	1.28	1.22
9	4	101	BCL	C3D-C2D	4.31	1.47	1.39
9	N	102	BCL	OBD-CAD	4.31	1.28	1.22
9	2	101	BCL	OBD-CAD	4.31	1.28	1.22
9	3	103	BCL	O2A-CGA	4.30	1.45	1.33
9	K	102	BCL	O2A-CGA	4.30	1.45	1.33
9	8	102	BCL	C3D-C2D	4.30	1.47	1.39
17	Y	102	CDL	OB8-CB7	4.30	1.45	1.33
9	A	703	BCL	C3D-C2D	4.30	1.47	1.39
9	Z	101	BCL	C3D-C2D	4.30	1.47	1.39
17	H	305	CDL	OA6-CA5	4.30	1.46	1.34
9	2	101	BCL	C3D-C2D	4.30	1.47	1.39
9	1	101	BCL	OBD-CAD	4.29	1.28	1.22
17	H	304	CDL	OA8-CA7	4.29	1.45	1.33
9	Q	104	BCL	C3D-C2D	4.28	1.47	1.39
12	H	307	PGV	O03-C19	4.28	1.45	1.33
9	7	101	BCL	O2A-CGA	4.28	1.45	1.33
17	H	305	CDL	OA8-CA7	4.27	1.45	1.33
9	O	101	BCL	O2A-CGA	4.26	1.45	1.33
12	Q	103	PGV	O03-C19	4.26	1.45	1.33
9	5	102	BCL	O2A-CGA	4.26	1.45	1.33
9	L	301	BCL	O2A-CGA	4.26	1.45	1.33
9	Y	103	BCL	OBD-CAD	4.26	1.28	1.22
9	5	102	BCL	C3D-C2D	4.25	1.47	1.39
17	H	304	CDL	OB8-CB7	4.25	1.45	1.33
9	L	309	BCL	OBD-CAD	4.25	1.28	1.22
12	X	101	PGV	O03-C19	4.25	1.45	1.33
9	O	101	BCL	OBD-CAD	4.25	1.28	1.22
9	6	101	BCL	O2A-CGA	4.24	1.45	1.33
9	6	101	BCL	C3D-C2D	4.24	1.47	1.39
17	Y	102	CDL	OA8-CA7	4.23	1.45	1.33
12	L	306	PGV	O03-C19	4.23	1.45	1.33
9	1	101	BCL	C3D-C2D	4.23	1.47	1.39
17	M	811	CDL	OA8-CA7	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	310	PGV	O03-C19	4.21	1.45	1.33
9	3	103	BCL	C3D-C2D	4.21	1.47	1.39
9	L	308	BCL	O2A-CGA	4.20	1.45	1.33
9	J	101	BCL	C3D-C2D	4.20	1.47	1.39
9	T	101	BCL	C3D-C2D	4.19	1.46	1.39
9	8	102	BCL	O2A-CGA	4.19	1.45	1.33
12	H	303	PGV	O03-C19	4.19	1.45	1.33
9	I	101	BCL	C3D-C2D	4.18	1.46	1.39
9	B	101	BCL	O2A-CGA	4.18	1.45	1.33
12	K	104	PGV	O03-C19	4.18	1.45	1.33
17	M	811	CDL	OB8-CB7	4.18	1.45	1.33
9	O	101	BCL	C3D-C2D	4.18	1.46	1.39
9	M	803	BCL	O2A-CGA	4.18	1.45	1.33
9	G	101	BCL	O2A-CGA	4.18	1.45	1.33
12	H	306	PGV	O01-C1	4.17	1.46	1.34
9	T	101	BCL	O2A-CGA	4.17	1.45	1.33
17	Y	102	CDL	OB6-CB5	4.17	1.46	1.34
17	M	811	CDL	OB6-CB5	4.17	1.46	1.34
9	L	309	BCL	O2A-CGA	4.17	1.45	1.33
9	N	102	BCL	C3D-C2D	4.16	1.46	1.39
9	S	102	BCL	O2A-CGA	4.16	1.45	1.33
12	L	305	PGV	O01-C1	4.16	1.46	1.34
12	L	305	PGV	O03-C19	4.16	1.45	1.33
9	L	308	BCL	C3D-C2D	4.15	1.46	1.39
9	S	102	BCL	C3D-C2D	4.15	1.46	1.39
9	7	101	BCL	C3D-C2D	4.15	1.46	1.39
17	H	304	CDL	OB6-CB5	4.15	1.46	1.34
9	4	101	BCL	O2A-CGA	4.14	1.45	1.33
9	F	102	BCL	C3D-C2D	4.14	1.46	1.39
9	F	102	BCL	O2A-CGA	4.14	1.45	1.33
9	R	102	BCL	C3D-C2D	4.14	1.46	1.39
9	Q	104	BCL	O2A-CGA	4.13	1.45	1.33
9	P	102	BCL	O2A-CGA	4.12	1.45	1.33
9	M	803	BCL	C3D-C2D	4.12	1.46	1.39
12	Y	104	PGV	O03-C19	4.12	1.45	1.33
12	K	104	PGV	O01-C1	4.11	1.45	1.34
9	D	101	BCL	O2A-CGA	4.11	1.45	1.33
12	3	102	PGV	O01-C1	4.11	1.45	1.34
9	J	101	BCL	O2A-CGA	4.10	1.45	1.33
9	Y	103	BCL	C3D-C2D	4.10	1.46	1.39
9	I	101	BCL	O2A-CGA	4.10	1.45	1.33
12	3	102	PGV	O03-C19	4.10	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	812	PGV	O01-C1	4.09	1.45	1.34
12	Q	103	PGV	O01-C1	4.09	1.45	1.34
9	W	101	BCL	C3D-C2D	4.09	1.46	1.39
17	H	305	CDL	OB8-CB7	4.09	1.45	1.33
9	D	101	BCL	C3D-C2D	4.09	1.46	1.39
17	H	304	CDL	OA6-CA5	4.09	1.45	1.34
9	Z	101	BCL	O2A-CGA	4.08	1.45	1.33
9	V	101	BCL	C3D-C2D	4.07	1.46	1.39
9	V	101	BCL	O2A-CGA	4.07	1.45	1.33
9	2	101	BCL	O2A-CGA	4.07	1.45	1.33
9	W	101	BCL	O2A-CGA	4.07	1.45	1.33
12	M	801	PGV	O03-C19	4.07	1.45	1.33
12	M	812	PGV	O03-C19	4.06	1.45	1.33
12	X	101	PGV	O01-C1	4.06	1.45	1.34
12	H	307	PGV	O01-C1	4.05	1.45	1.34
9	R	102	BCL	O2A-CGA	4.05	1.45	1.33
9	L	301	BCL	C3D-C2D	4.03	1.46	1.39
12	L	310	PGV	O01-C1	4.03	1.45	1.34
12	M	801	PGV	O01-C1	4.03	1.45	1.34
9	L	308	BCL	OBD-CAD	4.02	1.27	1.22
9	E	102	BCL	C3D-C2D	4.00	1.46	1.39
12	H	303	PGV	O01-C1	3.99	1.45	1.34
17	M	811	CDL	OA6-CA5	3.99	1.45	1.34
9	N	102	BCL	O2A-CGA	3.98	1.45	1.33
12	Y	104	PGV	O01-C1	3.96	1.45	1.34
9	1	101	BCL	O2A-CGA	3.94	1.44	1.33
9	Y	103	BCL	O2A-CGA	3.93	1.44	1.33
12	L	306	PGV	O01-C1	3.76	1.44	1.34
9	8	102	BCL	C2D-C1D	3.61	1.50	1.42
9	7	101	BCL	C2D-C1D	3.55	1.50	1.42
9	3	103	BCL	C2D-C1D	3.51	1.50	1.42
9	A	703	BCL	C2D-C1D	3.51	1.50	1.42
9	I	101	BCL	C2D-C1D	3.46	1.50	1.42
9	M	803	BCL	C2D-C1D	3.45	1.50	1.42
9	L	301	BCL	C2D-C1D	3.42	1.50	1.42
9	L	309	BCL	C2D-C1D	3.42	1.50	1.42
9	5	102	BCL	C2D-C1D	3.41	1.50	1.42
9	V	101	BCL	C2D-C1D	3.36	1.50	1.42
9	4	101	BCL	C2D-C1D	3.35	1.50	1.42
9	1	101	BCL	C2D-C1D	3.33	1.50	1.42
9	S	102	BCL	C2D-C1D	3.33	1.50	1.42
9	K	102	BCL	C2D-C1D	3.27	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	101	BCL	C2D-C1D	3.26	1.49	1.42
9	Q	104	BCL	C2D-C1D	3.25	1.49	1.42
9	F	102	BCL	C2D-C1D	3.24	1.49	1.42
9	L	308	BCL	C2D-C1D	3.24	1.49	1.42
9	O	101	BCL	C2D-C1D	3.23	1.49	1.42
9	R	102	BCL	C2D-C1D	3.22	1.49	1.42
9	J	101	BCL	C2D-C1D	3.22	1.49	1.42
9	P	102	BCL	C2D-C1D	3.20	1.49	1.42
9	Y	103	BCL	C2D-C1D	3.19	1.49	1.42
9	Z	101	BCL	C2D-C1D	3.19	1.49	1.42
9	E	102	BCL	C2D-C1D	3.15	1.49	1.42
9	W	101	BCL	C2D-C1D	3.14	1.49	1.42
9	2	101	BCL	C2D-C1D	3.13	1.49	1.42
9	B	101	BCL	C2D-C1D	3.13	1.49	1.42
9	N	102	BCL	C2D-C1D	3.12	1.49	1.42
9	6	101	BCL	C2D-C1D	3.11	1.49	1.42
9	T	101	BCL	C2D-C1D	3.09	1.49	1.42
9	G	101	BCL	C2D-C1D	3.09	1.49	1.42
9	1	101	BCL	MG-NA	-2.85	1.99	2.06
9	8	102	BCL	MG-NC	-2.78	1.99	2.06
11	L	304	U10	C3-C2	-2.75	1.41	1.48
11	L	303	U10	C3-C2	-2.72	1.41	1.48
9	8	102	BCL	MG-NA	-2.70	1.99	2.06
9	S	102	BCL	MG-NA	-2.64	2.00	2.06
11	M	806	U10	C4-C5	-2.58	1.41	1.48
10	L	302	BPH	C3A-C2A	-2.55	1.52	1.54
11	M	806	U10	C3-C2	-2.54	1.41	1.48
9	3	103	BCL	MG-NA	-2.52	2.00	2.06
9	4	101	BCL	MG-NC	-2.48	2.00	2.06
11	L	303	U10	C4-C5	-2.47	1.41	1.48
9	L	309	BCL	MG-NC	-2.47	2.00	2.06
9	E	102	BCL	MG-NC	-2.43	2.00	2.06
9	2	101	BCL	MG-NA	-2.43	2.00	2.06
9	A	703	BCL	MG-NC	-2.42	2.00	2.06
10	M	804	BPH	C3A-C2A	-2.42	1.52	1.54
9	L	309	BCL	MG-NA	-2.40	2.00	2.06
9	6	101	BCL	MG-NC	-2.40	2.00	2.06
9	J	101	BCL	MG-NA	-2.39	2.00	2.06
9	2	101	BCL	MG-NC	-2.37	2.00	2.06
9	L	308	BCL	MG-NA	-2.37	2.00	2.06
9	J	101	BCL	MG-NC	-2.37	2.00	2.06
9	G	101	BCL	MG-NC	-2.36	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	101	BCL	C1B-CHB	2.36	1.47	1.41
9	K	102	BCL	MG-NA	-2.36	2.00	2.06
9	R	102	BCL	MG-NA	-2.35	2.00	2.06
9	8	102	BCL	CHD-C4C	2.35	1.48	1.41
9	4	101	BCL	MG-NA	-2.35	2.00	2.06
9	8	102	BCL	C1B-CHB	2.34	1.47	1.41
9	R	102	BCL	MG-NC	-2.34	2.00	2.06
9	W	101	BCL	MG-NC	-2.33	2.00	2.06
9	N	102	BCL	MG-NC	-2.33	2.00	2.06
9	M	803	BCL	MG-NA	-2.32	2.00	2.06
9	Y	103	BCL	MG-NA	-2.31	2.00	2.06
9	E	102	BCL	MG-NA	-2.31	2.00	2.06
9	M	803	BCL	MG-NC	-2.30	2.00	2.06
9	7	101	BCL	MG-NC	-2.29	2.00	2.06
9	T	101	BCL	MG-NC	-2.29	2.00	2.06
9	3	103	BCL	MG-NC	-2.29	2.00	2.06
9	6	101	BCL	MG-NA	-2.29	2.00	2.06
9	D	101	BCL	MG-NA	-2.29	2.00	2.06
9	8	102	BCL	C4B-CHC	2.29	1.47	1.41
9	T	101	BCL	MG-NA	-2.28	2.00	2.06
9	Q	104	BCL	MG-NA	-2.27	2.00	2.06
9	V	101	BCL	MG-NC	-2.27	2.00	2.06
9	I	101	BCL	MG-NA	-2.27	2.00	2.06
9	N	102	BCL	MG-NA	-2.26	2.00	2.06
9	A	703	BCL	MG-NA	-2.26	2.00	2.06
9	L	301	BCL	C4B-CHC	2.26	1.47	1.41
9	F	102	BCL	MG-NC	-2.26	2.00	2.06
9	W	101	BCL	MG-NA	-2.24	2.00	2.06
9	5	102	BCL	MG-NC	-2.24	2.01	2.06
9	Z	101	BCL	MG-NC	-2.23	2.01	2.06
9	Z	101	BCL	C1B-CHB	2.23	1.47	1.41
9	G	101	BCL	MG-NA	-2.23	2.01	2.06
9	E	102	BCL	C4B-CHC	2.22	1.47	1.41
9	5	102	BCL	MG-NA	-2.22	2.01	2.06
9	L	308	BCL	C1B-CHB	2.22	1.47	1.41
9	B	101	BCL	MG-NC	-2.21	2.01	2.06
9	B	101	BCL	MG-NA	-2.21	2.01	2.06
9	K	102	BCL	MG-NC	-2.21	2.01	2.06
9	A	703	BCL	C1B-CHB	2.21	1.47	1.41
9	L	301	BCL	MG-NC	-2.21	2.01	2.06
9	Z	101	BCL	MG-NA	-2.21	2.01	2.06
9	4	101	BCL	C4B-CHC	2.21	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	101	BCL	MG-NC	-2.20	2.01	2.06
9	M	803	BCL	C1B-CHB	2.20	1.47	1.41
9	V	101	BCL	MG-NA	-2.19	2.01	2.06
9	L	308	BCL	MG-NC	-2.19	2.01	2.06
9	6	101	BCL	C4B-CHC	2.19	1.47	1.41
9	S	102	BCL	C1B-CHB	2.18	1.47	1.41
9	B	101	BCL	C1B-CHB	2.18	1.47	1.41
9	F	102	BCL	MG-NA	-2.18	2.01	2.06
9	B	101	BCL	C4B-CHC	2.17	1.47	1.41
9	4	101	BCL	C1B-CHB	2.17	1.47	1.41
9	7	101	BCL	MG-NA	-2.16	2.01	2.06
9	P	102	BCL	MG-NA	-2.16	2.01	2.06
9	P	102	BCL	MG-NC	-2.16	2.01	2.06
9	D	101	BCL	C1B-CHB	2.15	1.47	1.41
9	J	101	BCL	C3C-C4C	-2.15	1.48	1.51
9	6	101	BCL	C1B-CHB	2.14	1.46	1.41
9	I	101	BCL	C3C-C4C	-2.14	1.48	1.51
9	2	101	BCL	C1B-CHB	2.13	1.46	1.41
9	Y	103	BCL	C1B-CHB	2.12	1.46	1.41
9	O	101	BCL	MG-NA	-2.12	2.01	2.06
9	Q	104	BCL	C1B-CHB	2.12	1.46	1.41
9	W	101	BCL	C1B-CHB	2.12	1.46	1.41
9	A	703	BCL	CHD-C4C	2.12	1.47	1.41
9	N	102	BCL	C4B-CHC	2.10	1.46	1.41
11	L	304	U10	C4-C5	-2.10	1.42	1.48
9	T	101	BCL	C1B-CHB	2.10	1.46	1.41
9	2	101	BCL	C3C-C4C	-2.10	1.49	1.51
9	Y	103	BCL	MG-NC	-2.10	2.01	2.06
9	T	101	BCL	C4B-CHC	2.09	1.46	1.41
9	1	101	BCL	C1B-CHB	2.09	1.46	1.41
9	N	102	BCL	C1B-CHB	2.08	1.46	1.41
9	L	301	BCL	MG-NA	-2.08	2.01	2.06
9	G	101	BCL	C1B-CHB	2.08	1.46	1.41
9	G	101	BCL	C4B-CHC	2.07	1.46	1.41
9	R	102	BCL	C4B-CHC	2.07	1.46	1.41
9	P	102	BCL	C1B-CHB	2.07	1.46	1.41
9	Z	101	BCL	C3C-C4C	-2.07	1.49	1.51
9	L	309	BCL	C1B-CHB	2.06	1.46	1.41
9	W	101	BCL	C3C-C4C	-2.06	1.49	1.51
9	3	103	BCL	C1B-CHB	2.05	1.46	1.41
9	W	101	BCL	C4B-CHC	2.05	1.46	1.41
9	M	803	BCL	C3C-C4C	-2.05	1.49	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	101	BCL	MG-NC	-2.04	2.01	2.06
9	N	102	BCL	C3C-C4C	-2.04	1.49	1.51
9	7	101	BCL	CHD-C4C	2.04	1.47	1.41
9	E	102	BCL	C1B-CHB	2.04	1.46	1.41
9	M	803	BCL	C4B-CHC	2.04	1.46	1.41
9	R	102	BCL	C1B-CHB	2.04	1.46	1.41
10	L	302	BPH	CBD-CGD	-2.03	1.49	1.52
9	O	101	BCL	C4B-CHC	2.03	1.46	1.41
9	E	102	BCL	C3C-C4C	-2.03	1.49	1.51
9	S	102	BCL	MG-NC	-2.02	2.01	2.06
16	1	104	LMT	C5B-C4B	2.02	1.53	1.51
9	D	101	BCL	C4B-CHC	2.02	1.46	1.41
9	L	309	BCL	C4B-CHC	2.01	1.46	1.41
9	L	301	BCL	C1B-CHB	2.01	1.46	1.41
9	P	102	BCL	C4B-CHC	2.01	1.46	1.41
9	F	102	BCL	C4B-CHC	2.01	1.46	1.41

All (891) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	103	SPO	C10-C9-C7	-6.64	117.83	127.31
15	R	101	SPO	C10-C9-C7	-6.35	118.25	127.31
9	L	308	BCL	O2D-CGD-CBD	6.31	122.47	111.27
15	G	103	SPO	C5-C6-C7	-6.23	116.47	125.89
15	3	104	SPO	C5-C6-C7	-6.22	116.49	125.89
15	N	101	SPO	C10-C9-C7	-6.18	118.49	127.31
15	R	101	SPO	C21-C22-C23	-6.15	118.53	127.31
15	N	101	SPO	C5-C6-C7	-6.03	116.78	125.89
15	R	101	SPO	C5-C6-C7	-5.91	116.96	125.89
15	8	101	SPO	C21-C22-C23	-5.90	118.89	127.31
15	T	102	SPO	C10-C9-C7	-5.87	118.94	127.31
15	3	104	SPO	C10-C9-C7	-5.84	118.97	127.31
15	1	103	SPO	C5-C6-C7	-5.58	117.45	125.89
15	1	102	SPO	C20-C19-C17	-5.55	119.39	127.31
15	S	103	SPO	C20-C19-C17	-5.52	119.44	127.31
9	L	309	BCL	O2D-CGD-CBD	5.49	121.02	111.27
15	1	102	SPO	C21-C22-C23	-5.39	119.61	127.31
15	5	103	SPO	C21-C22-C23	-5.34	119.69	127.31
15	G	102	SPO	C21-C22-C23	-5.32	119.72	127.31
15	O	102	SPO	C21-C22-C23	-5.29	119.76	127.31
9	7	101	BCL	O2D-CGD-CBD	5.27	120.63	111.27
15	1	103	SPO	C10-C9-C7	-5.22	119.86	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	5	102	BCL	O2D-CGD-CBD	5.13	120.38	111.27
15	O	102	SPO	C20-C19-C17	-5.08	120.06	127.31
15	S	103	SPO	C21-C22-C23	-5.06	120.09	127.31
9	1	101	BCL	CHD-C4C-NC	5.04	130.68	125.08
9	O	101	BCL	O2D-CGD-CBD	5.03	120.20	111.27
9	K	102	BCL	O2D-CGD-CBD	5.01	120.17	111.27
17	M	811	CDL	OB6-CB5-C51	5.00	122.29	111.50
9	S	102	BCL	O2D-CGD-CBD	4.97	120.10	111.27
9	3	103	BCL	CHD-C4C-NC	4.94	130.57	125.08
9	8	102	BCL	O2D-CGD-CBD	4.92	120.02	111.27
9	S	102	BCL	CHD-C4C-NC	4.91	130.53	125.08
9	M	803	BCL	CHD-C4C-NC	4.91	130.53	125.08
9	W	101	BCL	CHD-C4C-NC	4.88	130.50	125.08
15	K	103	SPO	C21-C22-C23	-4.88	120.34	127.31
9	D	101	BCL	CHD-C4C-NC	4.87	130.49	125.08
9	O	101	BCL	CHD-C4C-NC	4.87	130.49	125.08
9	2	101	BCL	CHD-C4C-NC	4.86	130.47	125.08
9	1	101	BCL	C3C-C4C-CHD	-4.85	113.02	123.39
9	N	102	BCL	CHD-C4C-NC	4.82	130.43	125.08
15	F	104	SPO	C10-C9-C7	-4.81	120.44	127.31
9	I	101	BCL	CHD-C4C-NC	4.79	130.39	125.08
9	N	102	BCL	O2D-CGD-CBD	4.76	119.72	111.27
9	O	101	BCL	C3C-C4C-CHD	-4.76	113.23	123.39
9	1	101	BCL	O2D-CGD-CBD	4.76	119.72	111.27
9	M	803	BCL	O2D-CGD-CBD	4.75	119.71	111.27
9	Y	103	BCL	C3C-C4C-CHD	-4.75	113.25	123.39
15	X	102	SPO	C29-C28-C30	4.74	123.25	115.27
9	Y	103	BCL	CHD-C4C-NC	4.73	130.34	125.08
9	2	101	BCL	O2D-CGD-CBD	4.73	119.67	111.27
9	S	102	BCL	C3C-C4C-CHD	-4.72	113.30	123.39
9	D	101	BCL	C3C-C4C-CHD	-4.72	113.30	123.39
15	X	102	SPO	C21-C22-C23	-4.72	120.58	127.31
15	5	104	SPO	C20-C19-C17	-4.71	120.58	127.31
9	J	101	BCL	CHD-C4C-NC	4.71	130.31	125.08
15	5	103	SPO	C20-C19-C17	-4.71	120.59	127.31
9	Z	101	BCL	CHD-C4C-NC	4.70	130.30	125.08
9	L	308	BCL	CMB-C2B-C3B	4.69	133.44	124.68
9	I	101	BCL	O2D-CGD-CBD	4.68	119.58	111.27
9	Q	104	BCL	O2D-CGD-CBD	4.68	119.58	111.27
9	O	101	BCL	CMB-C2B-C3B	4.68	133.43	124.68
9	D	101	BCL	O2D-CGD-CBD	4.66	119.55	111.27
9	G	101	BCL	O2D-CGD-CBD	4.65	119.54	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	8	101	SPO	C10-C9-C7	-4.64	120.68	127.31
9	L	308	BCL	CHD-C4C-NC	4.64	130.23	125.08
9	R	102	BCL	O2D-CGD-CBD	4.63	119.50	111.27
9	Y	103	BCL	O2D-CGD-CBD	4.63	119.50	111.27
9	E	102	BCL	CHD-C4C-NC	4.63	130.22	125.08
9	7	101	BCL	CMB-C2B-C3B	4.63	133.33	124.68
9	P	102	BCL	CHD-C4C-NC	4.62	130.21	125.08
9	R	102	BCL	CHD-C4C-NC	4.62	130.21	125.08
9	N	102	BCL	C3C-C4C-CHD	-4.62	113.52	123.39
9	6	101	BCL	O2D-CGD-CBD	4.59	119.42	111.27
9	K	102	BCL	CHD-C4C-NC	4.59	130.17	125.08
9	M	803	BCL	CMB-C2B-C3B	4.58	133.25	124.68
15	V	103	SPO	C21-C22-C23	-4.58	120.78	127.31
9	Q	104	BCL	C3C-C4C-CHD	-4.57	113.64	123.39
9	2	101	BCL	C3C-C4C-CHD	-4.57	113.64	123.39
9	F	102	BCL	CMB-C2B-C3B	4.55	133.19	124.68
9	S	102	BCL	CMB-C2B-C3B	4.54	133.18	124.68
9	Q	104	BCL	CHD-C4C-NC	4.54	130.12	125.08
9	3	103	BCL	CMB-C2B-C3B	4.54	133.17	124.68
15	1	105	SPO	C20-C19-C17	-4.54	120.83	127.31
9	Z	101	BCL	C3C-C4C-CHD	-4.53	113.72	123.39
9	M	803	BCL	C3C-C4C-CHD	-4.52	113.74	123.39
9	5	102	BCL	CMB-C2B-C3B	4.52	133.13	124.68
15	P	101	SPO	C10-C9-C7	-4.51	120.87	127.31
9	T	101	BCL	CHD-C4C-NC	4.51	130.09	125.08
9	K	102	BCL	CMB-C2B-C3B	4.50	133.10	124.68
9	J	101	BCL	O2D-CGD-CBD	4.50	119.27	111.27
9	P	102	BCL	C3C-C4C-CHD	-4.50	113.78	123.39
9	4	101	BCL	CHD-C4C-NC	4.49	130.07	125.08
9	P	102	BCL	O2D-CGD-CBD	4.49	119.25	111.27
15	F	104	SPO	C5-C6-C7	-4.48	119.12	125.89
9	T	101	BCL	C3C-C4C-CHD	-4.47	113.83	123.39
15	8	101	SPO	C15-C14-C12	-4.47	120.93	127.31
9	3	103	BCL	C3C-C4C-CHD	-4.47	113.84	123.39
9	B	101	BCL	O2D-CGD-CBD	4.45	119.17	111.27
9	E	102	BCL	CMB-C2B-C3B	4.44	132.98	124.68
9	T	101	BCL	CMB-C2B-C3B	4.44	132.98	124.68
9	D	101	BCL	CMB-C2B-C3B	4.43	132.97	124.68
9	V	101	BCL	CMB-C2B-C3B	4.42	132.95	124.68
9	B	101	BCL	CHD-C4C-NC	4.42	129.99	125.08
9	A	703	BCL	O2D-CGD-CBD	4.41	119.10	111.27
9	I	101	BCL	C3C-C4C-CHD	-4.40	113.99	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	102	BCL	CHD-C4C-NC	4.40	129.97	125.08
9	L	301	BCL	CMB-C2B-C3B	4.40	132.91	124.68
9	R	102	BCL	C3C-C4C-CHD	-4.38	114.03	123.39
9	E	102	BCL	C3C-C4C-CHD	-4.38	114.03	123.39
9	N	102	BCL	CMB-C2B-C3B	4.38	132.87	124.68
9	L	309	BCL	CMB-C2B-C3B	4.37	132.85	124.68
9	F	102	BCL	C3C-C4C-CHD	-4.36	114.07	123.39
9	W	101	BCL	C3C-C4C-CHD	-4.36	114.08	123.39
9	B	101	BCL	C3C-C4C-CHD	-4.35	114.11	123.39
12	M	801	PGV	O01-C1-C2	4.33	120.82	111.50
9	5	102	BCL	CHD-C4C-NC	4.31	129.86	125.08
9	1	101	BCL	C4A-NA-C1A	4.30	108.64	106.71
15	8	101	SPO	C5-C6-C7	-4.30	119.39	125.89
15	O	103	SPO	C31-C32-C33	-4.30	117.31	127.66
9	W	101	BCL	O2D-CGD-CBD	4.29	118.89	111.27
9	1	101	BCL	CMB-C2B-C3B	4.29	132.70	124.68
9	I	101	BCL	CMB-C2B-C3B	4.28	132.69	124.68
9	G	101	BCL	CMB-C2B-C3B	4.27	132.67	124.68
15	5	104	SPO	C5-C6-C7	-4.27	119.44	125.89
9	1	101	BCL	C1C-NC-C4C	-4.27	104.79	106.71
12	3	102	PGV	O01-C1-C2	4.26	120.68	111.50
9	K	102	BCL	C3C-C4C-CHD	-4.26	114.30	123.39
9	3	103	BCL	O2D-CGD-CBD	4.25	118.82	111.27
9	J	101	BCL	C3C-C4C-CHD	-4.25	114.32	123.39
12	H	306	PGV	O01-C1-C2	4.24	120.64	111.50
9	6	101	BCL	CHD-C4C-NC	4.23	129.77	125.08
9	Z	101	BCL	O2D-CGD-CBD	4.23	118.78	111.27
15	K	103	SPO	C20-C19-C17	-4.22	121.28	127.31
9	G	101	BCL	CHD-C4C-NC	4.21	129.75	125.08
9	E	102	BCL	O2D-CGD-CBD	4.21	118.75	111.27
9	V	101	BCL	CHD-C4C-NC	4.20	129.74	125.08
15	T	102	SPO	C5-C6-C7	-4.19	119.56	125.89
9	L	308	BCL	C3C-C4C-CHD	-4.19	114.45	123.39
9	T	101	BCL	O2D-CGD-CBD	4.19	118.71	111.27
12	M	812	PGV	O01-C1-C2	4.18	120.51	111.50
9	5	102	BCL	C3C-C4C-CHD	-4.17	114.49	123.39
9	F	102	BCL	O2D-CGD-CBD	4.16	118.66	111.27
15	M	807	SPO	C21-C22-C23	-4.14	121.39	127.31
9	8	102	BCL	CHD-C4C-NC	4.14	129.68	125.08
9	6	101	BCL	CMB-C2B-C3B	4.14	132.42	124.68
9	L	301	BCL	CHD-C4C-NC	4.14	129.67	125.08
9	R	102	BCL	CMB-C2B-C3B	4.13	132.41	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	1	105	SPO	C21-C22-C23	-4.13	121.42	127.31
9	V	101	BCL	O2D-CGD-CBD	4.12	118.59	111.27
9	4	101	BCL	CMB-C2B-C3B	4.11	132.38	124.68
15	V	102	SPO	C21-C22-C23	-4.11	121.44	127.31
9	4	101	BCL	C3C-C4C-CHD	-4.11	114.62	123.39
15	V	103	SPO	C20-C19-C17	-4.10	121.45	127.31
9	4	101	BCL	O2D-CGD-CBD	4.10	118.56	111.27
12	K	104	PGV	O01-C1-C2	4.10	120.34	111.50
15	M	807	SPO	C31-C32-C33	-4.09	117.80	127.66
9	G	101	BCL	C3C-C4C-CHD	-4.09	114.65	123.39
15	R	101	SPO	C20-C19-C17	-4.09	121.48	127.31
15	5	104	SPO	C10-C9-C7	-4.08	121.48	127.31
9	7	101	BCL	CHD-C4C-NC	4.07	129.60	125.08
9	S	102	BCL	C4A-NA-C1A	4.06	108.53	106.71
9	P	102	BCL	CMB-C2B-C3B	4.04	132.24	124.68
12	L	310	PGV	O01-C1-C2	4.04	120.20	111.50
17	H	304	CDL	OB6-CB5-C51	4.04	120.20	111.50
9	6	101	BCL	C3C-C4C-CHD	-4.02	114.81	123.39
9	L	301	BCL	C3C-C4C-CHD	-4.00	114.85	123.39
9	Z	101	BCL	CMB-C2B-C3B	3.99	132.15	124.68
15	V	102	SPO	C20-C19-C17	-3.98	121.63	127.31
9	8	102	BCL	C1B-CHB-C4A	-3.98	122.23	130.12
9	L	301	BCL	O2D-CGD-CBD	3.98	118.34	111.27
15	O	103	SPO	C21-C22-C23	-3.98	121.63	127.31
15	G	102	SPO	C20-C19-C17	-3.97	121.64	127.31
9	B	101	BCL	C1-C2-C3	-3.97	119.17	126.04
17	M	811	CDL	OA6-CA5-C11	3.97	120.06	111.50
9	W	101	BCL	CMB-C2B-C3B	3.95	132.08	124.68
15	D	102	SPO	C21-C22-C23	-3.93	121.70	127.31
15	W	102	SPO	C21-C22-C23	-3.92	121.72	127.31
15	D	102	SPO	C20-C19-C17	-3.91	121.73	127.31
9	A	703	BCL	CHD-C4C-NC	3.91	129.42	125.08
9	Y	103	BCL	CMB-C2B-C3B	3.91	132.00	124.68
15	W	102	SPO	C20-C19-C17	-3.91	121.73	127.31
9	L	301	BCL	C4C-CHD-C1D	-3.91	120.11	125.88
17	H	304	CDL	OA6-CA5-C11	3.91	119.92	111.50
12	X	101	PGV	O01-C1-C2	3.90	119.90	111.50
12	Y	104	PGV	O01-C1-C2	3.88	119.86	111.50
15	X	102	SPO	C20-C19-C17	-3.86	121.80	127.31
9	N	102	BCL	C1-C2-C3	-3.86	119.37	126.04
9	7	101	BCL	C3C-C4C-CHD	-3.85	115.17	123.39
9	J	101	BCL	CMB-C2B-C3B	3.85	131.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Q	103	PGV	O01-C1-C2	3.84	119.78	111.50
9	V	101	BCL	C3C-C4C-CHD	-3.83	115.21	123.39
9	Y	103	BCL	C1-C2-C3	-3.82	119.43	126.04
9	2	101	BCL	C1-C2-C3	-3.82	119.44	126.04
9	L	308	BCL	C1-C2-C3	-3.82	119.44	126.04
9	Q	104	BCL	CMB-C2B-C3B	3.80	131.80	124.68
15	P	101	SPO	C5-C6-C7	-3.80	120.15	125.89
15	5	103	SPO	C31-C32-C33	-3.78	118.56	127.66
9	B	101	BCL	CMB-C2B-C3B	3.78	131.74	124.68
9	W	101	BCL	C1-C2-C3	-3.77	119.52	126.04
9	2	101	BCL	CMB-C2B-C3B	3.76	131.71	124.68
12	H	303	PGV	O01-C1-C2	3.76	119.60	111.50
17	Y	102	CDL	OB6-CB5-C51	3.76	119.60	111.50
15	R	101	SPO	C34-C33-C35	3.74	121.56	115.27
15	E	101	SPO	C10-C9-C7	-3.73	121.98	127.31
15	M	807	SPO	C20-C19-C17	-3.72	122.00	127.31
15	1	102	SPO	C29-C28-C30	3.72	121.52	115.27
15	N	101	SPO	C20-C19-C17	-3.71	122.01	127.31
9	1	101	BCL	C4C-CHD-C1D	-3.71	120.41	125.88
12	H	307	PGV	O01-C1-C2	3.70	119.47	111.50
9	L	309	BCL	CHD-C4C-NC	3.68	129.16	125.08
9	A	703	BCL	C4B-CHC-C1C	-3.68	122.84	130.12
16	H	301	LMT	O1B-C4'-C3'	3.67	117.05	107.28
15	5	104	SPO	C15-C14-C12	-3.64	122.11	127.31
15	8	101	SPO	C21-C20-C19	-3.64	116.03	123.47
12	L	305	PGV	O01-C1-C2	3.62	119.30	111.50
12	L	306	PGV	O01-C1-C2	3.61	119.27	111.50
15	R	101	SPO	C26-C25-C23	-3.60	116.31	126.42
15	W	102	SPO	C5-C6-C7	-3.59	120.47	125.89
15	F	103	SPO	C21-C22-C23	-3.59	122.19	127.31
15	1	102	SPO	C27-C26-C25	-3.59	112.03	123.22
15	8	101	SPO	C29-C28-C30	3.57	121.28	115.27
17	H	305	CDL	OA6-CA5-C11	3.56	119.17	111.50
15	F	103	SPO	C20-C19-C17	-3.56	122.23	127.31
9	S	102	BCL	C4C-CHD-C1D	-3.56	120.63	125.88
9	1	101	BCL	C1-C2-C3	-3.52	119.96	126.04
17	H	305	CDL	OB8-CB7-C71	3.51	120.59	111.38
9	L	308	BCL	C4C-CHD-C1D	-3.51	120.70	125.88
15	8	101	SPO	C20-C19-C17	-3.51	122.30	127.31
9	G	101	BCL	C4-C3-C5	3.49	121.14	115.27
9	8	102	BCL	CMB-C2B-C3B	3.48	131.19	124.68
9	O	101	BCL	C4C-CHD-C1D	-3.47	120.76	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	K	103	SPO	C15-C14-C12	-3.45	122.38	127.31
9	S	102	BCL	C1-C2-C3	-3.44	120.09	126.04
15	S	104	SPO	C34-C33-C35	3.44	121.06	115.27
9	I	101	BCL	C1-C2-C3	-3.42	120.12	126.04
9	6	101	BCL	C4C-CHD-C1D	-3.42	120.83	125.88
9	A	703	BCL	C4A-NA-C1A	3.41	108.24	106.71
9	A	703	BCL	C1B-CHB-C4A	-3.41	123.36	130.12
15	O	103	SPO	C15-C14-C12	-3.41	122.45	127.31
15	5	104	SPO	C20-C21-C22	-3.40	116.51	123.47
15	E	101	SPO	C20-C19-C17	-3.39	122.47	127.31
15	S	104	SPO	C29-C28-C30	3.39	120.97	115.27
9	P	102	BCL	C1-C2-C3	-3.39	120.19	126.04
9	J	101	BCL	C1-C2-C3	-3.38	120.19	126.04
9	K	102	BCL	C4C-CHD-C1D	-3.38	120.89	125.88
9	S	102	BCL	C1C-NC-C4C	-3.38	105.19	106.71
9	A	703	BCL	C4C-CHD-C1D	-3.37	120.91	125.88
9	L	301	BCL	O2A-CGA-CBA	3.35	122.42	111.91
15	V	103	SPO	C31-C32-C33	-3.34	119.62	127.66
9	8	102	BCL	C4B-CHC-C1C	-3.34	123.50	130.12
9	L	309	BCL	C3C-C4C-CHD	-3.34	116.26	123.39
9	A	703	BCL	C3C-C4C-CHD	-3.34	116.26	123.39
9	8	102	BCL	C3C-C4C-CHD	-3.34	116.26	123.39
15	G	103	SPO	C20-C19-C17	-3.33	122.55	127.31
9	A	703	BCL	O2A-CGA-CBA	3.33	122.37	111.91
12	M	801	PGV	O03-C19-C20	3.33	122.37	111.91
9	N	102	BCL	C4C-CHD-C1D	-3.33	120.96	125.88
15	5	103	SPO	C10-C9-C7	-3.32	122.57	127.31
15	D	102	SPO	C31-C32-C33	-3.32	119.68	127.66
15	N	101	SPO	C29-C28-C30	3.31	120.85	115.27
15	E	101	SPO	C5-C6-C7	-3.31	120.90	125.89
9	Y	103	BCL	C4C-CHD-C1D	-3.30	121.02	125.88
9	V	101	BCL	C4-C3-C5	3.29	120.81	115.27
15	P	101	SPO	C29-C28-C30	3.29	120.81	115.27
15	E	101	SPO	C29-C28-C30	3.26	120.75	115.27
15	5	104	SPO	C29-C28-C30	3.26	120.75	115.27
9	L	308	BCL	O2D-CGD-O1D	-3.26	117.47	123.84
15	1	105	SPO	C31-C32-C33	-3.26	119.82	127.66
9	J	101	BCL	C4C-CHD-C1D	-3.25	121.08	125.88
9	R	102	BCL	C4C-CHD-C1D	-3.25	121.08	125.88
9	Q	104	BCL	C1-C2-C3	-3.25	120.42	126.04
15	D	102	SPO	C29-C28-C30	3.25	120.74	115.27
9	M	803	BCL	C4C-CHD-C1D	-3.25	121.09	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	V	102	SPO	C31-C32-C33	-3.24	119.85	127.66
9	W	101	BCL	C4C-CHD-C1D	-3.24	121.10	125.88
9	I	101	BCL	C4C-CHD-C1D	-3.23	121.12	125.88
15	1	103	SPO	C31-C32-C33	-3.23	119.89	127.66
15	G	103	SPO	C15-C14-C12	-3.22	122.71	127.31
15	5	104	SPO	C31-C32-C33	-3.22	119.91	127.66
9	3	103	BCL	C4C-CHD-C1D	-3.22	121.13	125.88
9	Z	101	BCL	C4C-CHD-C1D	-3.21	121.14	125.88
15	R	101	SPO	C21-C20-C19	-3.21	116.89	123.47
9	V	101	BCL	C4C-CHD-C1D	-3.21	121.15	125.88
9	2	101	BCL	C4C-CHD-C1D	-3.20	121.15	125.88
9	1	101	BCL	CHC-C1C-NC	3.19	128.93	124.51
9	Q	104	BCL	C1C-NC-C4C	-3.19	105.27	106.71
9	Z	101	BCL	O2A-CGA-CBA	3.19	121.90	111.91
9	G	101	BCL	C4C-CHD-C1D	-3.18	121.19	125.88
9	7	101	BCL	C4-C3-C5	3.17	120.61	115.27
15	D	102	SPO	C9-C10-C11	-3.17	113.33	123.22
9	Z	101	BCL	C1-C2-C3	-3.17	120.56	126.04
9	Z	101	BCL	C4-C3-C5	3.17	120.60	115.27
15	N	101	SPO	C34-C33-C35	3.16	120.59	115.27
9	Q	104	BCL	C4C-CHD-C1D	-3.16	121.22	125.88
15	G	103	SPO	C8-C7-C9	-3.16	118.50	122.92
9	F	102	BCL	C4-C3-C5	3.15	120.58	115.27
9	P	102	BCL	C4-C3-C5	3.15	120.57	115.27
9	J	101	BCL	O2A-CGA-CBA	3.14	121.77	111.91
15	F	103	SPO	C34-C33-C35	3.14	120.56	115.27
15	S	103	SPO	C15-C14-C12	-3.14	122.83	127.31
15	M	807	SPO	C5-C6-C7	-3.14	121.15	125.89
9	D	101	BCL	C4C-CHD-C1D	-3.14	121.25	125.88
15	5	103	SPO	C29-C28-C30	3.14	120.55	115.27
9	S	102	BCL	CHC-C1C-NC	3.12	128.83	124.51
15	P	101	SPO	C34-C33-C35	3.12	120.52	115.27
9	P	102	BCL	C4C-CHD-C1D	-3.12	121.28	125.88
9	T	101	BCL	C4C-CHD-C1D	-3.12	121.28	125.88
9	5	102	BCL	C4-C3-C5	3.11	120.51	115.27
9	2	101	BCL	C4-C3-C5	3.11	120.50	115.27
9	F	102	BCL	C1-C2-C3	-3.11	120.66	126.04
9	4	101	BCL	C4C-CHD-C1D	-3.11	121.30	125.88
9	P	102	BCL	O2A-CGA-CBA	3.10	121.65	111.91
9	3	103	BCL	C4-C3-C5	3.10	120.49	115.27
15	K	103	SPO	C29-C28-C30	3.10	120.48	115.27
15	P	101	SPO	C21-C20-C19	-3.10	117.13	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	102	BCL	C4C-CHD-C1D	-3.09	121.32	125.88
15	F	104	SPO	C29-C28-C30	3.09	120.46	115.27
9	B	101	BCL	C4C-CHD-C1D	-3.09	121.33	125.88
15	F	104	SPO	C21-C22-C23	-3.08	122.91	127.31
9	B	101	BCL	C4-C3-C5	3.08	120.45	115.27
15	G	103	SPO	C21-C22-C23	-3.08	122.92	127.31
15	O	103	SPO	C21-C20-C19	-3.07	117.18	123.47
9	I	101	BCL	CHB-C4A-NA	3.07	128.76	124.51
9	5	102	BCL	C4C-CHD-C1D	-3.03	121.41	125.88
9	4	101	BCL	C4-C3-C5	3.02	120.36	115.27
12	L	306	PGV	O03-C19-C20	3.02	121.39	111.91
9	3	103	BCL	CHC-C1C-NC	3.02	128.69	124.51
15	F	104	SPO	C20-C19-C17	-3.02	123.00	127.31
15	G	103	SPO	C29-C28-C30	3.02	120.35	115.27
15	O	103	SPO	C9-C10-C11	-3.02	113.80	123.22
9	6	101	BCL	C1-C2-C3	-3.01	120.84	126.04
9	J	101	BCL	C4-C3-C5	3.00	120.33	115.27
9	T	101	BCL	C4-C3-C5	3.00	120.32	115.27
16	F	101	LMT	O1B-C4'-C3'	3.00	115.26	107.28
9	5	102	BCL	CHB-C4A-NA	3.00	128.66	124.51
9	3	103	BCL	O2A-CGA-CBA	2.99	121.30	111.91
15	3	104	SPO	C29-C28-C30	2.99	120.30	115.27
9	7	101	BCL	C4C-CHD-C1D	-2.99	121.47	125.88
15	1	103	SPO	C15-C14-C12	-2.99	123.05	127.31
9	S	102	BCL	C4-C3-C5	2.98	120.29	115.27
15	G	103	SPO	C6-C7-C9	2.98	123.52	118.94
9	O	101	BCL	O2A-CGA-CBA	2.98	121.26	111.91
9	E	102	BCL	C4C-CHD-C1D	-2.98	121.49	125.88
15	K	103	SPO	C9-C10-C11	-2.98	113.92	123.22
9	L	309	BCL	O2D-CGD-O1D	-2.97	118.03	123.84
9	R	102	BCL	C4-C3-C5	2.97	120.27	115.27
15	1	105	SPO	C9-C10-C11	-2.97	113.95	123.22
9	T	101	BCL	O2A-CGA-CBA	2.96	121.21	111.91
12	H	306	PGV	O03-C19-C20	2.96	121.21	111.91
15	S	104	SPO	C27-C26-C25	-2.96	113.98	123.22
9	K	102	BCL	C4-C3-C5	2.96	120.25	115.27
15	S	103	SPO	C31-C32-C33	-2.96	120.54	127.66
9	G	101	BCL	O2A-CGA-CBA	2.95	121.17	111.91
15	S	103	SPO	C34-C33-C35	2.95	120.23	115.27
15	V	103	SPO	C34-C33-C35	2.95	120.23	115.27
12	H	306	PGV	C02-O01-C1	-2.95	110.54	117.79
9	F	102	BCL	O2A-CGA-CBA	2.95	121.15	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	U	101	LMT	C1B-O1B-C4'	-2.94	110.69	117.96
15	V	102	SPO	C9-C10-C11	-2.94	114.04	123.22
15	G	102	SPO	C15-C14-C12	-2.94	123.11	127.31
15	F	103	SPO	C29-C28-C30	2.93	120.21	115.27
15	E	101	SPO	C31-C32-C33	-2.93	120.60	127.66
15	8	101	SPO	C34-C33-C35	2.93	120.20	115.27
9	Y	103	BCL	C4-C3-C5	2.93	120.20	115.27
15	S	103	SPO	C29-C28-C30	2.93	120.20	115.27
15	T	102	SPO	C29-C28-C30	2.92	120.19	115.27
15	X	102	SPO	C34-C33-C35	2.92	120.18	115.27
9	W	101	BCL	C4-C3-C5	2.91	120.17	115.27
9	Q	104	BCL	CHC-C1C-NC	2.91	128.54	124.51
9	6	101	BCL	C4B-CHC-C1C	-2.91	124.35	130.12
9	Y	103	BCL	O2A-CGA-CBA	2.91	121.03	111.91
9	L	309	BCL	C4C-CHD-C1D	-2.91	121.59	125.88
12	Y	104	PGV	C02-O01-C1	-2.90	110.64	117.79
15	E	101	SPO	C34-C33-C35	2.90	120.15	115.27
9	E	102	BCL	C4-C3-C5	2.90	120.15	115.27
9	7	101	BCL	O2A-CGA-CBA	2.90	121.00	111.91
9	M	803	BCL	C4-C3-C5	2.90	120.14	115.27
9	B	101	BCL	O2A-CGA-CBA	2.90	121.00	111.91
15	G	103	SPO	C31-C32-C33	-2.90	120.68	127.66
9	T	101	BCL	C1-C2-C3	-2.90	121.03	126.04
9	D	101	BCL	C4-C3-C5	2.90	120.14	115.27
9	I	101	BCL	O2A-CGA-CBA	2.90	120.99	111.91
15	G	102	SPO	C34-C33-C35	2.89	120.13	115.27
15	3	104	SPO	C34-C33-C35	2.89	120.13	115.27
15	V	103	SPO	C9-C10-C11	-2.89	114.21	123.22
9	F	102	BCL	CHC-C1C-NC	2.89	128.50	124.51
12	M	812	PGV	O03-C19-C20	2.88	120.96	111.91
9	5	102	BCL	O2A-CGA-CBA	2.88	120.95	111.91
15	R	101	SPO	C8-C7-C9	-2.88	118.89	122.92
15	F	103	SPO	C31-C32-C33	-2.88	120.73	127.66
9	K	102	BCL	O2A-CGA-CBA	2.87	120.92	111.91
15	1	102	SPO	C34-C33-C35	2.87	120.10	115.27
9	L	309	BCL	C1-C2-C3	-2.87	121.09	126.04
9	R	102	BCL	O2A-CGA-CBA	2.86	120.90	111.91
9	4	101	BCL	C1-C2-C3	-2.86	121.09	126.04
15	5	104	SPO	C34-C33-C35	2.86	120.08	115.27
15	T	102	SPO	C8-C7-C9	-2.86	118.92	122.92
15	G	103	SPO	C34-C33-C35	2.86	120.08	115.27
9	G	101	BCL	C4B-CHC-C1C	-2.86	124.46	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	104	SPO	C34-C33-C35	2.85	120.07	115.27
15	G	102	SPO	C31-C32-C33	-2.85	120.80	127.66
9	D	101	BCL	C1C-NC-C4C	-2.85	105.43	106.71
9	V	101	BCL	O2A-CGA-CBA	2.84	120.83	111.91
9	8	102	BCL	O2A-CGA-CBA	2.84	120.82	111.91
9	D	101	BCL	O2A-CGA-CBA	2.83	120.80	111.91
15	1	103	SPO	C20-C19-C17	-2.83	123.27	127.31
15	O	102	SPO	C29-C28-C30	2.83	120.03	115.27
15	O	103	SPO	C29-C28-C30	2.83	120.03	115.27
15	O	103	SPO	C20-C19-C17	-2.82	123.28	127.31
15	O	102	SPO	C15-C14-C12	-2.82	123.28	127.31
9	V	101	BCL	CHB-C4A-NA	2.82	128.41	124.51
9	4	101	BCL	O2A-CGA-CBA	2.82	120.75	111.91
9	Q	104	BCL	O2A-CGA-CBA	2.82	120.75	111.91
9	A	703	BCL	CMB-C2B-C3B	2.82	129.95	124.68
9	8	102	BCL	C1C-NC-C4C	2.82	107.97	106.71
9	V	101	BCL	C1-C2-C3	-2.82	121.17	126.04
9	R	102	BCL	CHB-C4A-NA	2.82	128.41	124.51
9	N	102	BCL	C4-C3-C5	2.81	120.00	115.27
9	6	101	BCL	C4-C3-C5	2.81	119.99	115.27
12	K	104	PGV	O03-C19-C20	2.80	120.70	111.91
9	4	101	BCL	C4B-CHC-C1C	-2.80	124.57	130.12
15	3	104	SPO	C20-C19-C17	-2.80	123.32	127.31
9	Q	104	BCL	CHB-C4A-NA	2.80	128.38	124.51
9	L	309	BCL	O2A-CGA-CBA	2.79	120.67	111.91
16	3	101	LMT	O1B-C4'-C3'	2.79	114.70	107.28
15	T	102	SPO	C15-C14-C12	-2.78	123.34	127.31
9	2	101	BCL	CHB-C4A-NA	2.78	128.36	124.51
9	6	101	BCL	O2A-CGA-CBA	2.78	120.64	111.91
9	Y	103	BCL	CHB-C4A-NA	2.78	128.35	124.51
15	P	101	SPO	C27-C26-C25	-2.78	114.55	123.22
16	M	810	LMT	O1'-C1'-C2'	2.77	112.63	108.30
9	7	101	BCL	CHC-C1C-NC	2.77	128.34	124.51
15	3	104	SPO	C31-C32-C33	-2.77	120.99	127.66
15	5	103	SPO	C9-C10-C11	-2.77	114.58	123.22
9	D	101	BCL	C1-C2-C3	-2.76	121.26	126.04
15	K	103	SPO	C31-C32-C33	-2.76	121.01	127.66
9	T	101	BCL	CHB-C4A-NA	2.76	128.33	124.51
9	P	102	BCL	CHB-C4A-NA	2.76	128.32	124.51
9	P	102	BCL	CHC-C1C-NC	2.75	128.32	124.51
9	K	102	BCL	CHC-C1C-NC	2.75	128.32	124.51
16	4	102	LMT	C1B-O1B-C4'	-2.75	111.15	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	102	SPO	C31-C32-C33	-2.75	121.04	127.66
9	D	101	BCL	CHC-C1C-NC	2.75	128.31	124.51
15	N	101	SPO	C31-C32-C33	-2.74	121.05	127.66
15	N	101	SPO	C14-C15-C16	-2.74	114.66	123.22
9	I	101	BCL	CHC-C1C-NC	2.74	128.30	124.51
9	Y	103	BCL	C1C-NC-C4C	-2.74	105.48	106.71
12	L	306	PGV	C02-O01-C1	-2.74	111.06	117.79
16	I	102	LMT	O1B-C4'-C3'	2.73	114.55	107.28
15	P	101	SPO	C21-C22-C23	-2.73	123.41	127.31
9	M	803	BCL	O2D-CGD-O1D	-2.73	118.50	123.84
15	V	103	SPO	C29-C28-C30	2.73	119.86	115.27
9	R	102	BCL	C1-C2-C3	-2.73	121.33	126.04
9	F	102	BCL	CHB-C4A-NA	2.73	128.28	124.51
15	1	105	SPO	C14-C15-C16	-2.73	114.71	123.22
16	D	103	LMT	C1B-O1B-C4'	-2.72	111.22	117.96
15	M	807	SPO	C15-C14-C12	-2.72	123.42	127.31
16	Q	101	LMT	O5'-C5'-C4'	2.72	114.63	109.69
15	X	102	SPO	C9-C10-C11	-2.72	114.73	123.22
15	W	102	SPO	C15-C14-C12	-2.72	123.43	127.31
17	M	811	CDL	OB8-CB7-C71	2.72	120.44	111.91
17	M	811	CDL	OA8-CA7-C31	2.72	120.43	111.91
15	V	103	SPO	C14-C15-C16	-2.71	114.75	123.22
15	D	102	SPO	C20-C21-C22	-2.70	117.93	123.47
9	1	101	BCL	O2A-CGA-CBA	2.70	120.39	111.91
15	1	105	SPO	C13-C12-C11	2.70	122.33	118.08
9	M	803	BCL	CHC-C1C-NC	2.70	128.24	124.51
15	O	103	SPO	C14-C15-C16	-2.69	114.81	123.22
9	J	101	BCL	C4B-CHC-C1C	-2.69	124.78	130.12
15	S	103	SPO	C40-C38-C39	2.69	120.55	114.60
15	N	101	SPO	C27-C26-C25	-2.69	114.81	123.22
15	G	102	SPO	C29-C28-C30	2.69	119.80	115.27
9	W	101	BCL	O2A-CGA-CBA	2.69	120.34	111.91
15	F	103	SPO	C9-C10-C11	-2.68	114.84	123.22
12	3	102	PGV	C02-O01-C1	-2.68	111.19	117.79
16	X	105	LMT	O1B-C4'-C3'	2.68	114.41	107.28
9	O	101	BCL	C4-C3-C5	2.67	119.77	115.27
9	8	102	BCL	O2D-CGD-O1D	-2.67	118.61	123.84
15	1	105	SPO	C29-C28-C30	2.67	119.77	115.27
9	8	102	BCL	C4C-CHD-C1D	-2.67	121.95	125.88
9	K	102	BCL	O2D-CGD-O1D	-2.66	118.63	123.84
9	D	101	BCL	CHB-C4A-NA	2.66	128.19	124.51
15	1	103	SPO	C40-C38-C39	2.66	120.48	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	102	SPO	C10-C9-C7	-2.66	123.51	127.31
15	1	103	SPO	C29-C28-C30	2.66	119.75	115.27
9	6	101	BCL	C1B-CHB-C4A	-2.66	124.85	130.12
9	S	102	BCL	CHB-C4A-NA	2.66	128.19	124.51
9	O	101	BCL	CHB-C4A-NA	2.65	128.18	124.51
16	M	810	LMT	C1'-C2'-C3'	2.65	115.52	110.00
12	M	801	PGV	C02-O01-C1	-2.64	111.28	117.79
15	D	102	SPO	C27-C26-C25	-2.64	114.97	123.22
15	5	103	SPO	C8-C7-C6	2.64	122.24	118.08
9	5	102	BCL	CHC-C1C-NC	2.63	128.15	124.51
12	H	303	PGV	O03-C19-C20	2.63	120.16	111.91
15	D	102	SPO	C15-C14-C12	-2.63	123.56	127.31
9	M	803	BCL	O2A-CGA-CBA	2.63	120.15	111.91
9	Z	101	BCL	O2D-CGD-O1D	-2.62	118.71	123.84
9	S	102	BCL	O2A-CGA-CBA	2.62	120.14	111.91
15	V	102	SPO	C29-C28-C30	2.62	119.68	115.27
16	A	702	LMT	C1B-O1B-C4'	-2.62	111.48	117.96
15	R	101	SPO	C14-C15-C16	-2.62	115.06	123.22
9	2	101	BCL	O2A-CGA-CBA	2.61	120.11	111.91
16	H	301	LMT	C1-O1'-C1'	-2.61	109.51	113.84
15	S	103	SPO	C8-C7-C6	2.61	122.19	118.08
15	X	102	SPO	C10-C9-C7	-2.61	123.58	127.31
15	V	103	SPO	C13-C12-C11	2.61	122.19	118.08
9	L	308	BCL	O2A-CGA-CBA	2.61	120.10	111.91
9	L	308	BCL	C4-C3-C5	2.61	119.66	115.27
15	K	103	SPO	C13-C12-C11	2.61	122.19	118.08
15	M	807	SPO	C9-C10-C11	-2.61	115.08	123.22
9	I	101	BCL	C4-C3-C5	2.61	119.66	115.27
9	D	101	BCL	C4A-NA-C1A	2.61	107.88	106.71
9	O	101	BCL	C1C-NC-C4C	-2.60	105.53	106.71
15	V	102	SPO	C14-C15-C16	-2.60	115.09	123.22
9	I	101	BCL	CAC-C3C-C4C	-2.60	106.81	112.58
9	Y	103	BCL	CHC-C1C-NC	2.60	128.11	124.51
15	R	101	SPO	C15-C14-C12	-2.60	123.60	127.31
15	5	103	SPO	C14-C15-C16	-2.60	115.11	123.22
12	H	307	PGV	O03-C19-C20	2.60	120.06	111.91
16	A	704	LMT	C1B-O1B-C4'	-2.59	111.55	117.96
17	H	305	CDL	OB4-PB2-OB3	2.59	120.83	110.68
9	N	102	BCL	CHB-C4A-NA	2.59	128.10	124.51
9	2	101	BCL	CHC-C1C-NC	2.59	128.09	124.51
15	T	102	SPO	C21-C20-C19	-2.59	118.17	123.47
9	A	703	BCL	C1-C2-C3	-2.59	121.57	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	101	BCL	CHB-C4A-NA	2.59	128.09	124.51
15	W	102	SPO	C31-C32-C33	-2.58	121.45	127.66
17	Y	102	CDL	OA8-CA7-C31	2.58	120.00	111.91
17	Y	102	CDL	OB8-CB7-C71	2.58	120.00	111.91
9	E	102	BCL	O2A-CGA-CBA	2.58	120.00	111.91
9	M	803	BCL	CAA-C2A-C3A	-2.58	105.72	112.78
15	1	102	SPO	C9-C10-C11	-2.58	115.18	123.22
15	E	101	SPO	C27-C26-C25	-2.57	115.18	123.22
15	F	104	SPO	C31-C32-C33	-2.57	121.47	127.66
9	W	101	BCL	CHB-C4A-NA	2.57	128.07	124.51
15	P	101	SPO	C20-C19-C17	-2.57	123.64	127.31
15	G	102	SPO	C40-C38-C39	2.57	120.28	114.60
15	3	104	SPO	C8-C7-C9	-2.57	119.33	122.92
9	B	101	BCL	CHB-C4A-NA	2.57	128.06	124.51
16	1	104	LMT	C1B-O1B-C4'	-2.56	111.62	117.96
9	1	101	BCL	C4-C3-C5	2.56	119.58	115.27
15	N	101	SPO	C8-C7-C9	-2.56	119.33	122.92
9	Z	101	BCL	CHB-C4A-NA	2.56	128.05	124.51
15	1	103	SPO	C34-C33-C35	2.56	119.57	115.27
9	1	101	BCL	CHB-C4A-NA	2.56	128.05	124.51
16	M	810	LMT	C1-O1'-C1'	-2.55	109.61	113.84
15	S	103	SPO	C36-C37-C38	-2.55	119.03	127.75
9	W	101	BCL	CHC-C1C-NC	2.55	128.04	124.51
15	F	104	SPO	C14-C15-C16	-2.55	115.26	123.22
15	D	102	SPO	C14-C15-C16	-2.55	115.27	123.22
15	8	101	SPO	C31-C32-C33	-2.54	121.54	127.66
15	K	103	SPO	C21-C20-C19	-2.54	118.27	123.47
15	S	104	SPO	C21-C20-C19	-2.54	118.27	123.47
12	Q	103	PGV	O03-C19-C20	2.54	119.88	111.91
17	H	304	CDL	OB8-CB7-C71	2.54	119.88	111.91
15	1	103	SPO	C8-C7-C9	-2.54	119.36	122.92
15	X	102	SPO	C40-C38-C39	2.54	120.21	114.60
9	N	102	BCL	CHC-C1C-NC	2.54	128.02	124.51
15	1	102	SPO	C31-C32-C33	-2.54	121.55	127.66
15	F	104	SPO	C27-C26-C25	-2.53	115.32	123.22
15	G	102	SPO	C9-C10-C11	-2.53	115.34	123.22
12	X	101	PGV	O03-C19-C20	2.52	119.82	111.91
15	D	102	SPO	C34-C33-C35	2.52	119.51	115.27
9	7	101	BCL	O2D-CGD-O1D	-2.51	118.92	123.84
15	N	101	SPO	C40-C38-C39	2.51	120.16	114.60
15	T	102	SPO	C20-C19-C17	-2.51	123.73	127.31
15	N	101	SPO	C21-C20-C19	-2.51	118.33	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	O	101	BCL	O2D-CGD-O1D	-2.51	118.93	123.84
15	1	102	SPO	C13-C12-C11	2.51	122.03	118.08
9	1	101	BCL	O2D-CGD-O1D	-2.51	118.94	123.84
15	F	104	SPO	C40-C38-C39	2.51	120.14	114.60
15	W	102	SPO	C14-C15-C16	-2.51	115.40	123.22
9	L	308	BCL	C4B-CHC-C1C	-2.50	125.16	130.12
15	3	104	SPO	C14-C15-C16	-2.50	115.41	123.22
9	2	101	BCL	C2A-C1A-CHA	-2.50	119.49	123.86
15	X	102	SPO	C14-C15-C16	-2.50	115.42	123.22
15	S	103	SPO	C20-C21-C22	-2.50	118.36	123.47
9	Q	104	BCL	O2D-CGD-O1D	-2.50	118.95	123.84
15	K	103	SPO	C34-C33-C35	2.50	119.47	115.27
15	3	104	SPO	C40-C38-C39	2.49	120.11	114.60
12	L	310	PGV	O03-C19-C20	2.49	119.73	111.91
9	L	301	BCL	C4-C3-C5	2.49	119.46	115.27
15	E	101	SPO	C14-C15-C16	-2.49	115.45	123.22
12	L	305	PGV	O03-C19-C20	2.49	119.71	111.91
15	F	104	SPO	C21-C20-C19	-2.48	118.39	123.47
15	R	101	SPO	C40-C38-C39	2.48	120.09	114.60
9	Y	103	BCL	O2D-CGD-O1D	-2.48	118.99	123.84
15	1	103	SPO	C6-C7-C9	2.48	122.75	118.94
15	1	105	SPO	C34-C33-C35	2.48	119.44	115.27
15	1	103	SPO	C13-C12-C11	2.47	121.98	118.08
9	G	101	BCL	O2D-CGD-O1D	-2.47	119.00	123.84
15	S	104	SPO	C40-C38-C39	2.47	120.06	114.60
9	S	102	BCL	O2D-CGD-O1D	-2.47	119.01	123.84
9	V	101	BCL	CHC-C1C-NC	2.47	127.92	124.51
16	K	101	LMT	C1-O1'-C1'	-2.47	109.75	113.84
9	O	101	BCL	CHC-C1C-NC	2.46	127.92	124.51
9	G	101	BCL	C1-C2-C3	-2.46	121.78	126.04
15	F	103	SPO	C40-C38-C39	2.46	120.03	114.60
9	L	308	BCL	C1C-NC-C4C	-2.45	105.61	106.71
9	L	309	BCL	C4B-CHC-C1C	-2.44	125.28	130.12
12	X	101	PGV	C02-O01-C1	-2.44	111.78	117.79
15	T	102	SPO	C21-C22-C23	-2.44	123.83	127.31
15	D	102	SPO	C40-C38-C39	2.44	119.99	114.60
15	V	102	SPO	C13-C12-C11	2.44	121.92	118.08
9	L	301	BCL	CHC-C1C-NC	2.43	127.88	124.51
15	D	102	SPO	C13-C12-C11	2.43	121.91	118.08
15	1	102	SPO	C40-C38-C39	2.43	119.96	114.60
9	V	101	BCL	C4B-CHC-C1C	-2.42	125.32	130.12
15	O	102	SPO	C9-C10-C11	-2.42	115.67	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	102	BCL	C2A-C1A-CHA	-2.42	119.63	123.86
17	H	305	CDL	OA4-PA1-OA3	2.41	120.11	110.68
16	H	302	LMT	O1B-C1B-C2B	2.41	114.34	108.10
15	S	103	SPO	C10-C9-C7	-2.41	123.88	127.31
15	S	104	SPO	C20-C19-C17	-2.41	123.88	127.31
9	Q	104	BCL	C4-C3-C5	2.41	119.32	115.27
15	G	102	SPO	C21-C20-C19	-2.41	118.55	123.47
15	V	103	SPO	C21-C20-C19	-2.40	118.55	123.47
10	L	302	BPH	CMA-C3A-C4A	-2.40	109.12	114.38
15	O	102	SPO	C10-C9-C7	-2.40	123.89	127.31
15	E	101	SPO	C40-C38-C39	2.40	119.90	114.60
9	L	308	BCL	C2A-C1A-CHA	-2.40	119.66	123.86
9	D	101	BCL	O2D-CGD-O1D	-2.40	119.15	123.84
9	Z	101	BCL	C2A-C1A-CHA	-2.40	119.67	123.86
9	K	102	BCL	C1-C2-C3	-2.40	121.90	126.04
9	5	102	BCL	O2D-CGD-O1D	-2.40	119.16	123.84
9	G	101	BCL	CHB-C4A-NA	2.39	127.82	124.51
15	5	103	SPO	C13-C12-C11	2.39	121.85	118.08
15	S	104	SPO	C8-C7-C6	2.39	121.84	118.08
9	P	102	BCL	O2D-CGD-O1D	-2.39	119.17	123.84
9	B	101	BCL	O2D-CGD-O1D	-2.39	119.17	123.84
9	P	102	BCL	C2A-C1A-CHA	-2.38	119.69	123.86
9	Z	101	BCL	CHC-C1C-NC	2.38	127.80	124.51
15	S	104	SPO	C14-C15-C16	-2.38	115.79	123.22
15	1	102	SPO	C21-C20-C19	-2.38	118.60	123.47
15	P	101	SPO	C15-C14-C12	-2.37	123.92	127.31
15	S	104	SPO	C13-C12-C11	2.37	121.82	118.08
15	5	103	SPO	C40-C38-C39	2.37	119.84	114.60
15	1	102	SPO	C15-C14-C12	-2.37	123.93	127.31
12	Y	104	PGV	O03-C19-C20	2.37	119.34	111.91
9	Y	103	BCL	C2A-C1A-CHA	-2.37	119.72	123.86
15	S	103	SPO	C9-C10-C11	-2.37	115.83	123.22
15	5	104	SPO	C40-C38-C39	2.37	119.83	114.60
9	L	309	BCL	C2A-C1A-CHA	-2.36	119.73	123.86
15	1	102	SPO	C15-C16-C17	-2.36	119.78	126.42
16	K	101	LMT	O1'-C1'-C2'	2.36	111.99	108.30
9	6	101	BCL	O2D-CGD-O1D	-2.36	119.22	123.84
15	O	103	SPO	C8-C7-C6	2.36	121.79	118.08
15	R	101	SPO	C24-C23-C22	-2.36	119.62	122.92
15	1	103	SPO	C21-C22-C23	-2.35	123.95	127.31
9	R	102	BCL	C11-C12-C13	-2.35	108.31	115.92
15	O	102	SPO	C34-C33-C35	2.35	119.22	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	301	BCL	O2A-CGA-O1A	-2.35	117.67	123.59
9	R	102	BCL	O2D-CGD-O1D	-2.35	119.25	123.84
15	8	101	SPO	C40-C38-C39	2.34	119.77	114.60
15	O	103	SPO	C34-C33-C35	2.34	119.20	115.27
12	K	104	PGV	C02-O01-C1	-2.34	112.04	117.79
15	5	103	SPO	C24-C23-C22	-2.34	119.65	122.92
9	J	101	BCL	O2A-CGA-O1A	-2.33	117.70	123.59
9	K	102	BCL	CHB-C4A-NA	2.33	127.73	124.51
15	8	101	SPO	C13-C12-C14	-2.33	119.66	122.92
15	3	104	SPO	C1-C4-C5	-2.33	106.89	113.06
15	N	101	SPO	C1-C4-C5	-2.33	106.89	113.06
12	M	812	PGV	C02-O01-C1	-2.33	112.06	117.79
15	P	101	SPO	C40-C38-C39	2.33	119.74	114.60
9	R	102	BCL	C4B-CHC-C1C	-2.33	125.51	130.12
15	F	103	SPO	C14-C15-C16	-2.32	115.97	123.22
9	M	803	BCL	CED-O2D-CGD	2.32	121.18	115.94
15	1	105	SPO	C40-C38-C39	2.32	119.72	114.60
9	F	102	BCL	CED-O2D-CGD	2.31	121.17	115.94
12	L	310	PGV	C02-O01-C1	-2.31	112.11	117.79
15	W	102	SPO	C9-C10-C11	-2.31	116.02	123.22
12	M	801	PGV	O03-C19-O04	-2.30	117.78	123.59
15	1	103	SPO	C13-C12-C14	-2.30	119.70	122.92
9	2	101	BCL	O2D-CGD-O1D	-2.30	119.34	123.84
15	V	102	SPO	C34-C33-C35	2.30	119.14	115.27
9	W	101	BCL	C2A-C1A-CHA	-2.30	119.84	123.86
9	E	102	BCL	CHB-C4A-NA	2.30	127.69	124.51
15	W	102	SPO	C34-C33-C35	2.30	119.13	115.27
15	D	102	SPO	C8-C7-C6	2.29	121.69	118.08
9	B	101	BCL	C4B-CHC-C1C	-2.29	125.57	130.12
9	4	101	BCL	O2D-CGD-O1D	-2.29	119.35	123.84
9	S	102	BCL	CAC-C3C-C4C	-2.29	107.50	112.58
15	G	103	SPO	C40-C38-C39	2.29	119.67	114.60
9	A	703	BCL	O2D-CGD-O1D	-2.29	119.36	123.84
9	Q	104	BCL	C4A-NA-C1A	2.29	107.73	106.71
9	3	103	BCL	CHB-C4A-NA	2.29	127.67	124.51
9	N	102	BCL	O2D-CGD-O1D	-2.29	119.37	123.84
15	V	103	SPO	C36-C37-C38	-2.28	119.96	127.75
9	R	102	BCL	C2A-C1A-CHA	-2.27	119.89	123.86
17	H	305	CDL	OA8-CA7-C31	2.27	119.03	111.91
15	5	103	SPO	C20-C21-C22	-2.27	118.82	123.47
9	J	101	BCL	CHB-C4A-NA	2.27	127.65	124.51
12	L	310	PGV	O14-P-O13	2.27	119.57	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	E	101	SPO	C24-C23-C25	2.27	121.65	118.08
9	L	308	BCL	CHC-C1C-NC	2.27	127.65	124.51
17	M	811	CDL	CA4-OA6-CA5	-2.27	112.20	117.79
16	F	101	LMT	O3'-C3'-C2'	-2.26	105.11	110.35
9	D	101	BCL	CAC-C3C-C4C	-2.26	107.57	112.58
15	1	102	SPO	C8-C7-C6	2.26	121.64	118.08
15	V	103	SPO	C8-C7-C6	2.26	121.63	118.08
15	3	104	SPO	C15-C14-C12	-2.26	124.09	127.31
9	M	803	BCL	CHB-C4A-NA	2.25	127.63	124.51
9	A	703	BCL	C4-C3-C5	2.25	119.06	115.27
15	O	102	SPO	C5-C6-C7	-2.25	122.50	125.89
15	X	102	SPO	C13-C12-C11	2.25	121.62	118.08
9	N	102	BCL	O2A-CGA-CBA	2.24	118.94	111.91
15	F	103	SPO	C13-C12-C11	2.24	121.61	118.08
15	3	104	SPO	C20-C21-C22	-2.24	118.88	123.47
15	F	103	SPO	C27-C26-C25	-2.24	116.23	123.22
15	R	101	SPO	C31-C32-C33	-2.24	122.27	127.66
15	5	104	SPO	C27-C26-C25	-2.24	116.23	123.22
9	F	102	BCL	CAD-C3D-C4D	2.24	109.72	108.47
16	M	809	LMT	C1B-O1B-C4'	-2.24	112.43	117.96
15	O	103	SPO	C40-C38-C39	2.24	119.54	114.60
15	S	103	SPO	C26-C25-C23	-2.24	120.13	126.42
9	I	101	BCL	O2D-CGD-O1D	-2.24	119.47	123.84
9	L	308	BCL	CHB-C4A-NA	2.24	127.60	124.51
9	P	102	BCL	O2A-CGA-O1A	-2.23	117.96	123.59
15	N	101	SPO	C24-C23-C25	2.23	121.59	118.08
9	M	803	BCL	C1-C2-C3	-2.23	122.19	126.04
17	H	304	CDL	OA8-CA7-C31	2.23	118.90	111.91
15	3	104	SPO	C6-C7-C9	2.23	122.36	118.94
15	T	102	SPO	C14-C15-C16	-2.23	116.27	123.22
12	3	102	PGV	O03-C19-C20	2.22	118.88	111.91
12	H	303	PGV	O14-P-O13	2.22	119.38	110.68
9	Z	101	BCL	O2A-CGA-O1A	-2.22	117.98	123.59
9	B	101	BCL	CHC-C1C-NC	2.22	127.58	124.51
9	4	101	BCL	C1B-CHB-C4A	-2.22	125.72	130.12
9	J	101	BCL	O2D-CGD-O1D	-2.22	119.50	123.84
12	L	305	PGV	C02-O01-C1	-2.21	112.34	117.79
9	2	101	BCL	C4B-CHC-C1C	-2.21	125.73	130.12
15	3	104	SPO	C36-C37-C38	-2.21	120.19	127.75
9	L	309	BCL	C1B-CHB-C4A	-2.21	125.74	130.12
9	F	102	BCL	O2D-CGD-O1D	-2.21	119.52	123.84
15	D	102	SPO	C24-C23-C25	2.21	121.55	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	R	101	SPO	C13-C12-C11	2.21	121.55	118.08
15	8	101	SPO	C10-C11-C12	-2.21	120.22	126.42
15	K	103	SPO	C14-C15-C16	-2.20	116.34	123.22
9	5	102	BCL	C1C-NC-C4C	-2.20	105.72	106.71
15	G	102	SPO	C14-C15-C16	-2.20	116.35	123.22
15	M	807	SPO	C40-C38-C39	2.20	119.46	114.60
12	H	307	PGV	C02-O01-C1	-2.20	112.38	117.79
9	D	101	BCL	CAD-C3D-C4D	2.20	109.69	108.47
15	E	101	SPO	C20-C21-C22	-2.19	118.98	123.47
15	O	103	SPO	C13-C12-C11	2.19	121.53	118.08
15	N	101	SPO	C36-C37-C38	-2.19	120.26	127.75
15	5	103	SPO	C34-C33-C35	2.19	118.96	115.27
15	1	103	SPO	C14-C15-C16	-2.19	116.38	123.22
15	D	102	SPO	C36-C37-C38	-2.19	120.27	127.75
15	V	102	SPO	C15-C14-C12	-2.19	124.19	127.31
9	T	101	BCL	O2A-CGA-O1A	-2.19	118.07	123.59
15	W	102	SPO	C21-C20-C19	-2.19	118.99	123.47
9	E	102	BCL	C1-O2A-CGA	2.19	122.19	116.44
9	5	102	BCL	C1-C2-C3	-2.18	122.27	126.04
9	E	102	BCL	CBA-CAA-C2A	-2.18	107.42	113.86
15	T	102	SPO	C34-C33-C35	2.18	118.94	115.27
9	R	102	BCL	CHC-C1C-NC	2.18	127.53	124.51
15	T	102	SPO	C40-C38-C39	2.18	119.42	114.60
15	T	102	SPO	C6-C7-C9	2.18	122.28	118.94
16	M	810	LMT	O5'-C1'-C2'	2.18	114.96	110.35
9	P	102	BCL	C4B-CHC-C1C	-2.18	125.81	130.12
9	S	102	BCL	C4B-CHC-C1C	-2.17	125.81	130.12
9	1	101	BCL	C4B-CHC-C1C	-2.17	125.81	130.12
9	5	102	BCL	CAC-C3C-C4C	-2.17	107.76	112.58
15	O	103	SPO	C36-C35-C33	-2.17	105.83	112.98
15	1	105	SPO	C8-C7-C6	2.17	121.50	118.08
15	1	105	SPO	C20-C21-C22	-2.17	119.03	123.47
15	S	104	SPO	C9-C10-C11	-2.17	116.45	123.22
9	L	308	BCL	O1D-CGD-CBD	-2.17	120.05	124.48
15	V	103	SPO	C40-C38-C39	2.16	119.39	114.60
9	L	309	BCL	CHC-C1C-NC	2.16	127.50	124.51
9	L	301	BCL	C4A-NA-C1A	-2.16	105.73	106.71
15	1	103	SPO	C20-C21-C22	-2.16	119.06	123.47
16	H	302	LMT	O5'-C5'-C4'	2.16	114.30	109.75
9	E	102	BCL	CHC-C1C-NC	2.16	127.49	124.51
15	V	103	SPO	C10-C9-C7	-2.15	124.24	127.31
9	L	301	BCL	CHB-C4A-NA	2.15	127.49	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	M	807	SPO	C13-C12-C11	2.15	121.47	118.08
15	P	101	SPO	C14-C15-C16	-2.15	116.50	123.22
15	W	102	SPO	C40-C38-C39	2.15	119.35	114.60
9	4	101	BCL	CAD-C3D-C4D	2.15	109.67	108.47
9	T	101	BCL	O2D-CGD-O1D	-2.15	119.64	123.84
9	4	101	BCL	CHB-C4A-NA	2.14	127.48	124.51
15	G	103	SPO	C27-C26-C25	-2.14	116.53	123.22
9	W	101	BCL	O2D-CGD-O1D	-2.14	119.65	123.84
15	G	103	SPO	C21-C20-C19	-2.14	119.09	123.47
9	A	703	BCL	O2A-CGA-O1A	-2.14	118.19	123.59
15	S	104	SPO	C31-C32-C33	-2.14	122.51	127.66
9	L	301	BCL	C2A-C1A-CHA	-2.14	120.12	123.86
15	V	102	SPO	C40-C38-C39	2.14	119.33	114.60
15	W	102	SPO	C20-C21-C22	-2.14	119.09	123.47
15	1	105	SPO	C36-C37-C38	-2.14	120.45	127.75
9	Q	104	BCL	C4B-CHC-C1C	-2.13	125.89	130.12
15	O	102	SPO	C40-C38-C39	2.13	119.31	114.60
17	M	811	CDL	OB6-CB5-OB7	-2.13	118.55	123.70
15	S	104	SPO	C10-C9-C7	-2.13	124.27	127.31
9	J	101	BCL	CAC-C3C-C4C	-2.13	107.87	112.58
15	V	103	SPO	C18-C17-C16	2.12	121.42	118.08
15	O	102	SPO	C31-C32-C33	-2.12	122.55	127.66
9	N	102	BCL	C11-C12-C13	-2.12	109.06	115.92
16	H	302	LMT	O5'-C1'-C2'	-2.12	105.86	110.35
15	W	102	SPO	C24-C23-C22	-2.12	119.95	122.92
9	L	301	BCL	C1B-CHB-C4A	-2.12	125.92	130.12
9	3	103	BCL	O2D-CGD-O1D	-2.12	119.70	123.84
15	S	104	SPO	C24-C23-C25	2.12	121.41	118.08
9	E	102	BCL	CAD-C3D-C4D	2.12	109.65	108.47
15	F	103	SPO	C20-C21-C22	-2.11	119.14	123.47
9	E	102	BCL	O2D-CGD-O1D	-2.11	119.71	123.84
9	R	102	BCL	O2A-CGA-O1A	-2.11	118.27	123.59
16	M	808	LMT	C1B-O1B-C4'	-2.11	112.74	117.96
9	1	101	BCL	CAD-C3D-C4D	2.11	109.64	108.47
9	F	102	BCL	CAC-C3C-C4C	-2.10	107.91	112.58
15	S	104	SPO	C15-C14-C12	-2.10	124.31	127.31
15	X	102	SPO	C15-C14-C12	-2.10	124.31	127.31
16	U	102	LMT	C1B-O1B-C4'	-2.10	112.76	117.96
12	H	303	PGV	C02-O01-C1	-2.10	112.63	117.79
15	G	102	SPO	C13-C12-C11	2.10	121.38	118.08
9	T	101	BCL	C2A-C1A-CHA	-2.10	120.19	123.86
9	Y	103	BCL	O2A-CGA-O1A	-2.10	118.30	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	1	102	SPO	C30-C31-C32	-2.09	105.01	111.88
15	P	101	SPO	C31-C32-C33	-2.09	122.63	127.66
9	E	102	BCL	CAC-C3C-C4C	-2.09	107.95	112.58
9	L	301	BCL	CED-O2D-CGD	2.09	120.65	115.94
9	3	103	BCL	C4B-CHC-C1C	-2.08	125.99	130.12
15	M	807	SPO	C34-C33-C35	2.08	118.78	115.27
9	I	101	BCL	CAD-C3D-C4D	2.08	109.63	108.47
9	E	102	BCL	C2A-C1A-CHA	-2.08	120.22	123.86
9	F	102	BCL	C2A-C1A-CHA	-2.07	120.23	123.86
15	S	103	SPO	C14-C15-C16	-2.07	116.74	123.22
15	V	102	SPO	C8-C7-C6	2.07	121.34	118.08
15	1	105	SPO	C26-C25-C23	-2.07	120.60	126.42
15	G	102	SPO	C8-C7-C6	2.07	121.34	118.08
9	1	101	BCL	CAC-C3C-C4C	-2.07	108.00	112.58
15	O	102	SPO	C26-C25-C23	-2.06	120.61	126.42
9	D	101	BCL	C4B-CHC-C1C	-2.06	126.03	130.12
15	V	102	SPO	C36-C37-C38	-2.06	120.70	127.75
9	F	102	BCL	O2A-CGA-O1A	-2.06	118.39	123.59
9	G	101	BCL	C1B-CHB-C4A	-2.06	126.03	130.12
9	E	102	BCL	C1B-CHB-C4A	-2.06	126.03	130.12
9	1	101	BCL	CBA-CAA-C2A	-2.06	107.79	113.86
15	O	102	SPO	C18-C17-C19	-2.06	120.04	122.92
15	G	103	SPO	C14-C15-C16	-2.06	116.80	123.22
15	F	103	SPO	C15-C14-C12	-2.06	124.37	127.31
17	H	305	CDL	OB8-CB7-OB9	-2.05	118.41	123.59
9	Z	101	BCL	C1C-NC-C4C	-2.05	105.78	106.71
15	3	104	SPO	C27-C26-C25	-2.05	116.81	123.22
9	L	301	BCL	C11-C12-C13	-2.05	109.29	115.92
9	G	101	BCL	O2A-CGA-O1A	-2.05	118.42	123.59
9	W	101	BCL	CAD-C3D-C4D	2.05	109.61	108.47
15	3	104	SPO	C21-C22-C23	-2.04	124.39	127.31
12	M	812	PGV	O03-C19-O04	-2.04	118.43	123.59
9	L	301	BCL	C1-C2-C3	-2.04	122.51	126.04
9	3	103	BCL	C1-C2-C3	-2.04	122.51	126.04
16	3	101	LMT	O3'-C3'-C2'	-2.04	105.63	110.35
15	N	101	SPO	C15-C14-C12	-2.04	124.40	127.31
10	M	804	BPH	CBA-CAA-C2A	-2.04	107.85	113.81
15	M	807	SPO	C24-C23-C22	-2.04	120.07	122.92
9	7	101	BCL	C2A-C1A-CHA	-2.04	120.30	123.86
9	B	101	BCL	O2A-CGA-O1A	-2.03	118.46	123.59
15	S	104	SPO	C8-C7-C9	-2.03	120.08	122.92
9	E	102	BCL	C4B-CHC-C1C	-2.03	126.09	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	104	SPO	C8-C7-C9	-2.03	120.08	122.92
15	S	104	SPO	C21-C22-C23	-2.03	124.41	127.31
15	S	103	SPO	C18-C17-C19	-2.03	120.08	122.92
9	I	101	BCL	C4B-CHC-C1C	-2.03	126.10	130.12
15	R	101	SPO	C6-C7-C9	2.03	122.05	118.94
9	K	102	BCL	CAD-C3D-C4D	2.03	109.60	108.47
9	I	101	BCL	O2A-CGA-O1A	-2.03	118.48	123.59
15	W	102	SPO	C24-C23-C25	2.03	121.27	118.08
15	N	101	SPO	C20-C21-C22	-2.02	119.33	123.47
15	5	104	SPO	C15-C16-C17	-2.02	120.73	126.42
15	X	102	SPO	C26-C25-C23	-2.02	120.73	126.42
9	V	101	BCL	CED-O2D-CGD	2.02	120.52	115.94
16	3	101	LMT	C1'-O5'-C5'	-2.02	109.72	113.69
9	B	101	BCL	CAC-C3C-C4C	-2.02	108.10	112.58
15	O	103	SPO	C34-C33-C32	-2.02	118.49	123.68
9	7	101	BCL	C1-C2-C3	-2.02	122.55	126.04
15	E	101	SPO	C9-C10-C11	-2.02	116.92	123.22
9	1	101	BCL	O2A-CGA-O1A	-2.02	118.50	123.59
9	D	101	BCL	O2A-CGA-O1A	-2.02	118.51	123.59
15	1	103	SPO	C36-C37-C38	-2.02	120.86	127.75
15	5	103	SPO	C26-C25-C23	-2.01	120.76	126.42
9	L	309	BCL	CHB-C4A-NA	2.01	127.29	124.51
15	1	103	SPO	C27-C26-C25	-2.01	116.94	123.22
15	5	103	SPO	C21-C20-C19	-2.01	119.36	123.47
9	M	803	BCL	C4B-CHC-C1C	-2.01	126.14	130.12
9	E	102	BCL	C1-C2-C3	-2.01	122.57	126.04
15	8	101	SPO	C36-C37-C38	-2.00	120.90	127.75
15	F	104	SPO	C20-C21-C22	-2.00	119.38	123.47
9	8	102	BCL	CMD-C2D-C3D	-2.00	120.94	124.68

There are no chirality outliers.

All (915) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	L	301	BCL	C2C-C3C-CAC-CBC
9	L	301	BCL	C4C-C3C-CAC-CBC
9	A	703	BCL	C2A-CAA-CBA-CGA
9	B	101	BCL	C1A-C2A-CAA-CBA
9	B	101	BCL	C3A-C2A-CAA-CBA
9	E	102	BCL	C6-C7-C8-C10
9	F	102	BCL	C2-C3-C5-C6
9	F	102	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	J	101	BCL	C1A-C2A-CAA-CBA
9	J	101	BCL	C3A-C2A-CAA-CBA
9	K	102	BCL	C2C-C3C-CAC-CBC
9	K	102	BCL	C4C-C3C-CAC-CBC
9	K	102	BCL	C2-C3-C5-C6
9	K	102	BCL	C4-C3-C5-C6
9	N	102	BCL	C1A-C2A-CAA-CBA
9	N	102	BCL	C3A-C2A-CAA-CBA
9	P	102	BCL	C1A-C2A-CAA-CBA
9	P	102	BCL	C3A-C2A-CAA-CBA
9	S	102	BCL	C4-C3-C5-C6
9	V	101	BCL	C2C-C3C-CAC-CBC
9	V	101	BCL	C4C-C3C-CAC-CBC
9	W	101	BCL	C1A-C2A-CAA-CBA
9	W	101	BCL	C3A-C2A-CAA-CBA
9	Z	101	BCL	C1A-C2A-CAA-CBA
9	2	101	BCL	C1A-C2A-CAA-CBA
9	2	101	BCL	C3A-C2A-CAA-CBA
9	2	101	BCL	C6-C7-C8-C9
9	4	101	BCL	C1A-C2A-CAA-CBA
9	6	101	BCL	C1A-C2A-CAA-CBA
9	7	101	BCL	C2-C3-C5-C6
9	7	101	BCL	C4-C3-C5-C6
9	8	102	BCL	C1A-C2A-CAA-CBA
12	L	305	PGV	C04-O12-P-O13
12	L	306	PGV	C03-O11-P-O12
12	L	306	PGV	C03-O11-P-O13
12	L	306	PGV	C04-O12-P-O14
12	L	306	PGV	C05-C04-O12-P
12	M	801	PGV	C03-O11-P-O12
12	M	801	PGV	C03-O11-P-O13
12	M	801	PGV	C03-O11-P-O14
12	M	812	PGV	C03-O11-P-O12
12	M	812	PGV	C03-O11-P-O13
12	M	812	PGV	C03-O11-P-O14
12	M	812	PGV	O01-C02-C03-O11
12	M	812	PGV	O02-C1-O01-C02
12	M	812	PGV	C2-C1-O01-C02
12	H	307	PGV	C03-O11-P-O14
12	H	307	PGV	C04-O12-P-O13
12	H	307	PGV	O01-C02-C03-O11
12	K	104	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
12	K	104	PGV	C2-C1-O01-C02
12	3	102	PGV	C03-O11-P-O13
12	3	102	PGV	C04-O12-P-O11
15	E	101	SPO	C2-C1-C4-C5
15	E	101	SPO	C3-C1-C4-C5
15	E	101	SPO	C33-C35-C36-C37
15	F	103	SPO	C28-C30-C31-C32
15	F	103	SPO	C33-C35-C36-C37
15	G	103	SPO	C3-C1-C4-C5
15	N	101	SPO	C5-C6-C7-C8
15	N	101	SPO	C5-C6-C7-C9
15	O	102	SPO	C10-C11-C12-C13
15	O	102	SPO	C10-C11-C12-C14
15	O	103	SPO	C32-C33-C35-C36
15	O	103	SPO	C34-C33-C35-C36
15	P	101	SPO	O1-C1-C4-C5
15	P	101	SPO	C2-C1-C4-C5
15	P	101	SPO	C3-C1-C4-C5
15	R	101	SPO	C22-C23-C25-C26
15	R	101	SPO	C24-C23-C25-C26
15	S	103	SPO	C10-C11-C12-C13
15	S	103	SPO	C10-C11-C12-C14
15	S	104	SPO	C32-C33-C35-C36
15	S	104	SPO	C34-C33-C35-C36
15	T	102	SPO	C2-C1-C4-C5
15	T	102	SPO	C33-C35-C36-C37
15	V	102	SPO	C32-C33-C35-C36
15	V	102	SPO	C34-C33-C35-C36
15	W	102	SPO	C2-C1-C4-C5
15	W	102	SPO	C3-C1-C4-C5
15	W	102	SPO	C5-C6-C7-C8
15	W	102	SPO	C5-C6-C7-C9
15	1	105	SPO	C28-C30-C31-C32
15	3	104	SPO	C5-C6-C7-C8
15	3	104	SPO	C5-C6-C7-C9
15	5	103	SPO	O1-C1-C4-C5
15	5	103	SPO	C2-C1-C4-C5
15	5	103	SPO	C3-C1-C4-C5
15	5	104	SPO	C28-C30-C31-C32
15	X	102	SPO	C5-C6-C7-C8
16	M	808	LMT	C2'-C1'-O1'-C1
16	M	808	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
16	M	809	LMT	C2-C1-O1'-C1'
16	F	101	LMT	O5'-C1'-O1'-C1
16	Q	101	LMT	C2-C1-O1'-C1'
16	U	101	LMT	O5'-C1'-O1'-C1
17	M	811	CDL	CA2-OA2-PA1-OA5
17	M	811	CDL	CA3-OA5-PA1-OA2
17	M	811	CDL	CA3-OA5-PA1-OA3
17	M	811	CDL	CA3-OA5-PA1-OA4
17	M	811	CDL	CB3-OB5-PB2-OB2
17	M	811	CDL	CB3-OB5-PB2-OB3
17	M	811	CDL	CB3-OB5-PB2-OB4
17	M	811	CDL	OB7-CB5-OB6-CB4
17	M	811	CDL	C51-CB5-OB6-CB4
17	H	304	CDL	CA2-OA2-PA1-OA5
17	H	304	CDL	CA3-OA5-PA1-OA3
17	H	304	CDL	C11-CA5-OA6-CA4
17	H	304	CDL	CB2-OB2-PB2-OB4
17	H	304	CDL	CB3-OB5-PB2-OB4
17	H	305	CDL	CA3-OA5-PA1-OA2
17	H	305	CDL	CA3-OA5-PA1-OA4
17	H	305	CDL	CB3-OB5-PB2-OB2
17	H	305	CDL	CB3-OB5-PB2-OB4
17	Y	102	CDL	CA2-OA2-PA1-OA3
17	Y	102	CDL	CA3-CA4-CA6-OA8
17	Y	102	CDL	OA6-CA4-CA6-OA8
17	Y	102	CDL	CB2-OB2-PB2-OB3
17	Y	102	CDL	CB3-OB5-PB2-OB3
16	H	301	LMT	C3'-C4'-O1B-C1B
16	I	102	LMT	C3'-C4'-O1B-C1B
16	H	302	LMT	C2B-C1B-O1B-C4'
16	3	101	LMT	C3'-C4'-O1B-C1B
9	L	301	BCL	CBD-CGD-O2D-CED
9	M	803	BCL	CBD-CGD-O2D-CED
16	K	101	LMT	C3'-C4'-O1B-C1B
16	X	105	LMT	C3'-C4'-O1B-C1B
9	6	101	BCL	CBD-CGD-O2D-CED
16	F	101	LMT	O5B-C1B-O1B-C4'
17	H	304	CDL	OA7-CA5-OA6-CA4
9	A	703	BCL	C3-C5-C6-C7
9	D	101	BCL	C3-C5-C6-C7
9	G	101	BCL	C3-C5-C6-C7
9	W	101	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	E	101	SPO	C29-C28-C30-C31
15	K	103	SPO	C34-C33-C35-C36
15	R	101	SPO	C34-C33-C35-C36
15	1	103	SPO	C29-C28-C30-C31
9	S	102	BCL	C2-C3-C5-C6
15	R	101	SPO	C32-C33-C35-C36
9	E	102	BCL	C2A-CAA-CBA-CGA
9	R	102	BCL	C2A-CAA-CBA-CGA
9	L	301	BCL	C3-C5-C6-C7
9	G	101	BCL	CBD-CGD-O2D-CED
9	L	301	BCL	O1D-CGD-O2D-CED
16	H	301	LMT	O5'-C5'-C6'-O6'
16	5	101	LMT	C3'-C4'-O1B-C1B
9	N	102	BCL	CBD-CGD-O2D-CED
12	L	306	PGV	O12-C04-C05-O05
9	J	101	BCL	C3-C5-C6-C7
16	M	809	LMT	O5'-C5'-C6'-O6'
9	M	803	BCL	O1D-CGD-O2D-CED
12	L	305	PGV	C2-C1-O01-C02
16	S	105	LMT	O5B-C5B-C6B-O6B
9	V	101	BCL	C4-C3-C5-C6
9	5	102	BCL	C4-C3-C5-C6
11	L	304	U10	C12-C11-C9-C10
15	G	102	SPO	C34-C33-C35-C36
15	N	101	SPO	C34-C33-C35-C36
15	S	103	SPO	C34-C33-C35-C36
15	V	103	SPO	C34-C33-C35-C36
15	5	104	SPO	C29-C28-C30-C31
15	8	101	SPO	C29-C28-C30-C31
9	V	101	BCL	C2-C3-C5-C6
9	W	101	BCL	C2-C3-C5-C6
9	5	102	BCL	C2-C3-C5-C6
11	L	304	U10	C12-C11-C9-C8
15	E	101	SPO	C27-C28-C30-C31
15	G	102	SPO	C32-C33-C35-C36
15	K	103	SPO	C32-C33-C35-C36
15	N	101	SPO	C32-C33-C35-C36
15	S	103	SPO	C32-C33-C35-C36
15	V	103	SPO	C32-C33-C35-C36
15	5	104	SPO	C27-C28-C30-C31
15	8	101	SPO	C27-C28-C30-C31
9	P	102	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	M	806	U10	C24-C26-C27-C28
15	K	103	SPO	C28-C30-C31-C32
15	N	101	SPO	C33-C35-C36-C37
15	O	102	SPO	C28-C30-C31-C32
15	O	103	SPO	C33-C35-C36-C37
15	S	103	SPO	C28-C30-C31-C32
15	V	102	SPO	C33-C35-C36-C37
15	V	103	SPO	C28-C30-C31-C32
15	1	103	SPO	C28-C30-C31-C32
15	1	105	SPO	C33-C35-C36-C37
15	5	103	SPO	C28-C30-C31-C32
15	5	103	SPO	C33-C35-C36-C37
12	H	307	PGV	C2-C1-O01-C02
9	P	102	BCL	CBD-CGD-O2D-CED
12	L	305	PGV	O02-C1-O01-C02
9	3	103	BCL	C3-C5-C6-C7
9	G	101	BCL	C8-C10-C11-C12
16	F	101	LMT	C3'-C4'-O1B-C1B
9	F	102	BCL	C15-C16-C17-C18
9	K	102	BCL	C8-C10-C11-C12
9	K	102	BCL	C15-C16-C17-C18
9	R	102	BCL	C8-C10-C11-C12
12	M	812	PGV	O12-C04-C05-O05
17	M	811	CDL	OA6-CA4-CA6-OA8
15	1	103	SPO	C27-C28-C30-C31
9	L	301	BCL	C14-C13-C15-C16
9	L	308	BCL	C11-C10-C8-C9
9	B	101	BCL	C6-C7-C8-C9
9	D	101	BCL	C11-C10-C8-C9
9	G	101	BCL	C11-C10-C8-C9
9	J	101	BCL	C11-C10-C8-C9
9	R	102	BCL	C6-C7-C8-C9
9	T	101	BCL	C6-C7-C8-C9
9	W	101	BCL	C11-C12-C13-C14
9	Y	103	BCL	C11-C10-C8-C9
9	Z	101	BCL	C11-C10-C8-C9
9	6	101	BCL	C6-C7-C8-C9
9	8	102	BCL	C6-C7-C8-C9
9	K	102	BCL	C5-C6-C7-C8
15	G	102	SPO	C10-C11-C12-C13
15	O	103	SPO	C5-C6-C7-C8
15	S	104	SPO	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	S	104	SPO	C10-C11-C12-C13
15	V	103	SPO	C10-C11-C12-C13
15	1	102	SPO	C10-C11-C12-C13
15	1	105	SPO	C15-C16-C17-C18
15	X	102	SPO	C10-C11-C12-C13
15	S	104	SPO	C5-C6-C7-C9
9	L	308	BCL	C13-C15-C16-C17
9	S	102	BCL	C15-C16-C17-C18
9	6	101	BCL	O1D-CGD-O2D-CED
9	A	703	BCL	C5-C6-C7-C8
9	O	101	BCL	C15-C16-C17-C18
9	T	101	BCL	C10-C11-C12-C13
9	Y	103	BCL	C5-C6-C7-C8
9	1	101	BCL	C8-C10-C11-C12
9	2	101	BCL	C10-C11-C12-C13
9	6	101	BCL	C10-C11-C12-C13
9	J	101	BCL	C13-C15-C16-C17
9	S	102	BCL	C5-C6-C7-C8
12	L	306	PGV	C1-C2-C3-C4
12	M	812	PGV	C1-C2-C3-C4
9	J	101	BCL	C10-C11-C12-C13
9	R	102	BCL	C15-C16-C17-C18
9	5	102	BCL	C5-C6-C7-C8
9	Z	101	BCL	C8-C10-C11-C12
12	L	305	PGV	C19-C20-C21-C22
12	H	306	PGV	C1-C2-C3-C4
9	J	101	BCL	C5-C6-C7-C8
9	P	102	BCL	C6-C7-C8-C10
9	S	102	BCL	C6-C7-C8-C10
9	W	101	BCL	C11-C10-C8-C7
9	1	101	BCL	C11-C10-C8-C7
9	2	101	BCL	C11-C10-C8-C7
9	3	103	BCL	C6-C7-C8-C10
9	6	101	BCL	C11-C10-C8-C7
9	T	101	BCL	C2A-CAA-CBA-CGA
9	7	101	BCL	C5-C6-C7-C8
9	F	102	BCL	C5-C6-C7-C8
15	D	102	SPO	C28-C30-C31-C32
15	G	102	SPO	C33-C35-C36-C37
15	O	103	SPO	C28-C30-C31-C32
15	S	103	SPO	C33-C35-C36-C37
15	1	103	SPO	C33-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
16	F	101	LMT	C5'-C4'-O1B-C1B
17	H	304	CDL	CB5-C51-C52-C53
12	L	305	PGV	O12-C04-C05-O05
12	H	307	PGV	O02-C1-O01-C02
16	M	809	LMT	C4'-C5'-C6'-O6'
16	H	301	LMT	C4'-C5'-C6'-O6'
9	K	102	BCL	C10-C11-C12-C13
9	N	102	BCL	C13-C15-C16-C17
9	V	101	BCL	C15-C16-C17-C18
9	Y	103	BCL	C10-C11-C12-C13
17	M	811	CDL	C17-C18-C19-C20
9	I	101	BCL	C10-C11-C12-C13
9	R	102	BCL	C5-C6-C7-C8
9	R	102	BCL	C13-C15-C16-C17
9	1	101	BCL	C10-C11-C12-C13
12	L	305	PGV	C03-O11-P-O12
12	L	306	PGV	C04-O12-P-O11
12	H	307	PGV	C03-O11-P-O12
17	M	811	CDL	CB2-OB2-PB2-OB5
17	H	304	CDL	CB2-OB2-PB2-OB5
17	H	304	CDL	CB3-OB5-PB2-OB2
9	B	101	BCL	C8-C10-C11-C12
12	L	305	PGV	O12-C04-C05-C06
9	G	101	BCL	C2A-CAA-CBA-CGA
9	3	103	BCL	C16-C17-C18-C19
15	W	102	SPO	C25-C26-C27-C28
9	6	101	BCL	C8-C10-C11-C12
9	T	101	BCL	C16-C17-C18-C19
9	V	101	BCL	C16-C17-C18-C19
9	4	101	BCL	C16-C17-C18-C19
12	Q	103	PGV	C24-C25-C26-C27
9	G	101	BCL	O1D-CGD-O2D-CED
12	L	305	PGV	C21-C22-C23-C24
16	H	301	LMT	C6-C7-C8-C9
13	L	307	LDA	C3-C4-C5-C6
9	L	301	BCL	C15-C16-C17-C18
9	W	101	BCL	CBA-CGA-O2A-C1
9	2	101	BCL	CBA-CGA-O2A-C1
9	E	102	BCL	C6-C7-C8-C9
9	I	101	BCL	C6-C7-C8-C9
9	4	101	BCL	C2A-CAA-CBA-CGA
12	Y	104	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
16	M	809	LMT	C5-C6-C7-C8
9	D	101	BCL	C8-C10-C11-C12
9	Z	101	BCL	C5-C6-C7-C8
12	K	104	PGV	C22-C23-C24-C25
13	X	103	LDA	C2-C3-C4-C5
12	K	104	PGV	C25-C26-C27-C28
12	3	102	PGV	C4-C5-C6-C7
9	T	101	BCL	C15-C16-C17-C18
9	V	101	BCL	C5-C6-C7-C8
12	Q	103	PGV	C01-C02-C03-O11
15	G	103	SPO	C33-C35-C36-C37
12	Y	104	PGV	C24-C25-C26-C27
13	L	307	LDA	C2-C3-C4-C5
12	K	104	PGV	C23-C24-C25-C26
12	Q	103	PGV	C22-C23-C24-C25
9	N	102	BCL	O1D-CGD-O2D-CED
9	G	101	BCL	C3A-C2A-CAA-CBA
9	R	102	BCL	C3A-C2A-CAA-CBA
9	T	101	BCL	C3A-C2A-CAA-CBA
9	Y	103	BCL	C3A-C2A-CAA-CBA
9	Z	101	BCL	C3A-C2A-CAA-CBA
9	4	101	BCL	C3A-C2A-CAA-CBA
9	6	101	BCL	C3A-C2A-CAA-CBA
9	O	101	BCL	C13-C15-C16-C17
9	8	102	BCL	C8-C10-C11-C12
16	S	105	LMT	C1-C2-C3-C4
16	M	810	LMT	C2-C1-O1'-C1'
9	E	102	BCL	C16-C17-C18-C19
9	W	101	BCL	C3-C5-C6-C7
16	5	101	LMT	O5'-C5'-C6'-O6'
12	H	307	PGV	C5-C6-C7-C8
9	2	101	BCL	C15-C16-C17-C18
9	6	101	BCL	C4-C3-C5-C6
15	W	102	SPO	C29-C28-C30-C31
15	W	102	SPO	C27-C28-C30-C31
12	L	310	PGV	C4-C5-C6-C7
9	L	309	BCL	C16-C17-C18-C19
16	S	105	LMT	C4B-C5B-C6B-O6B
9	E	102	BCL	C2-C1-O2A-CGA
13	M	802	LDA	C11-C10-C9-C8
9	T	101	BCL	C8-C10-C11-C12
9	W	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	Y	104	PGV	C3-C4-C5-C6
9	Y	103	BCL	C3-C5-C6-C7
16	D	103	LMT	O5B-C5B-C6B-O6B
9	8	102	BCL	CBA-CGA-O2A-C1
9	L	309	BCL	C15-C16-C17-C18
9	M	803	BCL	C5-C6-C7-C8
9	N	102	BCL	C8-C10-C11-C12
9	2	101	BCL	O1A-CGA-O2A-C1
16	U	102	LMT	O5'-C5'-C6'-O6'
15	S	104	SPO	C29-C28-C30-C31
15	T	102	SPO	C29-C28-C30-C31
15	1	102	SPO	C34-C33-C35-C36
9	L	301	BCL	C12-C13-C15-C16
9	M	803	BCL	C6-C7-C8-C10
9	I	101	BCL	C6-C7-C8-C10
9	K	102	BCL	C11-C12-C13-C15
9	R	102	BCL	C6-C7-C8-C10
9	T	101	BCL	C6-C7-C8-C10
9	2	101	BCL	C6-C7-C8-C10
9	6	101	BCL	C2-C3-C5-C6
9	4	101	BCL	C16-C17-C18-C20
12	L	305	PGV	C11-C10-C9-C8
16	F	105	LMT	O1'-C1-C2-C3
9	J	101	BCL	C2A-CAA-CBA-CGA
9	Z	101	BCL	C2A-CAA-CBA-CGA
9	Q	104	BCL	C5-C6-C7-C8
9	P	102	BCL	O1D-CGD-O2D-CED
12	M	801	PGV	C13-C14-C15-C16
16	Q	101	LMT	C1-C2-C3-C4
9	Y	103	BCL	CBA-CGA-O2A-C1
9	Q	104	BCL	C16-C17-C18-C19
9	Y	103	BCL	C8-C10-C11-C12
15	D	102	SPO	C33-C35-C36-C37
15	S	104	SPO	C33-C35-C36-C37
16	3	101	LMT	C4-C5-C6-C7
12	L	306	PGV	C2-C1-O01-C02
17	H	304	CDL	OA5-CA3-CA4-OA6
16	3	101	LMT	C2-C3-C4-C5
9	5	102	BCL	C15-C16-C17-C18
17	Y	102	CDL	O1-C1-CA2-OA2
12	L	306	PGV	O02-C1-O01-C02
16	H	302	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
16	I	102	LMT	O5'-C5'-C6'-O6'
16	K	101	LMT	O5'-C5'-C6'-O6'
10	M	804	BPH	C4-C3-C5-C6
15	1	102	SPO	C32-C33-C35-C36
9	M	803	BCL	C6-C7-C8-C9
9	Q	104	BCL	C11-C12-C13-C14
9	1	101	BCL	C11-C10-C8-C9
9	2	101	BCL	C11-C10-C8-C9
9	7	101	BCL	C11-C10-C8-C9
9	6	101	BCL	C2A-CAA-CBA-CGA
16	M	810	LMT	C2-C3-C4-C5
16	A	701	LMT	O5B-C5B-C6B-O6B
15	N	101	SPO	C24-C23-C25-C26
9	8	102	BCL	O1A-CGA-O2A-C1
9	L	309	BCL	C1A-C2A-CAA-CBA
9	G	101	BCL	C1A-C2A-CAA-CBA
9	R	102	BCL	C1A-C2A-CAA-CBA
9	T	101	BCL	C1A-C2A-CAA-CBA
9	Y	103	BCL	C1A-C2A-CAA-CBA
16	Q	102	LMT	O5'-C5'-C6'-O6'
9	Q	104	BCL	C16-C17-C18-C20
9	1	101	BCL	C16-C17-C18-C19
9	3	103	BCL	C16-C17-C18-C20
12	Y	104	PGV	C2-C1-O01-C02
9	1	101	BCL	C5-C6-C7-C8
9	4	101	BCL	C15-C16-C17-C18
12	M	812	PGV	C01-C02-C03-O11
16	M	810	LMT	O5B-C1B-O1B-C4'
9	7	101	BCL	C15-C16-C17-C18
15	5	104	SPO	C1-C4-C5-C6
12	L	306	PGV	O12-C04-C05-C06
16	3	101	LMT	O5'-C5'-C6'-O6'
16	4	102	LMT	O5B-C5B-C6B-O6B
15	S	104	SPO	C27-C28-C30-C31
15	T	102	SPO	C27-C28-C30-C31
16	3	101	LMT	C3-C4-C5-C6
9	V	101	BCL	C16-C17-C18-C20
12	M	812	PGV	C2-C3-C4-C5
12	H	306	PGV	O03-C01-C02-C03
17	M	811	CDL	CA3-CA4-CA6-OA8
9	Z	101	BCL	C15-C16-C17-C18
16	5	101	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
9	Y	103	BCL	O1A-CGA-O2A-C1
9	G	101	BCL	C15-C16-C17-C18
16	X	105	LMT	O5'-C1'-O1'-C1
16	A	701	LMT	O5'-C5'-C6'-O6'
16	1	104	LMT	O5'-C5'-C6'-O6'
9	L	308	BCL	C15-C16-C17-C18
16	D	103	LMT	O5'-C5'-C6'-O6'
12	M	812	PGV	C6-C7-C8-C9
16	A	702	LMT	O5B-C5B-C6B-O6B
16	A	702	LMT	O5'-C5'-C6'-O6'
9	G	101	BCL	C4-C3-C5-C6
9	Q	104	BCL	C4-C3-C5-C6
15	M	807	SPO	C29-C28-C30-C31
16	H	302	LMT	C3'-C4'-O1B-C1B
9	W	101	BCL	C16-C17-C18-C19
17	H	304	CDL	C31-CA7-OA8-CA6
17	H	304	CDL	C51-C52-C53-C54
9	S	102	BCL	C8-C10-C11-C12
9	V	101	BCL	C13-C15-C16-C17
9	L	301	BCL	C2-C1-O2A-CGA
16	4	102	LMT	O5'-C5'-C6'-O6'
9	2	101	BCL	C8-C10-C11-C12
12	L	310	PGV	C03-O11-P-O13
12	L	305	PGV	C2-C3-C4-C5
17	M	811	CDL	C14-C15-C16-C17
9	E	102	BCL	C13-C15-C16-C17
9	P	102	BCL	C5-C6-C7-C8
12	Q	103	PGV	O03-C01-C02-O01
17	H	304	CDL	OA9-CA7-OA8-CA6
9	1	101	BCL	C16-C17-C18-C20
15	M	807	SPO	C3-C1-C4-C5
15	G	103	SPO	C2-C1-C4-C5
15	T	102	SPO	C3-C1-C4-C5
9	L	309	BCL	C4-C3-C5-C6
9	T	101	BCL	C4-C3-C5-C6
15	M	807	SPO	C34-C33-C35-C36
9	L	309	BCL	C6-C7-C8-C10
9	B	101	BCL	C6-C7-C8-C10
9	D	101	BCL	C6-C7-C8-C10
9	G	101	BCL	C2-C3-C5-C6
9	J	101	BCL	C11-C10-C8-C7
9	O	101	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
9	Q	104	BCL	C6-C7-C8-C10
9	Y	103	BCL	C11-C10-C8-C7
9	Z	101	BCL	C11-C10-C8-C7
9	5	102	BCL	C6-C7-C8-C10
9	6	101	BCL	C6-C7-C8-C10
9	7	101	BCL	C11-C10-C8-C7
9	8	102	BCL	C6-C7-C8-C10
10	M	804	BPH	C2-C3-C5-C6
15	M	807	SPO	C27-C28-C30-C31
9	A	703	BCL	C11-C10-C8-C9
9	P	102	BCL	C6-C7-C8-C9
9	Q	104	BCL	C6-C7-C8-C9
9	S	102	BCL	C6-C7-C8-C9
9	W	101	BCL	C6-C7-C8-C9
9	6	101	BCL	C11-C10-C8-C9
9	L	301	BCL	C13-C15-C16-C17
9	D	101	BCL	C15-C16-C17-C18
15	E	101	SPO	O1-C1-C4-C5
15	G	103	SPO	O1-C1-C4-C5
15	W	102	SPO	O1-C1-C4-C5
15	5	104	SPO	C10-C11-C12-C13
15	X	102	SPO	C5-C6-C7-C9
9	N	102	BCL	CBA-CGA-O2A-C1
16	A	701	LMT	C4-C5-C6-C7
9	G	101	BCL	C5-C6-C7-C8
9	O	101	BCL	C5-C6-C7-C8
9	Y	103	BCL	C13-C15-C16-C17
16	S	105	LMT	C2-C3-C4-C5
17	H	304	CDL	OA5-CA3-CA4-CA6
9	I	101	BCL	C5-C6-C7-C8
9	R	102	BCL	C4-C3-C5-C6
10	L	302	BPH	C4-C3-C5-C6
15	P	101	SPO	C34-C33-C35-C36
9	Q	104	BCL	C2-C3-C5-C6
9	T	101	BCL	C2-C3-C5-C6
15	M	807	SPO	C32-C33-C35-C36
16	I	102	LMT	O1'-C1-C2-C3
16	S	101	LMT	C3-C4-C5-C6
12	Y	104	PGV	C5-C6-C7-C8
9	V	101	BCL	C8-C10-C11-C12
9	S	102	BCL	CBA-CGA-O2A-C1
9	8	102	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	L	306	PGV	C2-C3-C4-C5
12	K	104	PGV	C14-C15-C16-C17
9	J	101	BCL	C15-C16-C17-C18
12	M	801	PGV	O03-C01-C02-C03
17	H	305	CDL	CA3-CA4-CA6-OA8
12	Y	104	PGV	O02-C1-O01-C02
12	H	306	PGV	C19-C20-C21-C22
16	S	101	LMT	C2-C3-C4-C5
9	L	301	BCL	C4-C3-C5-C6
9	R	102	BCL	C2-C3-C5-C6
12	K	104	PGV	C7-C8-C9-C10
17	Y	102	CDL	CA2-OA2-PA1-OA5
17	Y	102	CDL	C71-C72-C73-C74
12	M	801	PGV	O01-C02-C03-O11
12	Q	103	PGV	O01-C02-C03-O11
9	L	309	BCL	C16-C17-C18-C20
12	M	812	PGV	C4-C5-C6-C7
12	M	801	PGV	O03-C01-C02-O01
12	H	306	PGV	O03-C01-C02-O01
12	K	104	PGV	C26-C27-C28-C29
9	1	101	BCL	C13-C15-C16-C17
9	7	101	BCL	C8-C10-C11-C12
15	F	104	SPO	C33-C35-C36-C37
15	K	103	SPO	C33-C35-C36-C37
15	N	101	SPO	C28-C30-C31-C32
9	V	101	BCL	C2-C1-O2A-CGA
10	L	302	BPH	C2-C3-C5-C6
9	L	301	BCL	C11-C10-C8-C9
9	D	101	BCL	C6-C7-C8-C9
9	O	101	BCL	C6-C7-C8-C9
9	P	102	BCL	C11-C10-C8-C9
9	3	103	BCL	C11-C10-C8-C9
16	H	302	LMT	C5'-C4'-O1B-C1B
9	T	101	BCL	C16-C17-C18-C20
9	W	101	BCL	C16-C17-C18-C20
15	G	103	SPO	C10-C11-C12-C13
12	M	812	PGV	C23-C24-C25-C26
15	V	103	SPO	C10-C11-C12-C14
15	1	102	SPO	C10-C11-C12-C14
15	1	105	SPO	C15-C16-C17-C19
12	K	104	PGV	C15-C16-C17-C18
12	K	104	PGV	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
9	E	102	BCL	C16-C17-C18-C20
9	6	101	BCL	C16-C17-C18-C19
16	5	101	LMT	C5'-C4'-O1B-C1B
9	I	101	BCL	C15-C16-C17-C18
12	M	801	PGV	C01-C02-C03-O11
12	H	307	PGV	C01-C02-C03-O11
9	A	703	BCL	C11-C10-C8-C7
9	F	102	BCL	C6-C7-C8-C10
9	G	101	BCL	C11-C10-C8-C7
9	J	101	BCL	C6-C7-C8-C10
9	P	102	BCL	C11-C10-C8-C7
9	Q	104	BCL	C11-C10-C8-C7
9	S	102	BCL	C11-C12-C13-C15
9	W	101	BCL	C6-C7-C8-C10
9	1	101	BCL	C6-C7-C8-C10
9	3	103	BCL	C11-C10-C8-C7
9	5	102	BCL	C12-C13-C15-C16
9	7	101	BCL	C6-C7-C8-C10
9	N	102	BCL	O1A-CGA-O2A-C1
12	H	306	PGV	C2-C1-O01-C02
17	M	811	CDL	C13-C14-C15-C16
16	A	702	LMT	C3-C4-C5-C6
9	L	301	BCL	CAD-CBD-CGD-O2D
9	L	309	BCL	CAD-CBD-CGD-O2D
9	6	101	BCL	CAD-CBD-CGD-O2D
12	H	303	PGV	C20-C21-C22-C23
9	L	301	BCL	C10-C11-C12-C13
9	6	101	BCL	C16-C17-C18-C20
17	M	811	CDL	OB5-CB3-CB4-OB6
9	8	102	BCL	CAA-CBA-CGA-O2A
12	Y	104	PGV	O12-C04-C05-O05
17	Y	102	CDL	O1-C1-CB2-OB2
9	M	803	BCL	CHA-CBD-CGD-O1D
9	M	803	BCL	CHA-CBD-CGD-O2D
9	2	101	BCL	C5-C6-C7-C8
9	8	102	BCL	CBD-CGD-O2D-CED
9	S	102	BCL	O1A-CGA-O2A-C1
17	H	305	CDL	OA6-CA4-CA6-OA8
9	7	101	BCL	C3-C5-C6-C7
9	N	102	BCL	C4-C3-C5-C6
15	W	102	SPO	C34-C33-C35-C36
15	W	102	SPO	C32-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
12	H	306	PGV	O02-C1-O01-C02
12	H	303	PGV	C22-C23-C24-C25
17	H	304	CDL	C16-C17-C18-C19
17	M	811	CDL	C60-C61-C62-C63
15	1	102	SPO	C24-C23-C25-C26
16	A	702	LMT	O1'-C1-C2-C3
15	G	102	SPO	C10-C11-C12-C14
15	X	102	SPO	C10-C11-C12-C14
9	L	308	BCL	C1A-C2A-CAA-CBA
9	E	102	BCL	C1A-C2A-CAA-CBA
9	F	102	BCL	C1A-C2A-CAA-CBA
9	Q	104	BCL	C1A-C2A-CAA-CBA
9	L	301	BCL	C16-C17-C18-C19
9	M	803	BCL	C16-C17-C18-C19
9	5	102	BCL	C16-C17-C18-C19
9	W	101	BCL	C15-C16-C17-C18
17	H	304	CDL	CA3-OA5-PA1-OA2
17	Y	102	CDL	CB2-OB2-PB2-OB5
17	Y	102	CDL	CB3-OB5-PB2-OB2
12	H	306	PGV	O12-C04-C05-O05
11	L	303	U10	C12-C11-C9-C10
15	1	105	SPO	C34-C33-C35-C36
9	3	103	BCL	C13-C15-C16-C17
12	M	812	PGV	C02-C03-O11-P
17	H	304	CDL	CA4-CA3-OA5-PA1
12	L	305	PGV	C03-O11-P-O13
12	3	102	PGV	C04-O12-P-O14
17	M	811	CDL	CA2-OA2-PA1-OA4
17	M	811	CDL	CB2-OB2-PB2-OB3
17	H	304	CDL	CA2-OA2-PA1-OA4
17	H	304	CDL	CB3-OB5-PB2-OB3
9	8	102	BCL	O2A-C1-C2-C3
12	X	101	PGV	C01-C02-C03-O11
17	M	811	CDL	OB5-CB3-CB4-CB6
9	Y	103	BCL	C15-C16-C17-C18
12	H	306	PGV	C21-C22-C23-C24
9	E	102	BCL	C8-C10-C11-C12
15	M	807	SPO	C1-C4-C5-C6
12	X	101	PGV	C1-C2-C3-C4
12	M	812	PGV	O12-C04-C05-C06
9	R	102	BCL	C16-C17-C18-C19
9	L	301	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	L	301	BCL	C11-C10-C8-C7
9	L	308	BCL	C11-C10-C8-C7
9	M	803	BCL	C11-C10-C8-C7
9	I	101	BCL	C11-C12-C13-C15
9	S	102	BCL	C11-C10-C8-C7
9	V	101	BCL	C6-C7-C8-C10
9	8	102	BCL	C11-C10-C8-C7
12	X	101	PGV	O01-C02-C03-O11
12	X	101	PGV	C22-C23-C24-C25
13	Y	101	LDA	C3-C4-C5-C6
16	M	809	LMT	C3-C4-C5-C6
17	M	811	CDL	C38-C39-C40-C41
11	L	303	U10	C15-C14-C16-C17
9	L	309	BCL	C5-C6-C7-C8
9	L	309	BCL	C6-C7-C8-C9
9	E	102	BCL	C11-C10-C8-C9
9	F	102	BCL	C6-C7-C8-C9
9	Q	104	BCL	C11-C10-C8-C9
9	S	102	BCL	C11-C12-C13-C14
9	V	101	BCL	C6-C7-C8-C9
9	W	101	BCL	C11-C10-C8-C9
9	1	101	BCL	C6-C7-C8-C9
9	5	102	BCL	C14-C13-C15-C16
9	7	101	BCL	C6-C7-C8-C9
13	L	311	LDA	C11-C10-C9-C8
13	L	311	LDA	C6-C7-C8-C9
16	5	101	LMT	C6-C7-C8-C9
9	P	102	BCL	C15-C16-C17-C18
9	7	101	BCL	C13-C15-C16-C17
12	3	102	PGV	C13-C14-C15-C16
9	S	102	BCL	C10-C11-C12-C13
12	Y	104	PGV	C20-C21-C22-C23
16	U	102	LMT	C7-C8-C9-C10
9	L	301	BCL	C2A-CAA-CBA-CGA
9	7	101	BCL	C10-C11-C12-C13
9	S	102	BCL	C2-C1-O2A-CGA
16	H	302	LMT	O5'-C5'-C6'-O6'
17	M	811	CDL	C71-CB7-OB8-CB6
9	N	102	BCL	C2-C3-C5-C6
15	P	101	SPO	C32-C33-C35-C36
9	W	101	BCL	C10-C11-C12-C13
12	M	801	PGV	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
15	O	103	SPO	C3-C1-O1-CM1
10	M	804	BPH	C1-C2-C3-C5
12	L	305	PGV	C04-O12-P-O11
12	M	812	PGV	C04-O12-P-O11
12	H	307	PGV	C04-O12-P-O11
12	Q	103	PGV	C03-O11-P-O12
12	Q	103	PGV	C04-O12-P-O11
12	Y	104	PGV	C03-O11-P-O12
12	Y	104	PGV	C04-O12-P-O11
12	3	102	PGV	C03-O11-P-O12
12	X	101	PGV	C03-O11-P-O12
12	X	101	PGV	C04-O12-P-O11
17	Y	102	CDL	CA3-OA5-PA1-OA2
12	3	102	PGV	C21-C22-C23-C24
15	M	807	SPO	C2-C1-C4-C5
15	O	102	SPO	C2-C1-C4-C5
15	3	104	SPO	C3-C1-C4-C5
9	A	703	BCL	C10-C11-C12-C13
12	Q	103	PGV	O03-C01-C02-C03
9	2	101	BCL	C4-C3-C5-C6
9	D	101	BCL	C11-C10-C8-C7
9	W	101	BCL	C11-C12-C13-C15
9	4	101	BCL	C6-C7-C8-C10
9	I	101	BCL	C11-C12-C13-C14
9	J	101	BCL	C6-C7-C8-C9
9	S	102	BCL	C11-C10-C8-C9
9	3	103	BCL	C6-C7-C8-C9
9	5	102	BCL	C6-C7-C8-C9
15	P	101	SPO	C25-C26-C27-C28
17	M	811	CDL	C73-C74-C75-C76
15	M	807	SPO	O1-C1-C4-C5
15	N	101	SPO	C22-C23-C25-C26
15	S	104	SPO	C10-C11-C12-C14
9	3	103	BCL	C8-C10-C11-C12
17	M	811	CDL	OB9-CB7-OB8-CB6
9	L	309	BCL	C2-C3-C5-C6
17	M	811	CDL	C31-CA7-OA8-CA6
15	R	101	SPO	C28-C30-C31-C32
9	T	101	BCL	C3-C5-C6-C7
11	L	303	U10	C25-C24-C26-C27
17	Y	102	CDL	C34-C35-C36-C37
12	H	307	PGV	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
9	F	102	BCL	C3A-C2A-CAA-CBA
9	Q	104	BCL	C3A-C2A-CAA-CBA
9	Z	101	BCL	C16-C17-C18-C19
16	M	809	LMT	C7-C8-C9-C10
11	L	303	U10	C13-C14-C16-C17
9	N	102	BCL	CAA-CBA-CGA-O2A
9	P	102	BCL	C14-C13-C15-C16
9	V	101	BCL	C14-C13-C15-C16
9	4	101	BCL	C11-C10-C8-C9
12	Y	104	PGV	C19-C20-C21-C22
17	H	304	CDL	C52-C53-C54-C55
16	1	104	LMT	C1-C2-C3-C4
9	B	101	BCL	C15-C16-C17-C18
9	R	102	BCL	C16-C17-C18-C20
10	L	302	BPH	O2A-C1-C2-C3
16	M	810	LMT	C3-C4-C5-C6
9	3	103	BCL	C1A-C2A-CAA-CBA
9	F	102	BCL	C11-C12-C13-C15
9	G	101	BCL	C6-C7-C8-C10
9	8	102	BCL	O1D-CGD-O2D-CED
17	M	811	CDL	OA9-CA7-OA8-CA6
9	K	102	BCL	C13-C15-C16-C17
9	Q	104	BCL	C13-C15-C16-C17
9	7	101	BCL	C16-C17-C18-C19
17	H	304	CDL	CA5-C11-C12-C13
12	H	306	PGV	C7-C8-C9-C10
9	I	101	BCL	C4-C3-C5-C6
9	Y	103	BCL	C4-C3-C5-C6
12	H	307	PGV	C1-C2-C3-C4
12	L	310	PGV	C22-C23-C24-C25
17	H	304	CDL	C14-C15-C16-C17
16	M	809	LMT	C1-C2-C3-C4
9	E	102	BCL	O1D-CGD-O2D-CED
15	R	101	SPO	C1-C4-C5-C6
16	F	101	LMT	C1-C2-C3-C4
9	5	102	BCL	C10-C11-C12-C13
12	Y	104	PGV	O12-C04-C05-C06
9	A	703	BCL	C2-C1-O2A-CGA
9	B	101	BCL	C2-C1-O2A-CGA
9	D	101	BCL	C2-C1-O2A-CGA
9	Q	104	BCL	C2-C1-O2A-CGA
11	L	303	U10	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
9	Q	104	BCL	O1A-CGA-O2A-C1
11	L	303	U10	C21-C22-C23-C24
12	3	102	PGV	O03-C19-C20-C21
17	M	811	CDL	O1-C1-CB2-OB2
12	L	310	PGV	C29-C30-C31-C32
12	M	801	PGV	C22-C23-C24-C25
15	O	103	SPO	C12-C14-C15-C16
9	A	703	BCL	C4-C3-C5-C6
9	Z	101	BCL	C4-C3-C5-C6
15	G	103	SPO	C10-C11-C12-C14
15	O	103	SPO	C5-C6-C7-C9
9	P	102	BCL	C16-C17-C18-C19
9	2	101	BCL	C2-C3-C5-C6
11	L	303	U10	C12-C11-C9-C8
9	L	309	BCL	C3-C5-C6-C7
11	L	303	U10	C11-C12-C13-C14
9	Y	103	BCL	C2A-CAA-CBA-CGA
17	M	811	CDL	C61-C62-C63-C64
9	5	102	BCL	C3-C5-C6-C7
9	1	101	BCL	C4-C3-C5-C6
11	L	304	U10	C9-C11-C12-C13
16	A	702	LMT	C7-C8-C9-C10
17	H	304	CDL	C17-C18-C19-C20
10	M	804	BPH	C1-C2-C3-C4
15	O	103	SPO	C25-C26-C27-C28
9	Q	104	BCL	CBA-CGA-O2A-C1
16	X	105	LMT	C4-C5-C6-C7
15	F	103	SPO	C34-C33-C35-C36
15	P	101	SPO	C29-C28-C30-C31
15	T	102	SPO	C34-C33-C35-C36
12	Y	104	PGV	C2-C3-C4-C5
16	M	809	LMT	C6-C7-C8-C9
9	A	703	BCL	C2-C3-C5-C6
15	1	105	SPO	C32-C33-C35-C36
12	H	303	PGV	C7-C8-C9-C10
9	M	803	BCL	C11-C10-C8-C9
9	O	101	BCL	C11-C10-C8-C9
9	Q	104	BCL	C14-C13-C15-C16
9	4	101	BCL	C11-C12-C13-C14
9	8	102	BCL	C11-C10-C8-C9
9	O	101	BCL	C3-C5-C6-C7
9	E	102	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	3	103	BCL	C3A-C2A-CAA-CBA
12	M	801	PGV	C9-C10-C11-C12
12	K	104	PGV	C9-C10-C11-C12
16	H	302	LMT	O1'-C1-C2-C3
12	M	801	PGV	O02-C1-O01-C02
16	3	101	LMT	C5-C6-C7-C8
12	H	306	PGV	C23-C24-C25-C26
15	G	102	SPO	C29-C28-C30-C31
16	M	810	LMT	O5'-C1'-O1'-C1
9	I	101	BCL	C2-C3-C5-C6
9	Y	103	BCL	C2-C3-C5-C6
15	5	104	SPO	C10-C11-C12-C14
17	M	811	CDL	C11-C12-C13-C14
12	H	307	PGV	O03-C01-C02-C03
12	L	305	PGV	O01-C02-C03-O11
17	Y	102	CDL	OB5-CB3-CB4-OB6
9	O	101	BCL	C8-C10-C11-C12
12	M	801	PGV	O01-C1-C2-C3
12	H	307	PGV	C22-C23-C24-C25
9	E	102	BCL	O2A-C1-C2-C3
17	H	305	CDL	OA9-CA7-OA8-CA6
16	S	105	LMT	C4'-C5'-C6'-O6'
16	A	702	LMT	C5-C6-C7-C8
9	Z	101	BCL	C16-C17-C18-C20
9	D	101	BCL	O1D-CGD-O2D-CED
12	L	306	PGV	C6-C7-C8-C9
17	M	811	CDL	C63-C64-C65-C66
9	L	308	BCL	CHA-CBD-CGD-O1D
9	L	308	BCL	CHA-CBD-CGD-O2D
9	J	101	BCL	CHA-CBD-CGD-O1D
9	J	101	BCL	CHA-CBD-CGD-O2D
9	7	101	BCL	CHA-CBD-CGD-O1D
13	L	307	LDA	C2-C1-N1-CM1
13	L	307	LDA	C2-C1-N1-CM2
15	O	103	SPO	C2-C1-O1-CM1
15	P	101	SPO	C3-C1-O1-CM1
15	T	102	SPO	C3-C1-O1-CM1
12	M	812	PGV	O03-C01-C02-O01
9	P	102	BCL	C10-C11-C12-C13
10	M	804	BPH	CHA-CBD-CGD-O1D
9	Z	101	BCL	C2-C3-C5-C6
15	G	102	SPO	C27-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
16	3	101	LMT	C5'-C4'-O1B-C1B
12	H	306	PGV	C9-C10-C11-C12
9	W	101	BCL	CAA-CBA-CGA-O2A
12	K	104	PGV	O03-C19-C20-C21
9	L	301	BCL	C6-C7-C8-C9
9	G	101	BCL	C6-C7-C8-C9
9	K	102	BCL	C11-C12-C13-C14
9	N	102	BCL	C11-C10-C8-C9
15	F	103	SPO	C17-C19-C20-C21
15	N	101	SPO	C25-C26-C27-C28
17	Y	102	CDL	C73-C74-C75-C76
12	M	801	PGV	O02-C1-C2-C3
12	M	812	PGV	O01-C1-C2-C3
15	5	104	SPO	C5-C6-C7-C8
9	1	101	BCL	C2-C3-C5-C6
12	X	101	PGV	C25-C26-C27-C28
15	R	101	SPO	C10-C11-C12-C14
15	5	104	SPO	C5-C6-C7-C9
17	H	305	CDL	C31-CA7-OA8-CA6
16	M	810	LMT	C2B-C1B-O1B-C4'
9	O	101	BCL	C1A-C2A-CAA-CBA
12	K	104	PGV	O04-C19-C20-C21
16	S	101	LMT	C1-C2-C3-C4
16	M	810	LMT	C5'-C4'-O1B-C1B
15	O	102	SPO	C29-C28-C30-C31
12	H	306	PGV	C04-O12-P-O13
12	Q	103	PGV	C04-O12-P-O13
12	X	101	PGV	C04-O12-P-O13
13	M	802	LDA	C6-C7-C8-C9
12	L	310	PGV	O03-C19-C20-C21
9	7	101	BCL	C16-C17-C18-C20
12	H	306	PGV	O03-C19-C20-C21
9	I	101	BCL	C13-C15-C16-C17
12	3	102	PGV	C22-C23-C24-C25
16	S	101	LMT	O1'-C1-C2-C3
16	U	102	LMT	C9-C10-C11-C12
11	L	304	U10	C2-C3-O3-C3M
11	L	303	U10	C16-C17-C18-C19
9	O	101	BCL	CAD-CBD-CGD-O1D
12	L	306	PGV	O01-C1-C2-C3
9	N	102	BCL	C6-C7-C8-C9
12	L	310	PGV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
17	Y	102	CDL	C72-C73-C74-C75
16	Q	102	LMT	C1-C2-C3-C4
9	V	101	BCL	O1A-CGA-O2A-C1
9	5	102	BCL	C13-C15-C16-C17
16	A	701	LMT	C9-C10-C11-C12
9	O	101	BCL	C4-C3-C5-C6
9	L	301	BCL	C6-C7-C8-C10
9	N	102	BCL	C11-C10-C8-C7
9	O	101	BCL	C3A-C2A-CAA-CBA
10	M	804	BPH	C6-C7-C8-C10
12	L	310	PGV	C19-C20-C21-C22
9	2	101	BCL	CAA-CBA-CGA-O2A
16	X	105	LMT	C3-C4-C5-C6
15	3	104	SPO	C11-C10-C9-C7
12	K	104	PGV	C24-C25-C26-C27
9	P	102	BCL	C16-C17-C18-C20
9	L	309	BCL	CAA-CBA-CGA-O2A
11	L	304	U10	C4-C3-O3-C3M
16	A	701	LMT	C5-C6-C7-C8
12	M	812	PGV	O02-C1-C2-C3
12	H	306	PGV	O04-C19-C20-C21
15	S	104	SPO	C28-C30-C31-C32
9	W	101	BCL	C5-C6-C7-C8
9	8	102	BCL	CAA-CBA-CGA-O1A
12	3	102	PGV	C24-C25-C26-C27

There are no ring outliers.

97 monomers are involved in 363 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	104	SPO	2	0
15	V	102	SPO	4	0
9	S	102	BCL	6	0
12	L	310	PGV	1	0
15	X	102	SPO	5	0
15	1	102	SPO	3	0
9	4	101	BCL	5	0
9	F	102	BCL	4	0
9	K	102	BCL	7	0
9	O	101	BCL	6	0
17	Y	102	CDL	2	0
15	5	103	SPO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	M	811	CDL	6	0
13	L	311	LDA	2	0
15	E	101	SPO	3	0
16	A	702	LMT	6	0
11	L	304	U10	4	0
9	T	101	BCL	5	0
12	M	801	PGV	2	0
9	M	803	BCL	3	0
10	M	804	BPH	6	0
15	R	101	SPO	5	0
9	L	308	BCL	6	0
15	S	104	SPO	5	0
12	L	306	PGV	3	0
12	Q	103	PGV	1	0
15	K	103	SPO	7	0
12	H	307	PGV	3	0
15	F	104	SPO	3	0
9	3	103	BCL	4	0
15	V	103	SPO	5	0
16	H	302	LMT	4	0
9	D	101	BCL	6	0
9	8	102	BCL	7	0
9	Z	101	BCL	4	0
9	W	101	BCL	8	0
12	X	101	PGV	3	0
15	T	102	SPO	10	0
15	G	102	SPO	8	0
9	1	101	BCL	6	0
9	E	102	BCL	8	0
16	M	810	LMT	2	0
16	U	102	LMT	2	0
11	M	806	U10	1	0
12	Y	104	PGV	7	0
15	1	105	SPO	6	0
9	7	101	BCL	6	0
15	O	103	SPO	5	0
9	P	102	BCL	4	0
9	B	101	BCL	9	0
17	H	304	CDL	6	0
15	S	103	SPO	6	0
9	J	101	BCL	4	0
15	N	101	SPO	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	309	BCL	5	0
15	1	103	SPO	4	0
16	A	701	LMT	1	0
16	K	101	LMT	2	0
16	Q	101	LMT	3	0
15	F	103	SPO	5	0
9	R	102	BCL	4	0
13	Y	101	LDA	5	0
12	L	305	PGV	4	0
16	3	101	LMT	3	0
12	K	104	PGV	3	0
9	Q	104	BCL	1	0
10	L	302	BPH	5	0
9	G	101	BCL	4	0
16	5	101	LMT	2	0
15	8	101	SPO	5	0
15	G	103	SPO	8	0
9	I	101	BCL	9	0
9	N	102	BCL	2	0
16	S	105	LMT	1	0
15	D	102	SPO	4	0
9	V	101	BCL	9	0
9	Y	103	BCL	7	0
12	H	306	PGV	3	0
12	M	812	PGV	4	0
15	O	102	SPO	8	0
9	5	102	BCL	6	0
9	L	301	BCL	6	0
16	Q	102	LMT	1	0
15	M	807	SPO	4	0
9	A	703	BCL	2	0
15	P	101	SPO	2	0
16	S	101	LMT	1	0
16	M	809	LMT	2	0
16	M	808	LMT	2	0
9	2	101	BCL	5	0
12	3	102	PGV	1	0
13	X	103	LDA	2	0
16	H	301	LMT	1	0
9	6	101	BCL	5	0
11	L	303	U10	3	0
15	W	102	SPO	4	0

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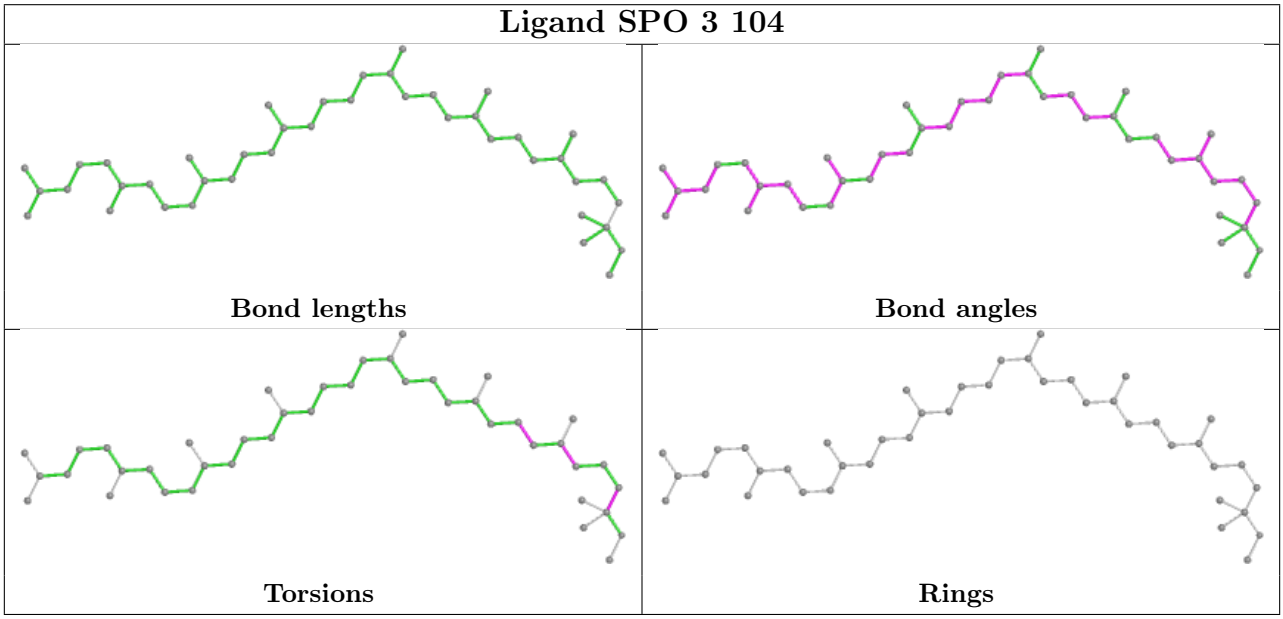
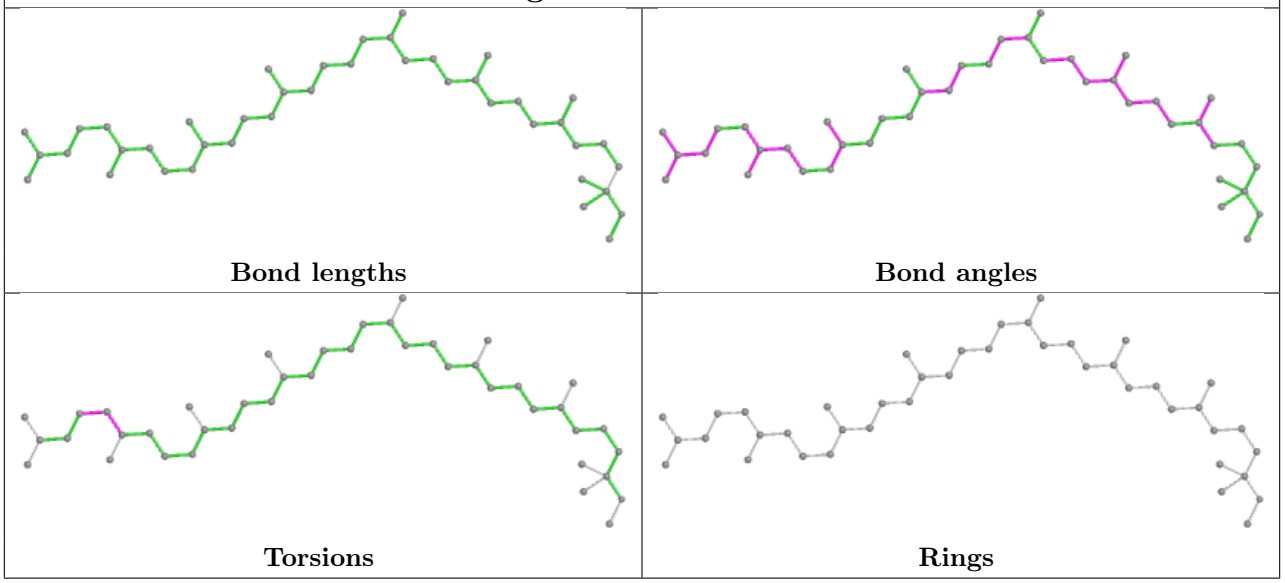
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	5	104	SPO	7	0

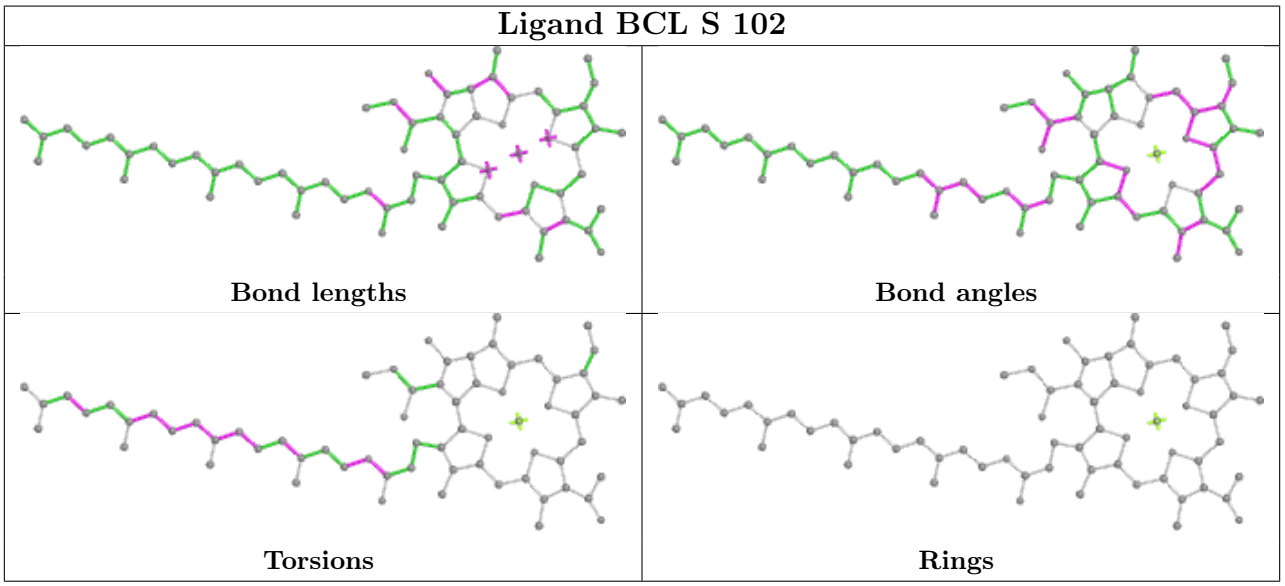
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



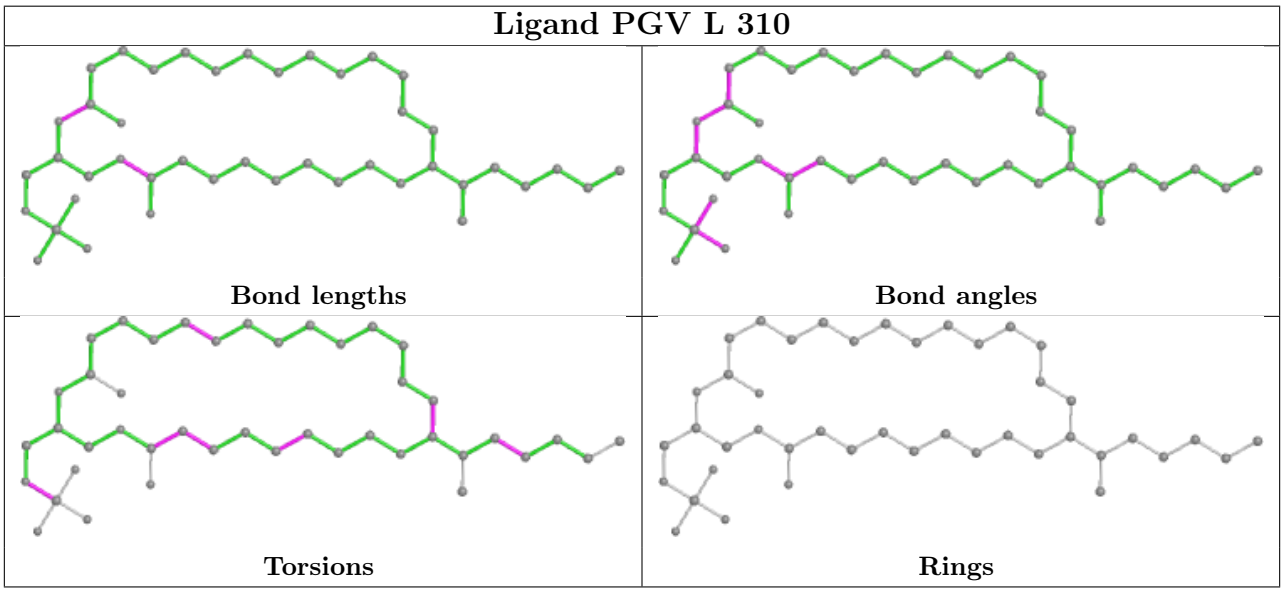
Ligand SPO V 102



Ligand BCL S 102



Ligand PGV L 310



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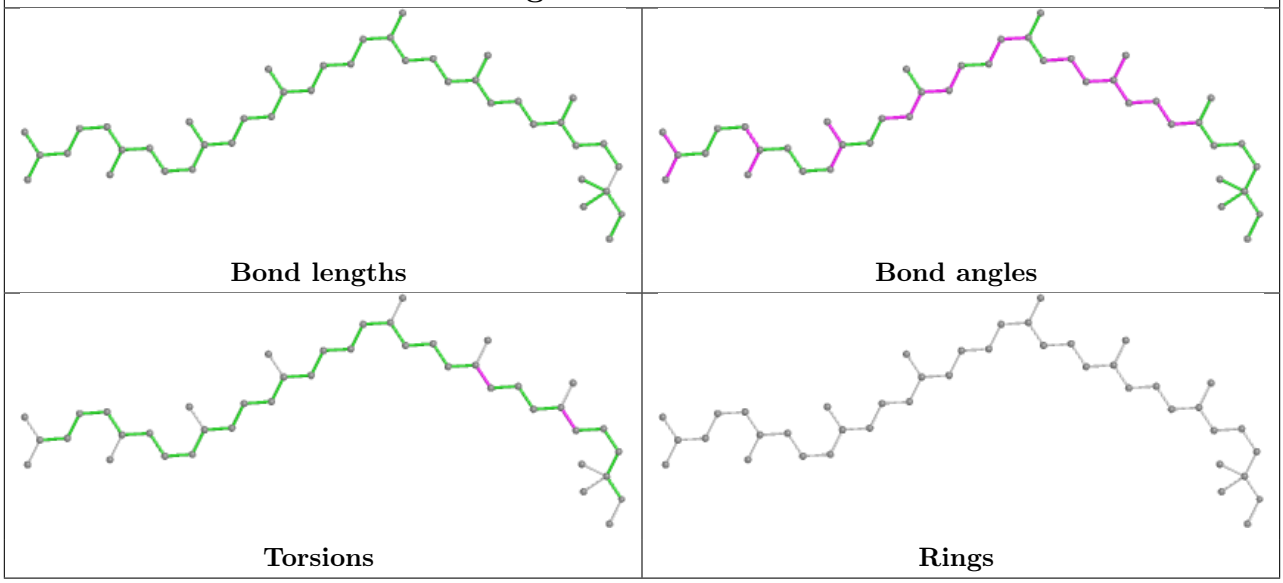

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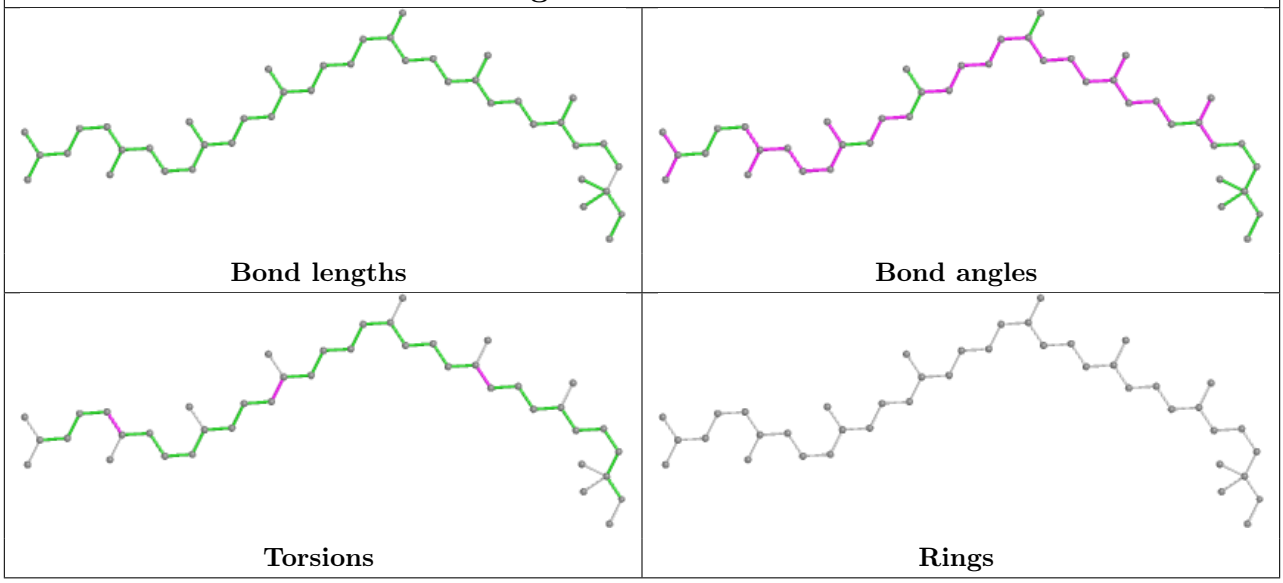
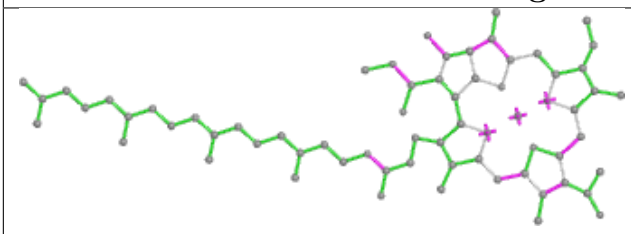
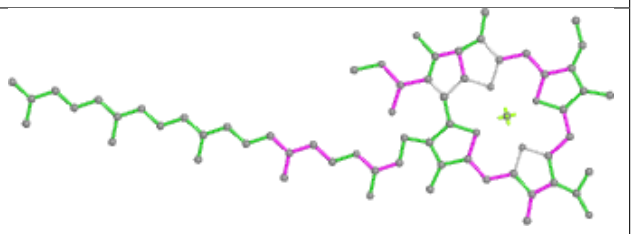


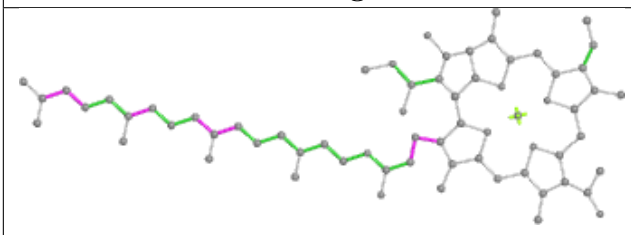
Ligand BCL 4 101



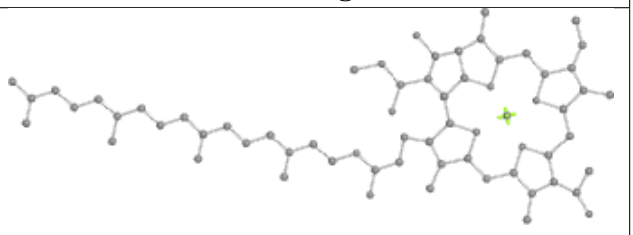
Bond lengths



Bond angles

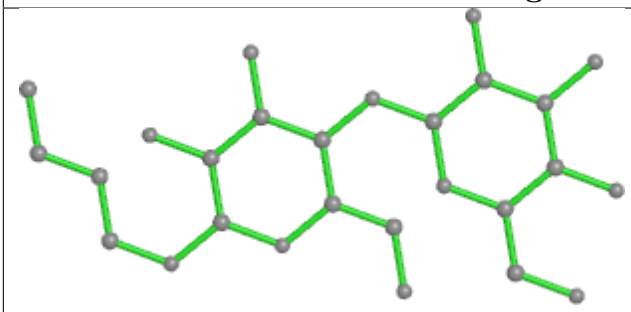


Torsions

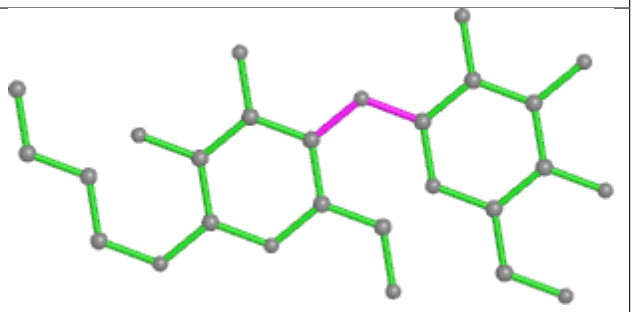


Rings

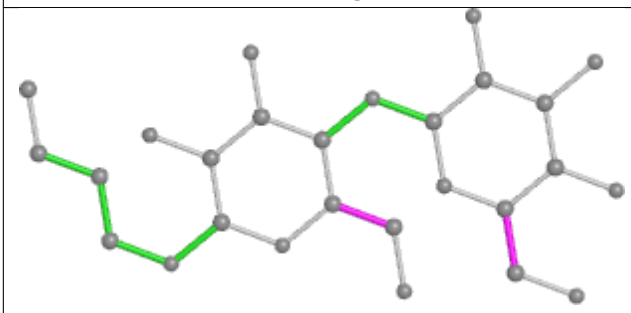
Ligand LMT 4 102



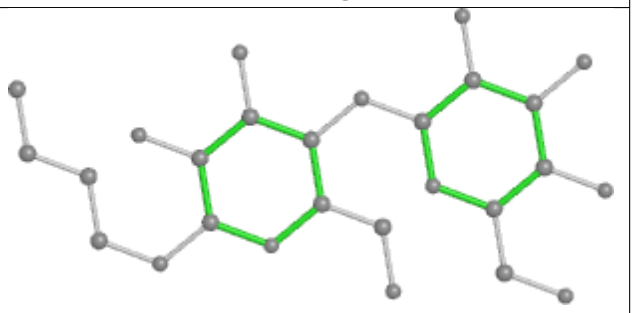
Bond lengths



Bond angles

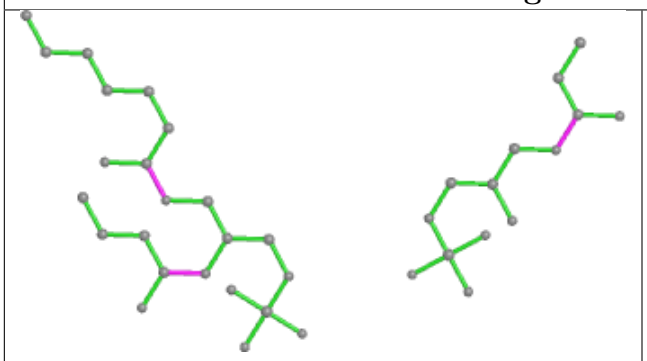


Torsions

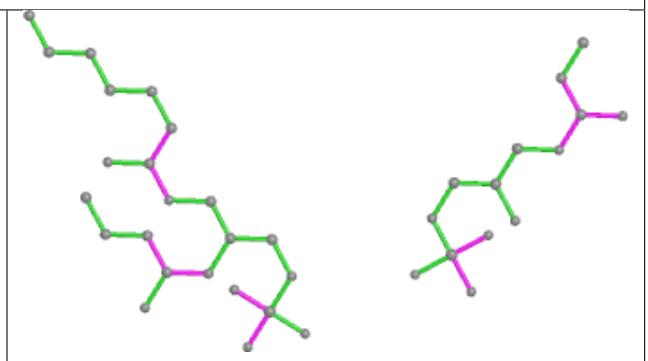


Rings

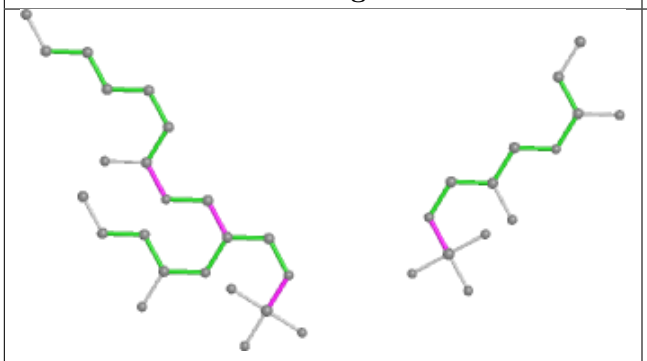
Ligand CDL H 305



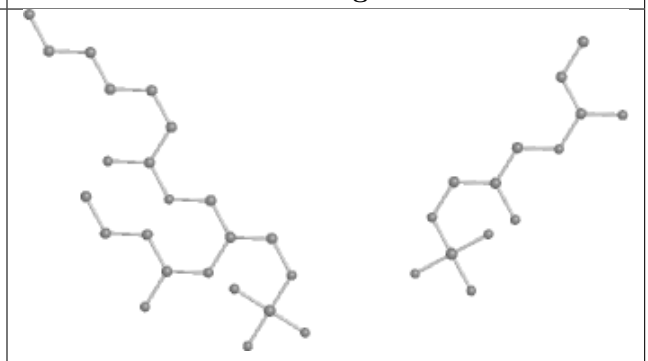
Bond lengths



Bond angles

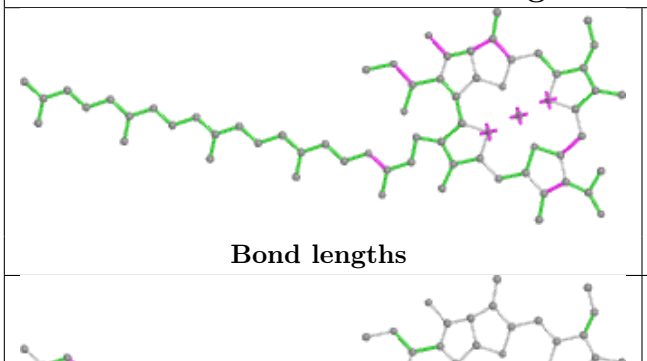


Torsions

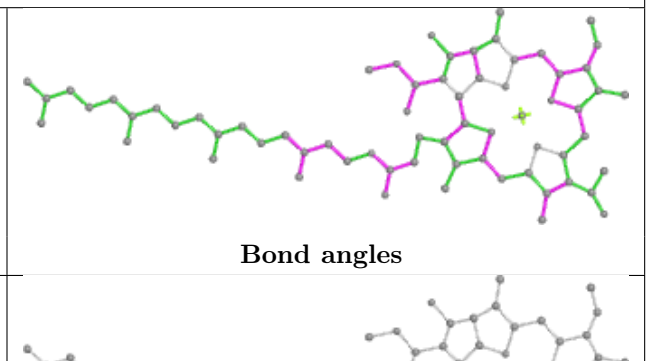


Rings

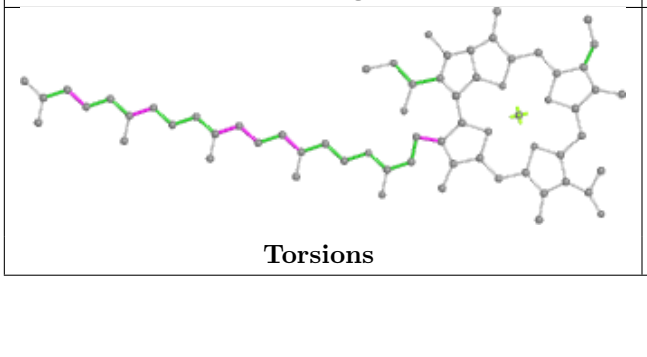
Ligand BCL F 102



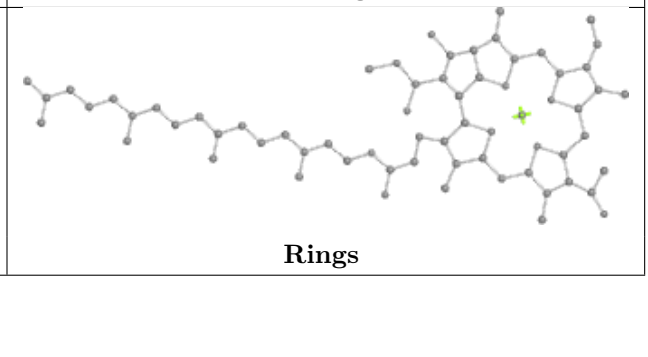
Bond lengths



Bond angles

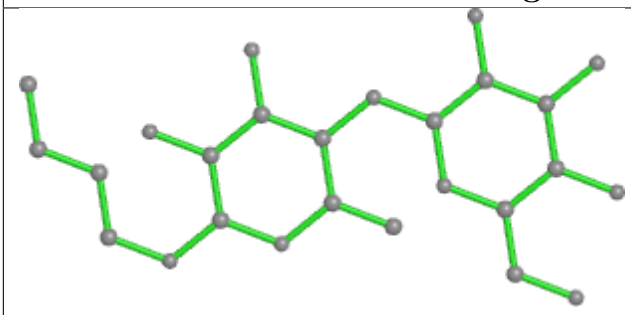


Torsions

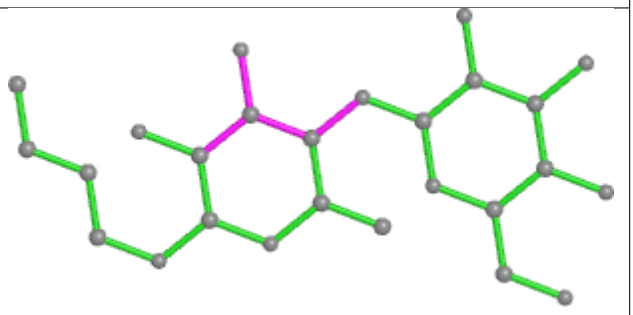


Rings

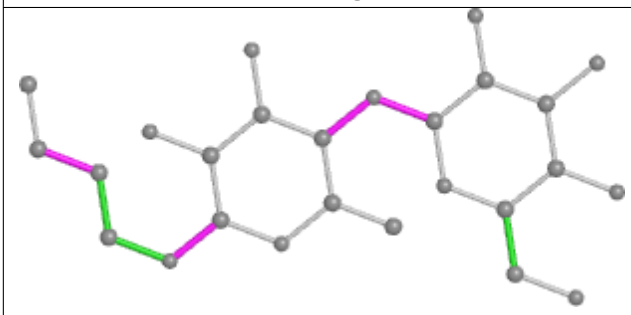
Ligand LMT F 101



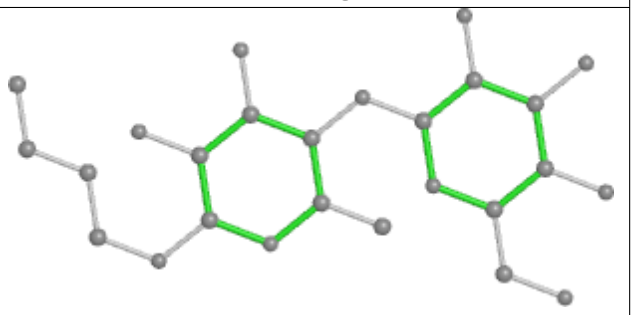
Bond lengths



Bond angles

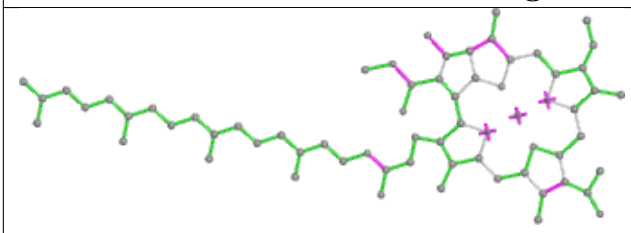


Torsions

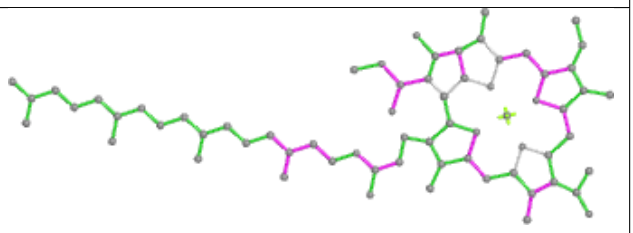


Rings

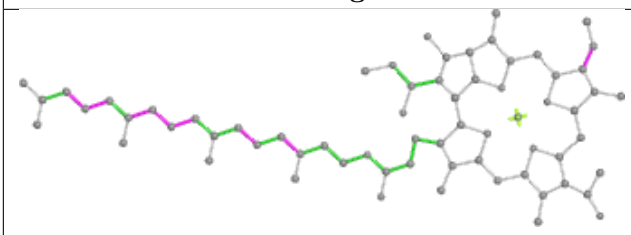
Ligand BCL K 102



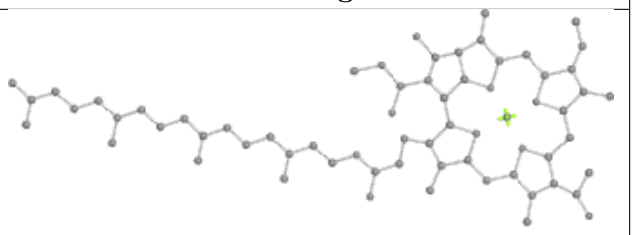
Bond lengths



Bond angles

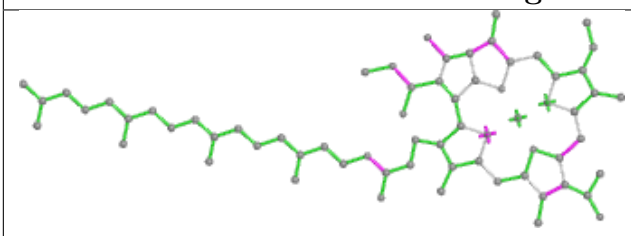


Torsions

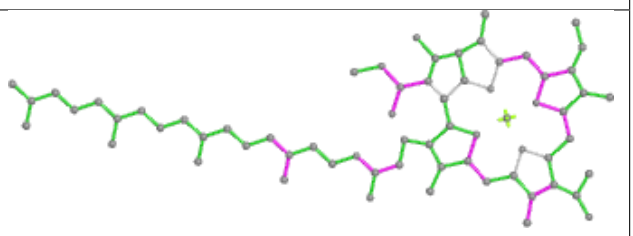


Rings

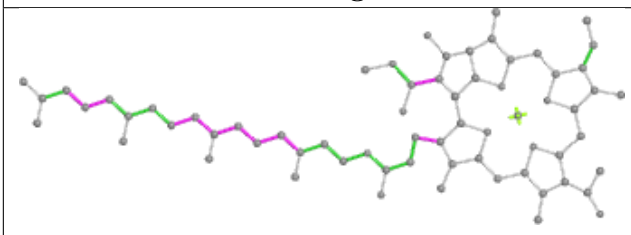
Ligand BCL O 101



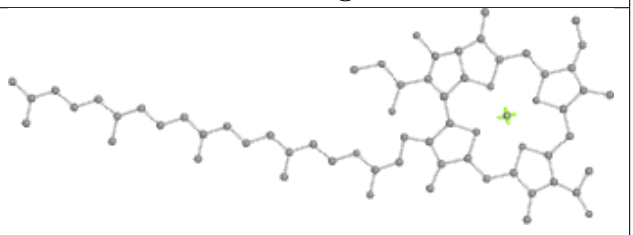
Bond lengths



Bond angles

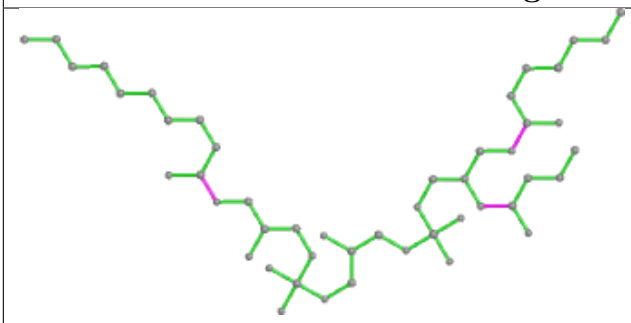


Torsions

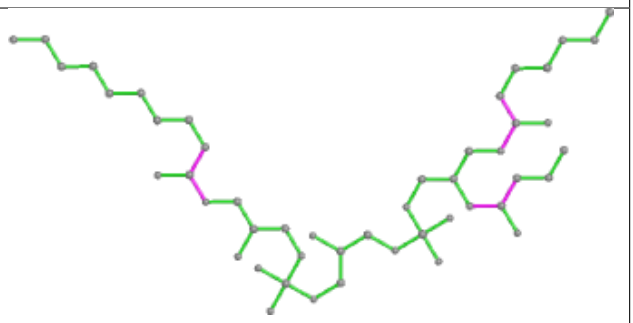


Rings

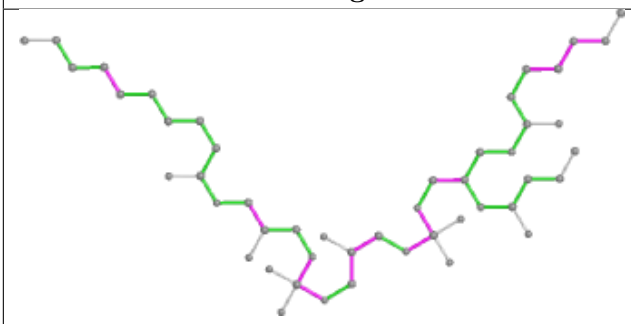
Ligand CDL Y 102



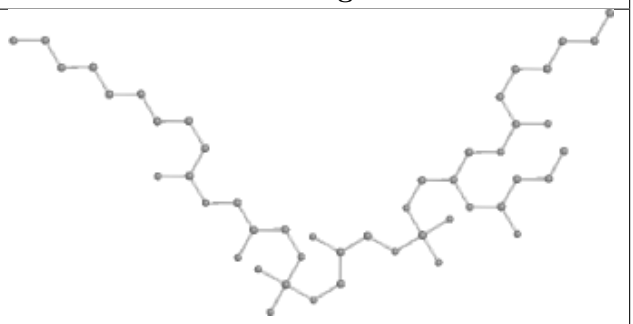
Bond lengths



Bond angles

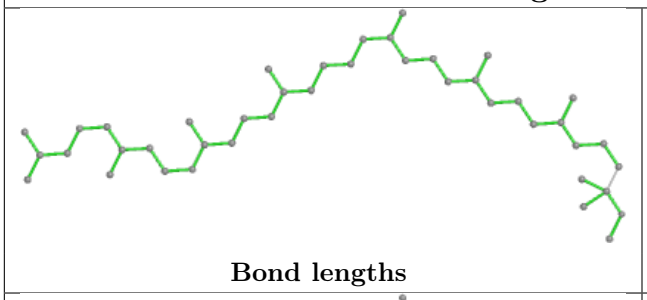


Torsions

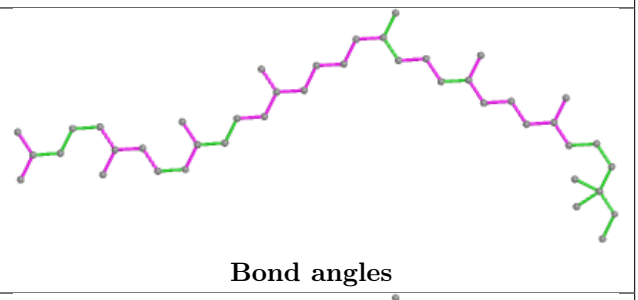


Rings

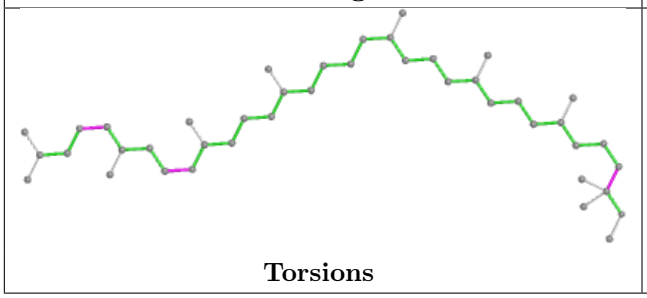
Ligand SPO 5 103



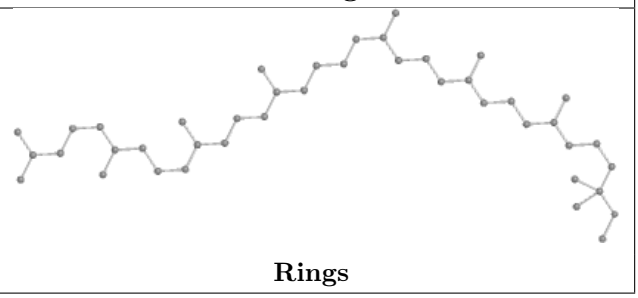
Bond lengths



Bond angles

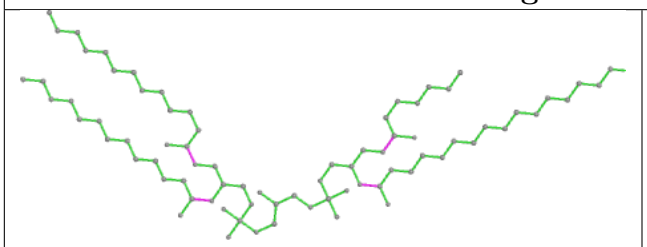


Torsions

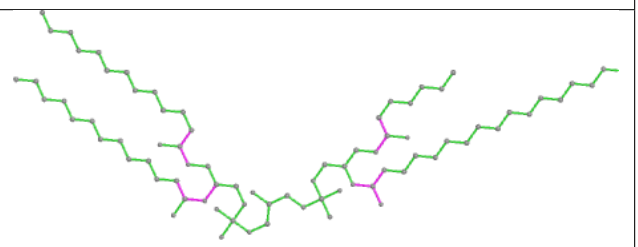


Rings

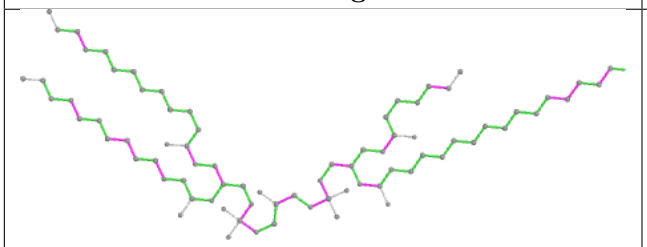
Ligand CDL M 811



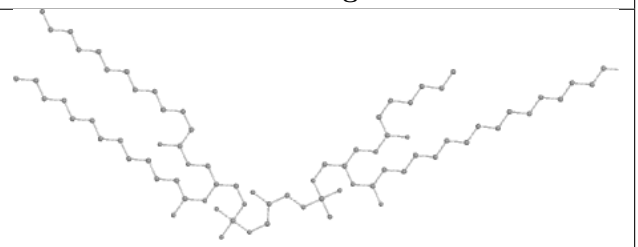
Bond lengths



Bond angles

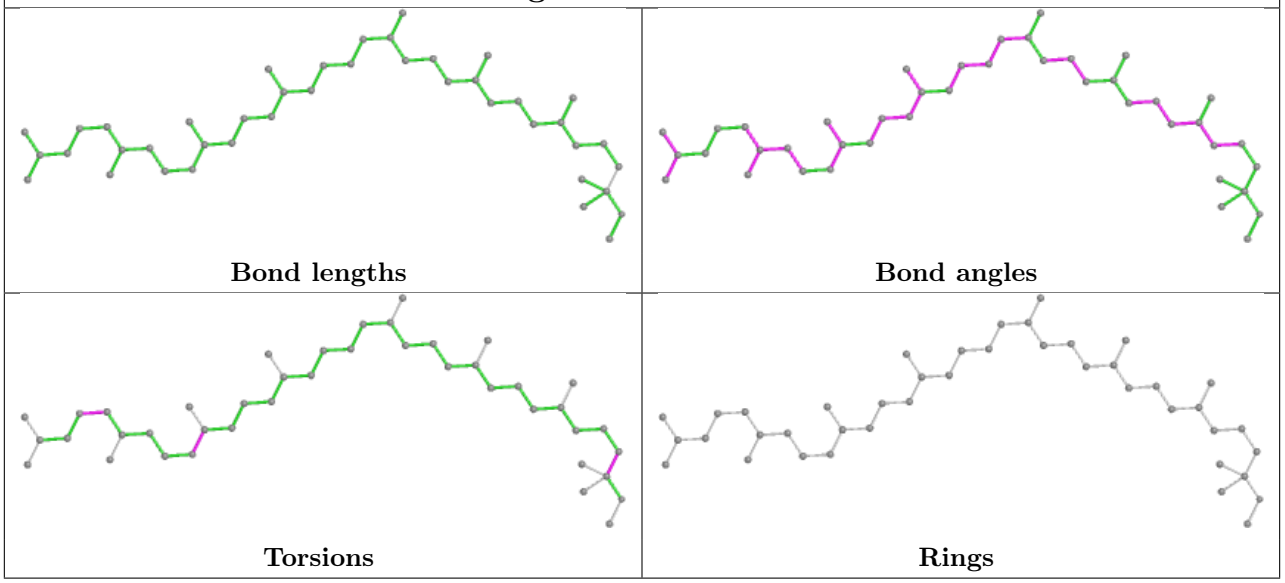


Torsions

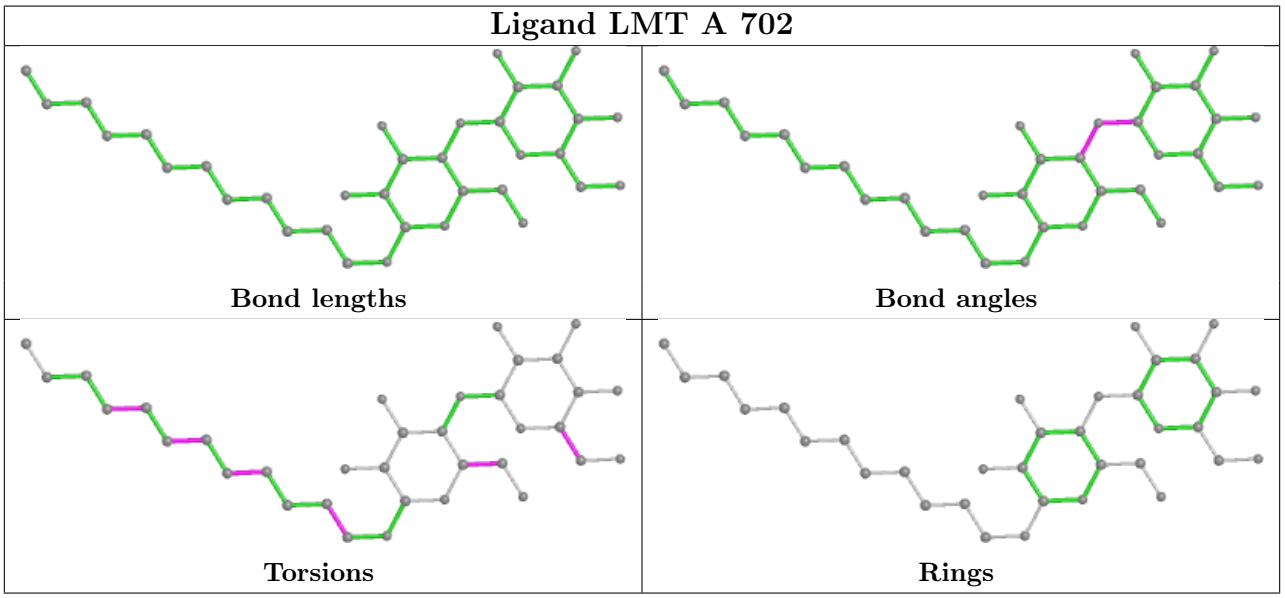


Rings

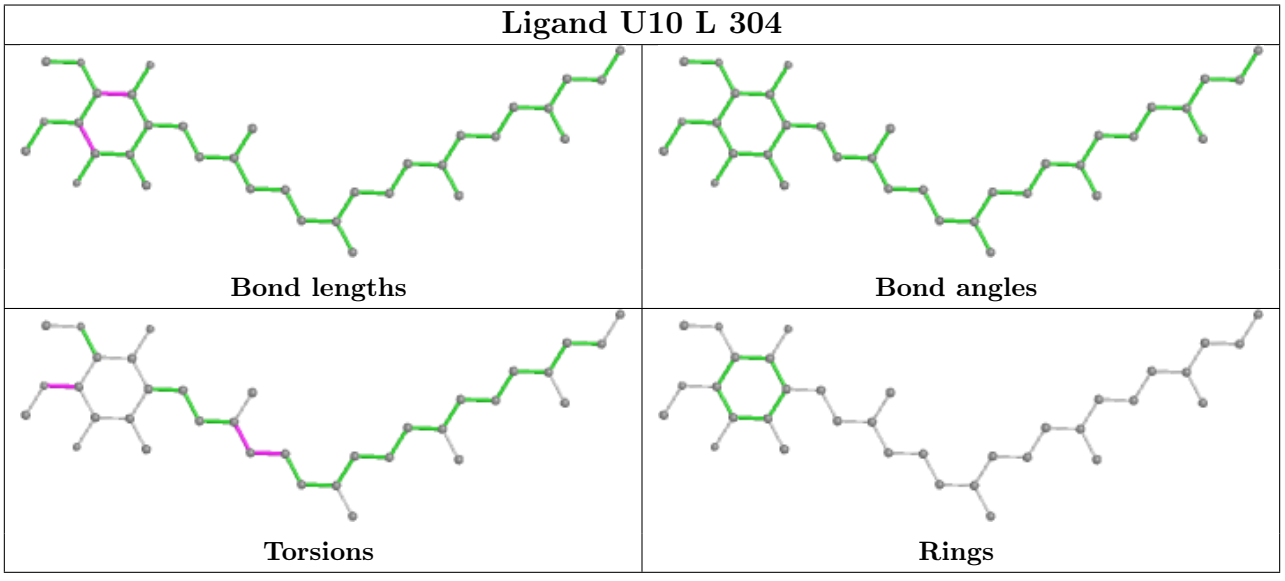
Ligand SPO E 101



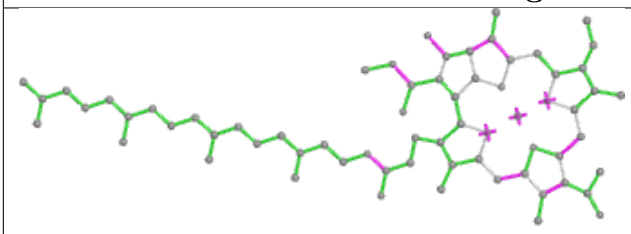
Ligand LMT A 702



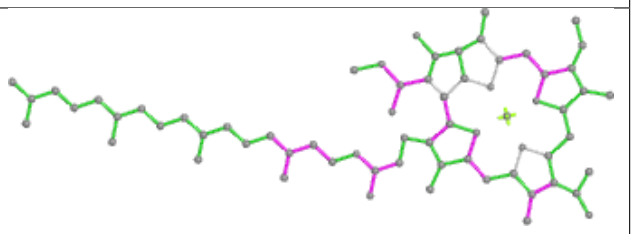
Ligand U10 L 304



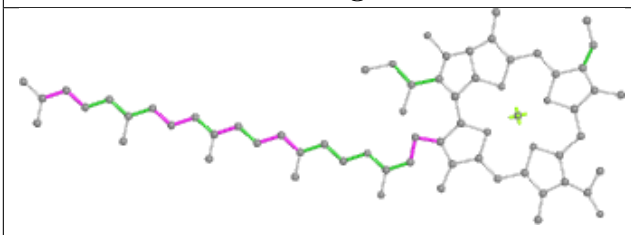
Ligand BCL T 101



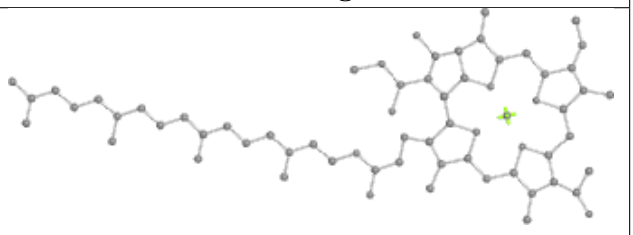
Bond lengths



Bond angles

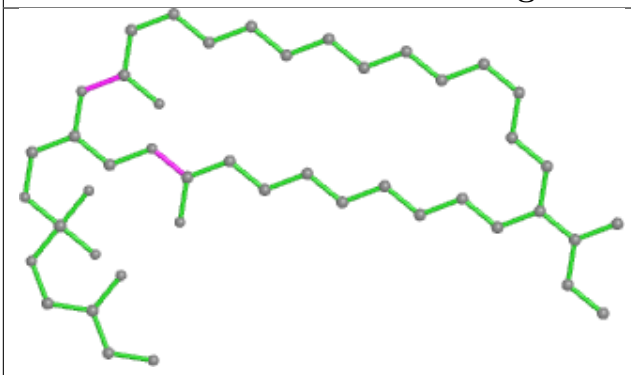


Torsions

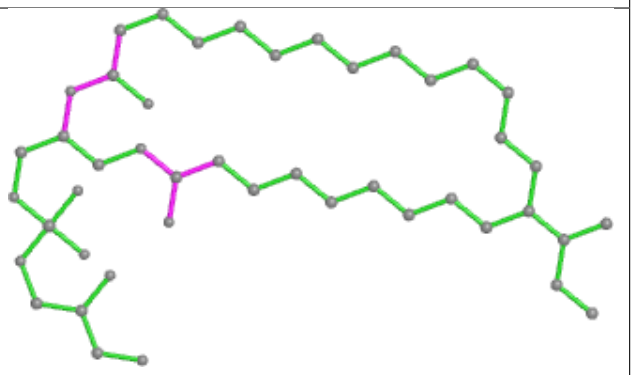


Rings

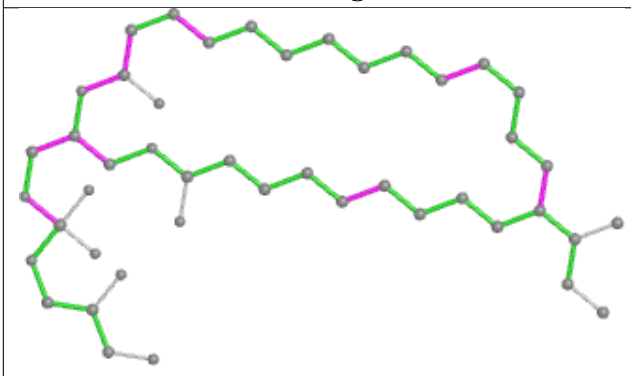
Ligand PGV M 801



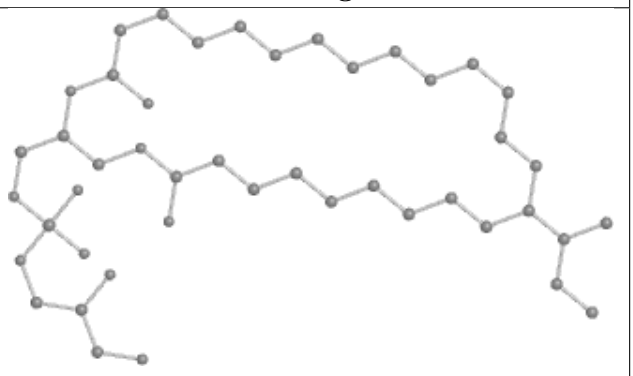
Bond lengths



Bond angles

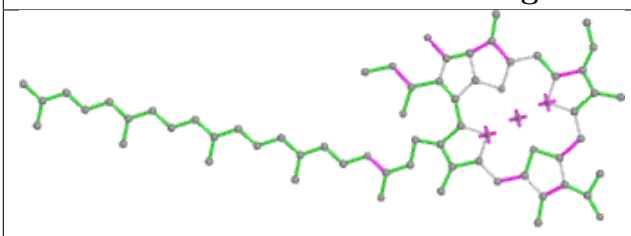


Torsions

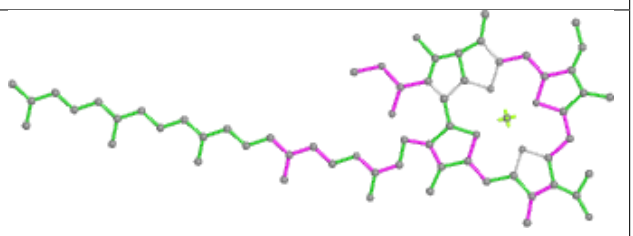


Rings

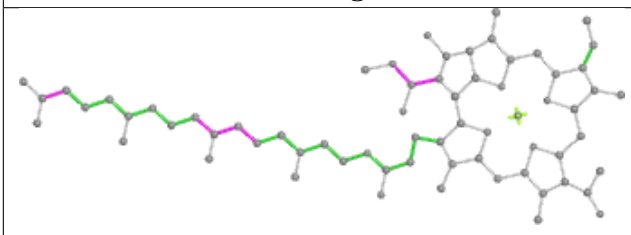
Ligand BCL M 803



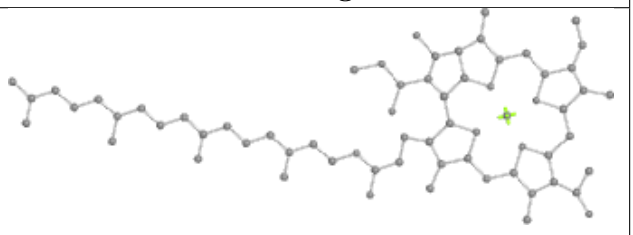
Bond lengths



Bond angles

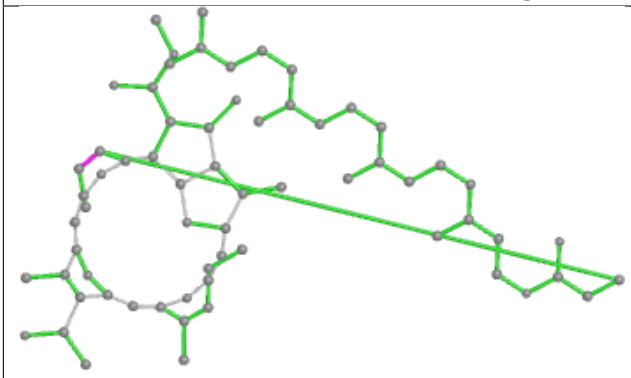


Torsions

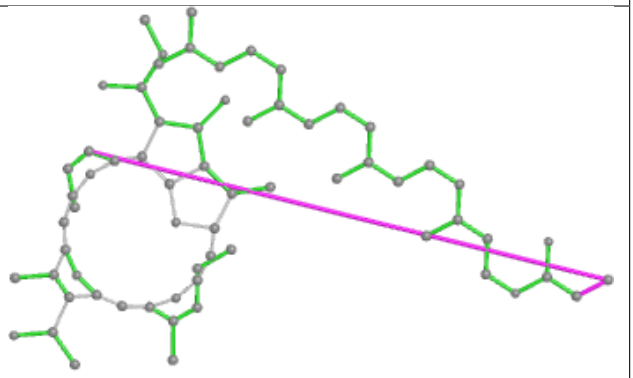


Rings

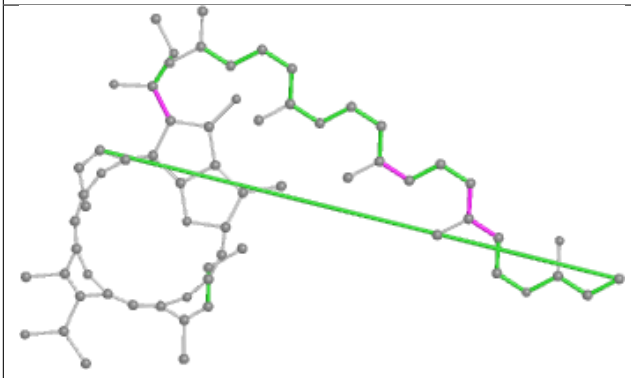
Ligand BPH M 804



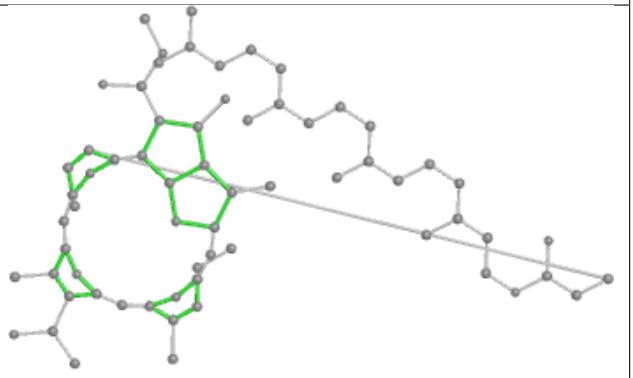
Bond lengths



Bond angles

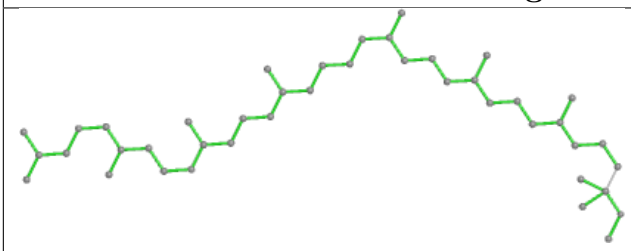


Torsions

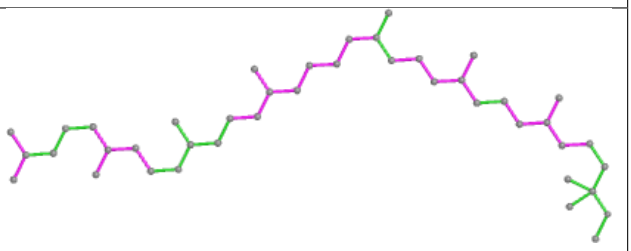


Rings

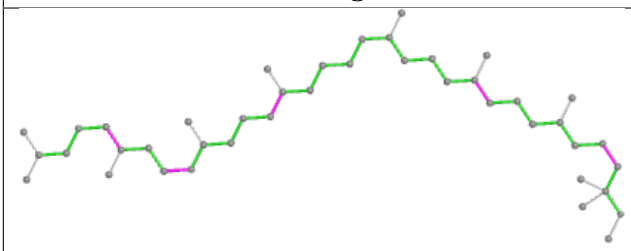
Ligand SPO R 101



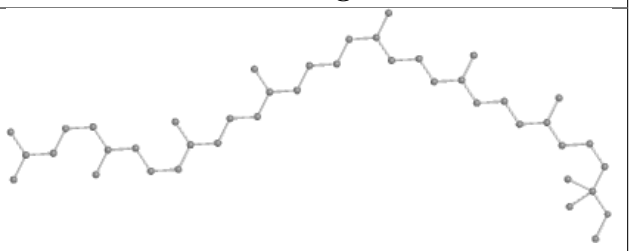
Bond lengths



Bond angles

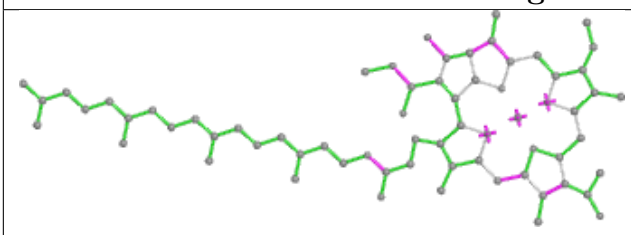


Torsions

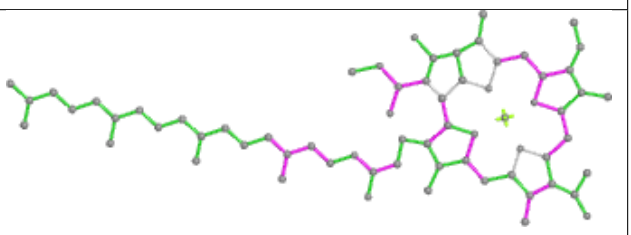


Rings

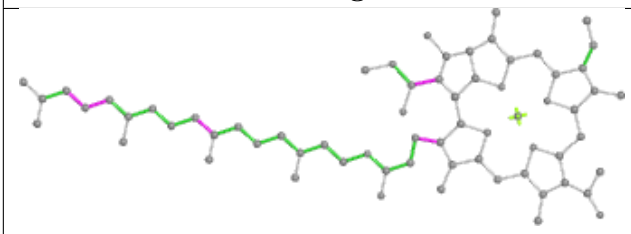
Ligand BCL L 308



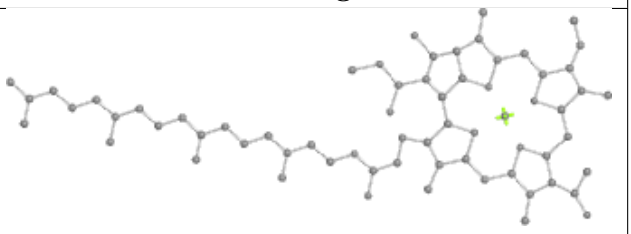
Bond lengths



Bond angles

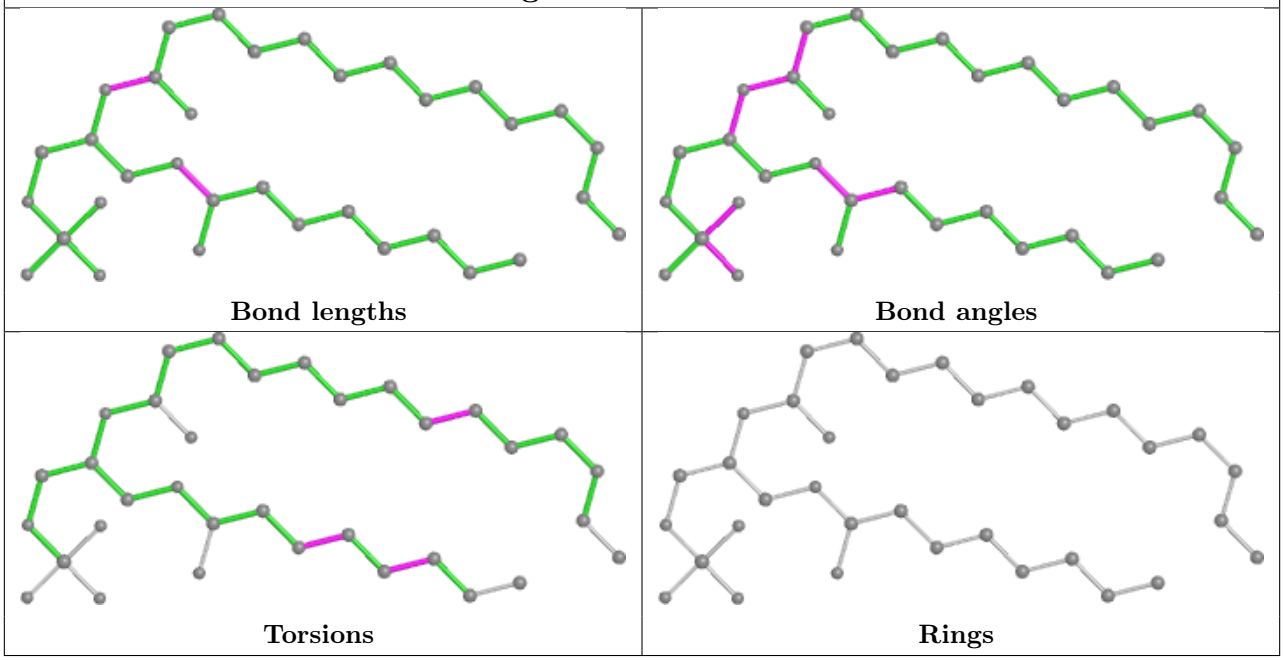


Torsions

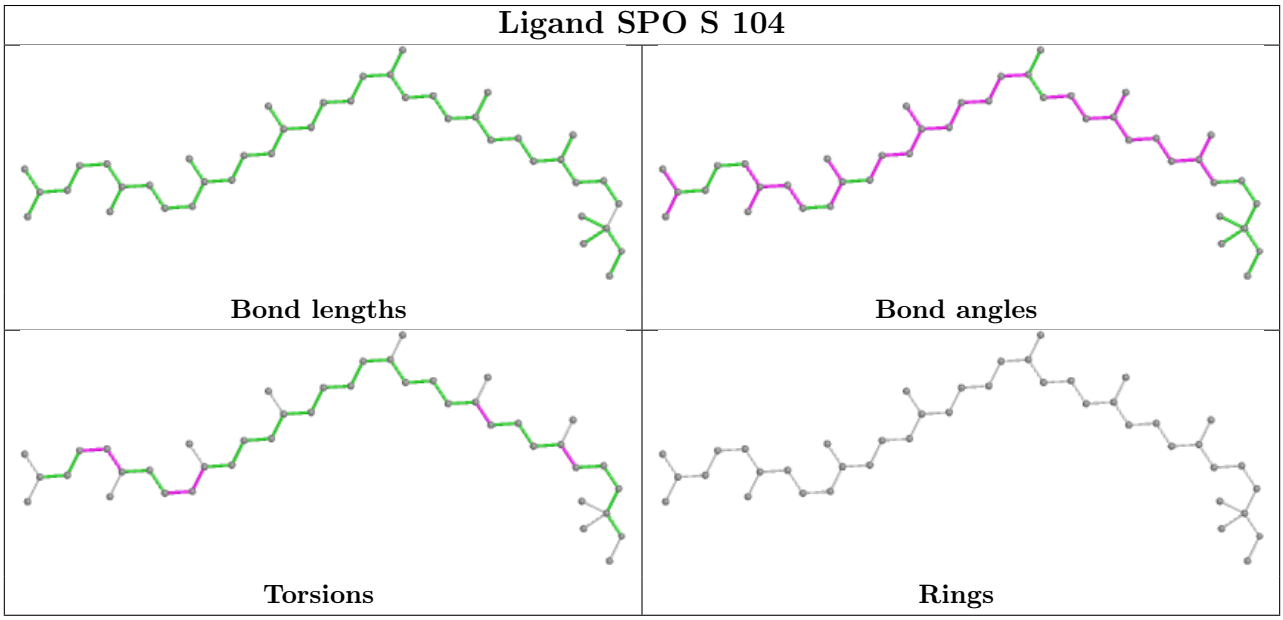


Rings

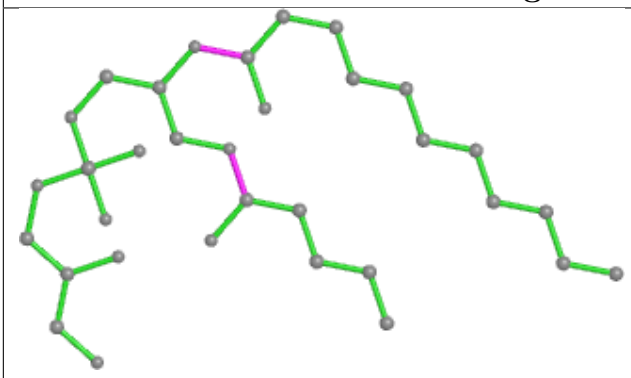
Ligand PGV H 303



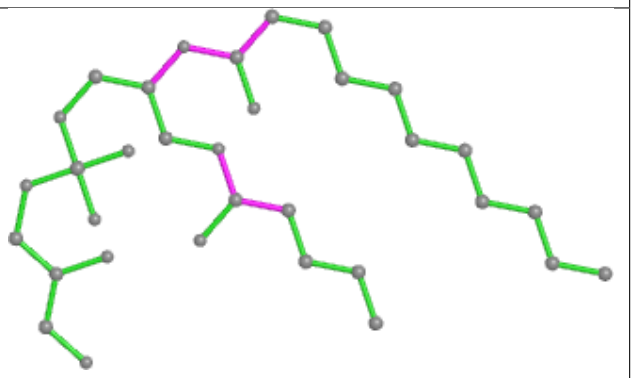
Ligand SPO S 104



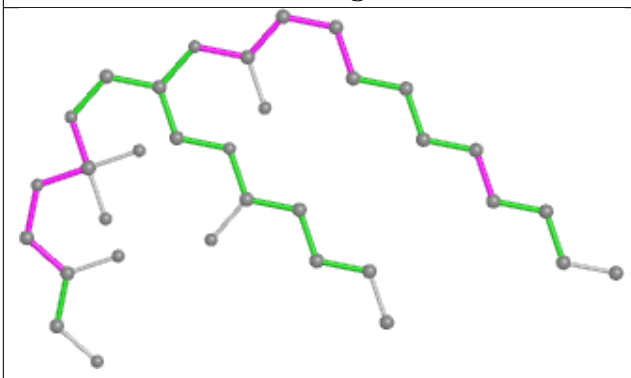
Ligand PGV L 306



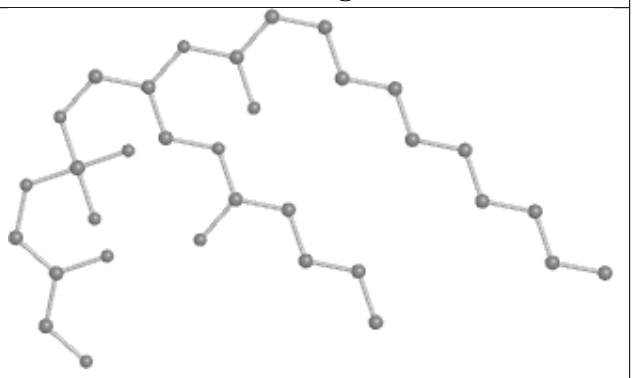
Bond lengths



Bond angles

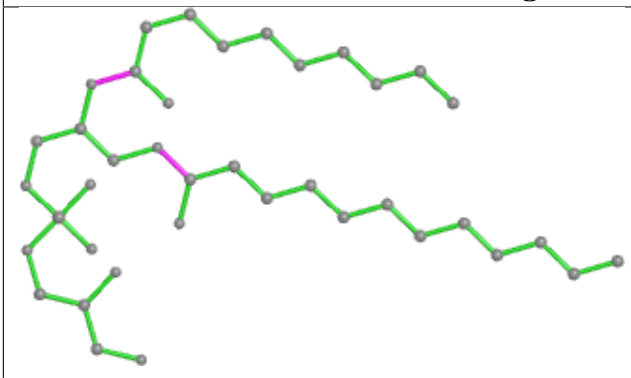


Torsions

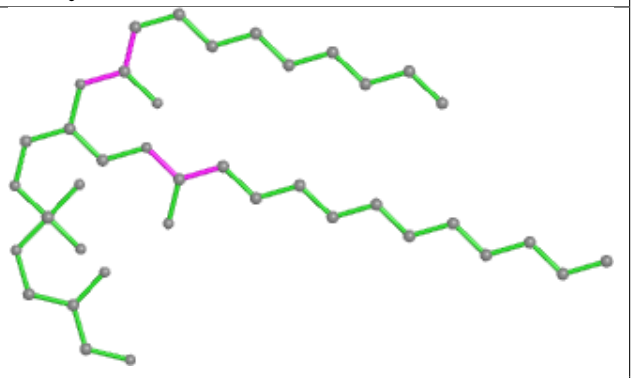


Rings

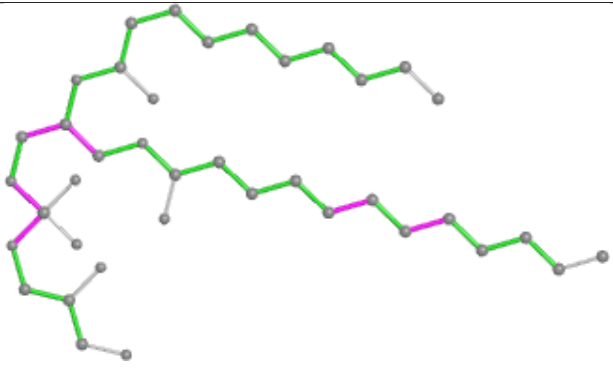
Ligand PGV Q 103



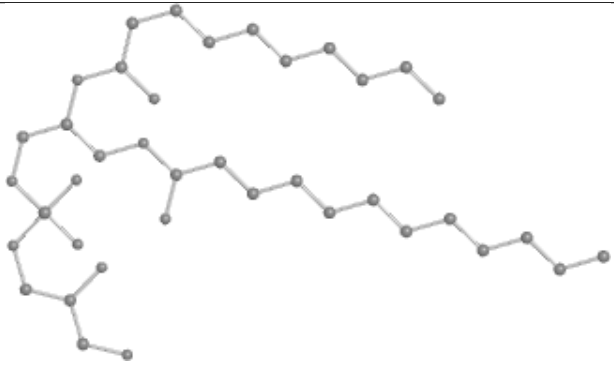
Bond lengths



Bond angles

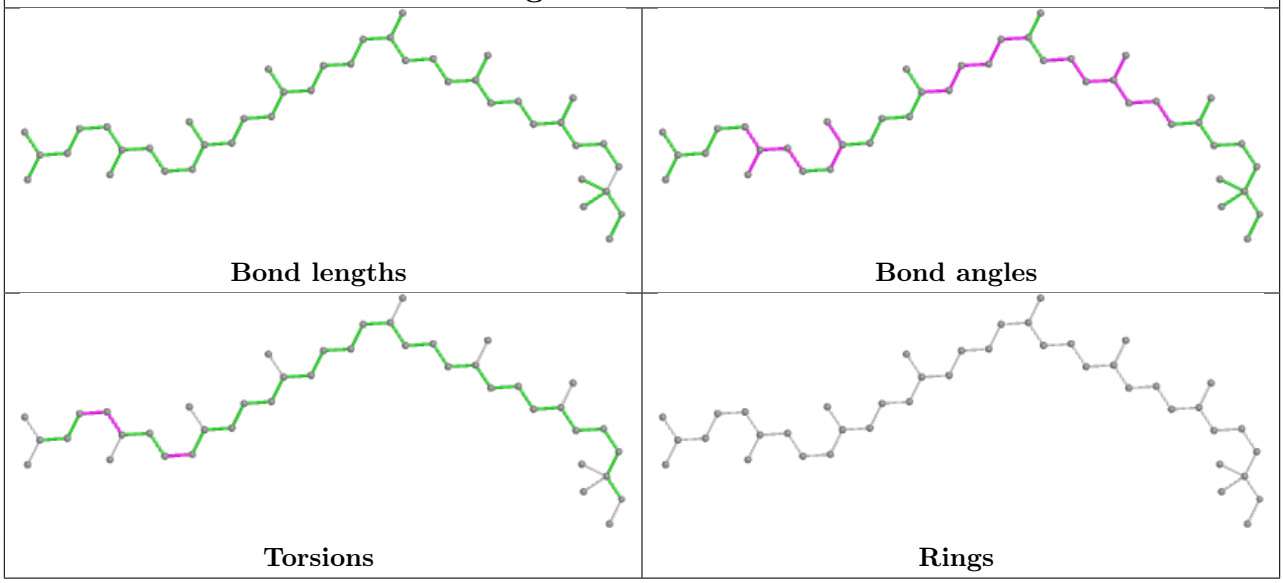


Torsions

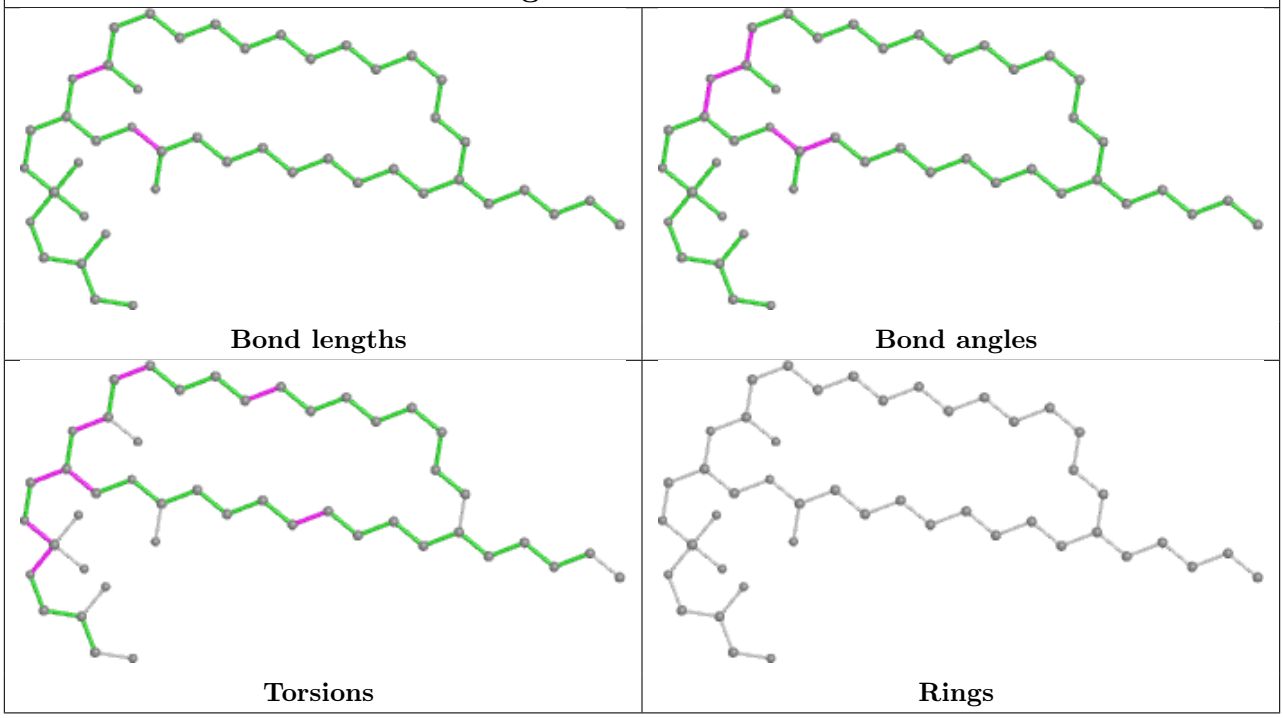


Rings

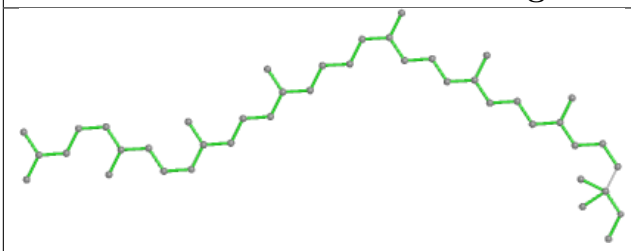
Ligand SPO K 103



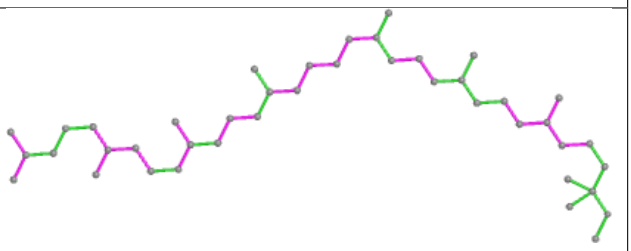
Ligand PGV H 307



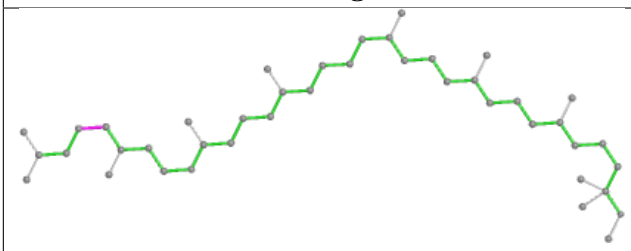
Ligand SPO F 104



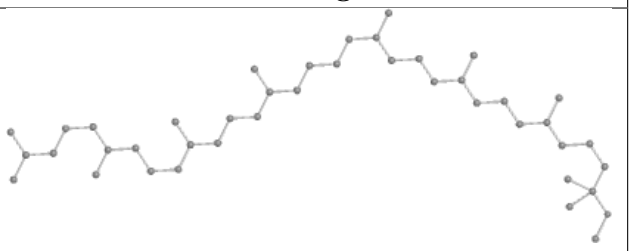
Bond lengths



Bond angles

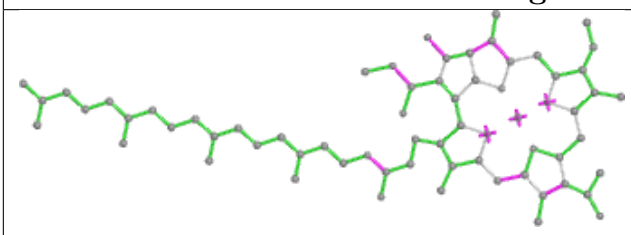


Torsions

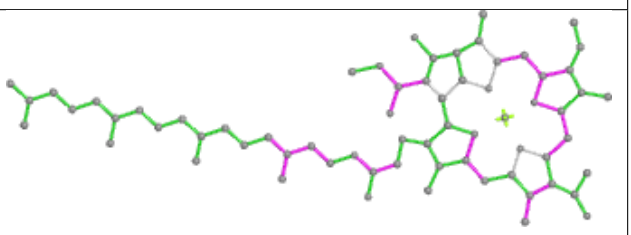


Rings

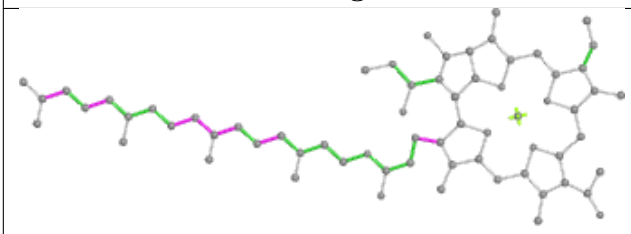
Ligand BCL 3 103



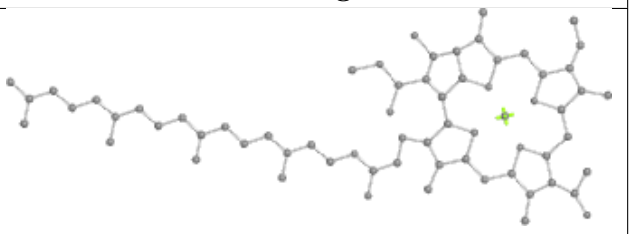
Bond lengths



Bond angles

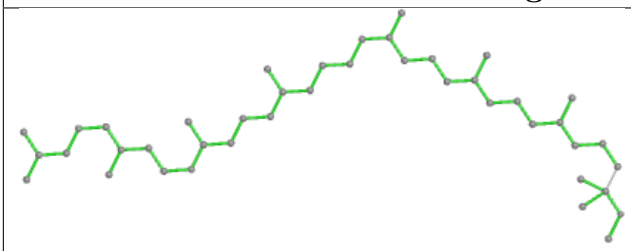


Torsions

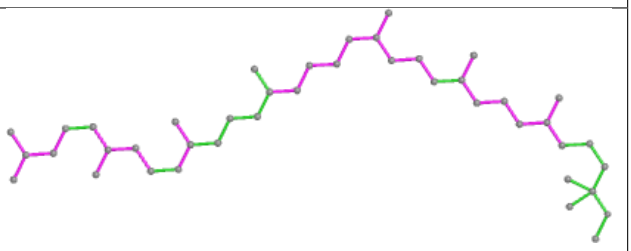


Rings

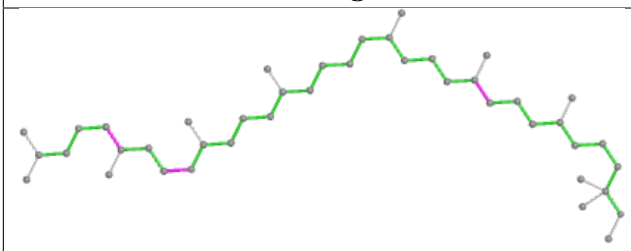
Ligand SPO V 103



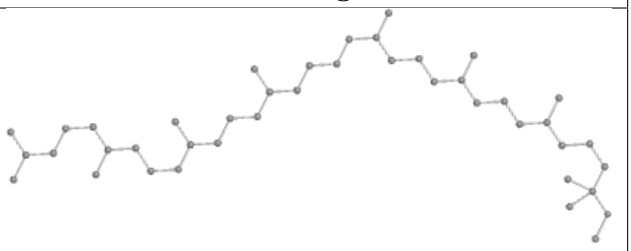
Bond lengths



Bond angles

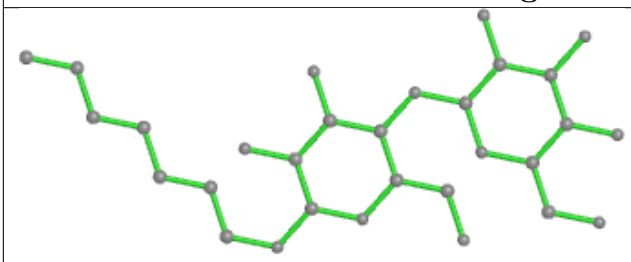


Torsions

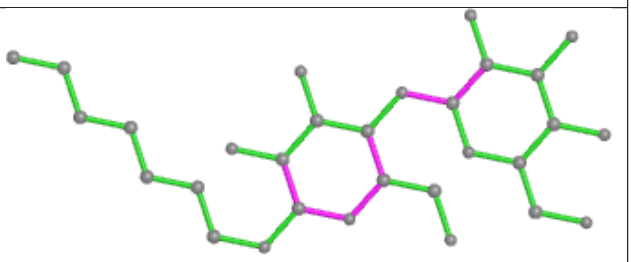


Rings

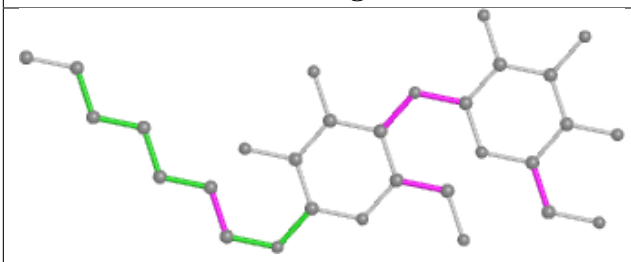
Ligand LMT H 302



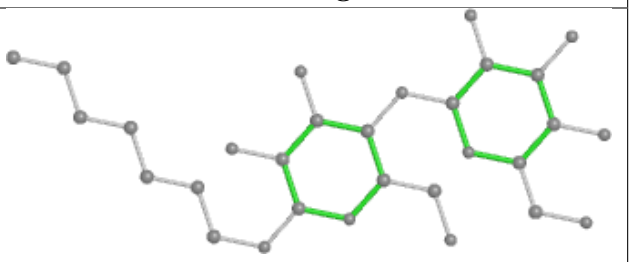
Bond lengths



Bond angles

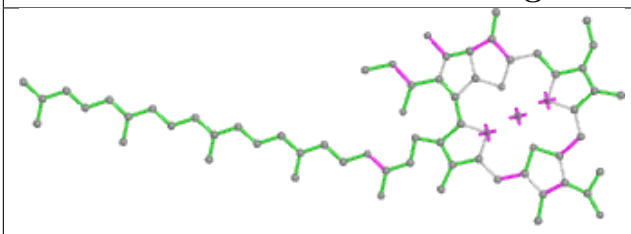


Torsions

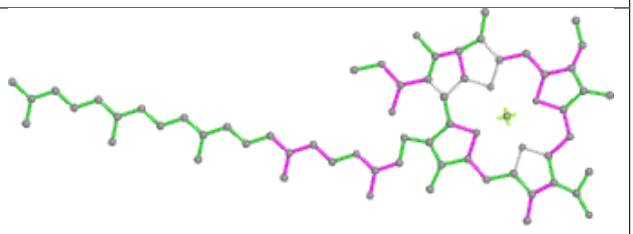


Rings

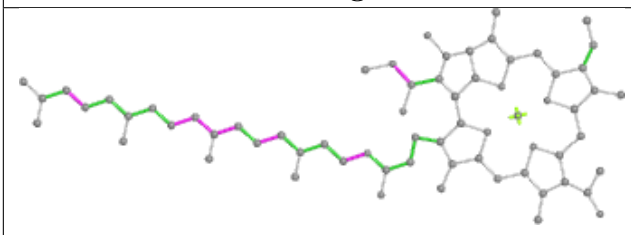
Ligand BCL D 101



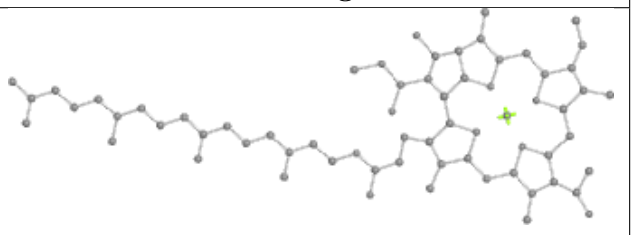
Bond lengths



Bond angles

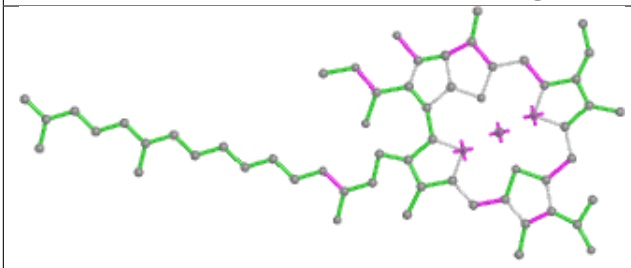


Torsions

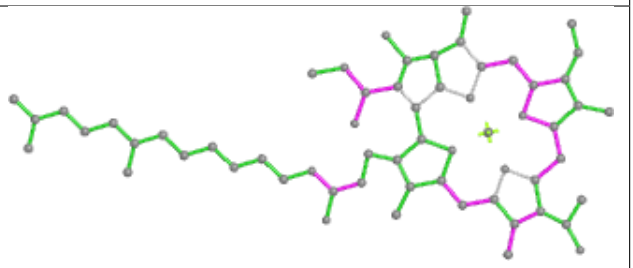


Rings

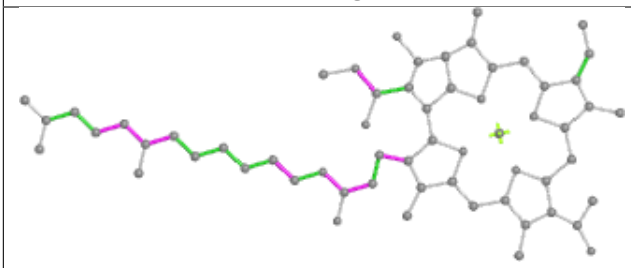
Ligand BCL 8 102



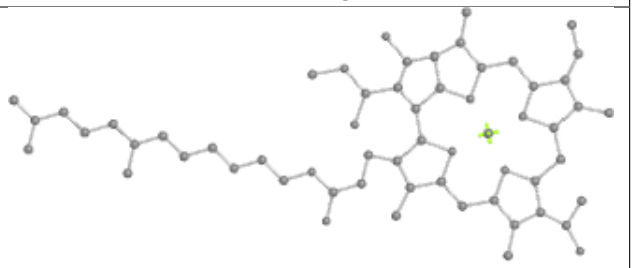
Bond lengths



Bond angles

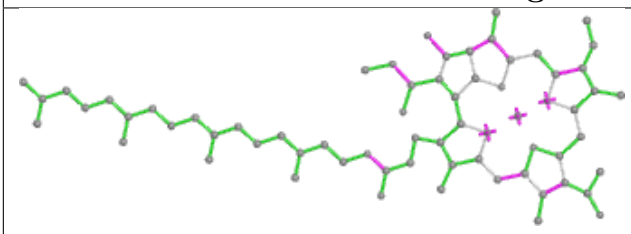


Torsions

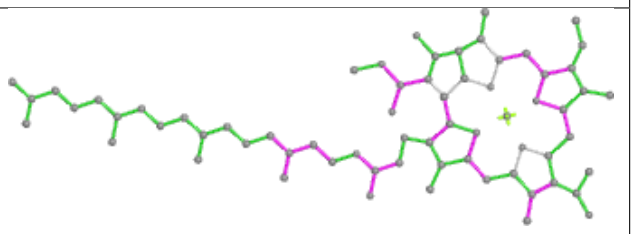


Rings

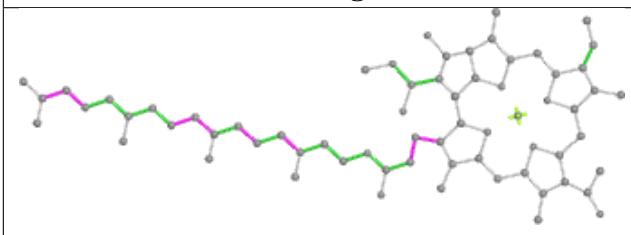
Ligand BCL Z 101



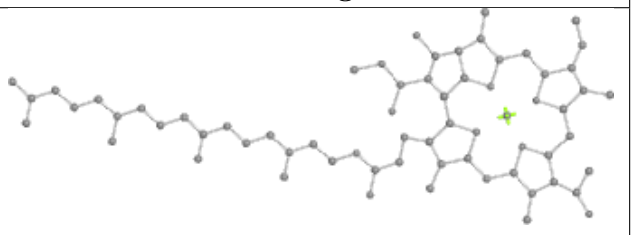
Bond lengths



Bond angles

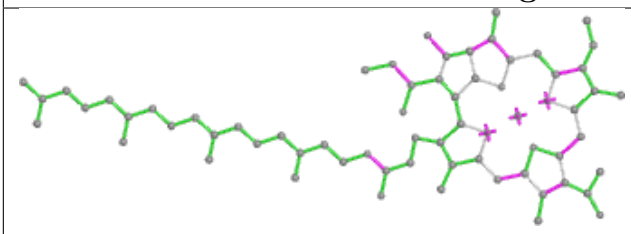


Torsions

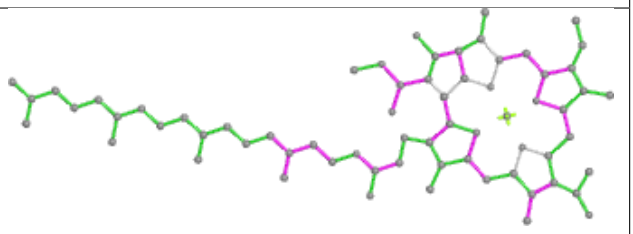


Rings

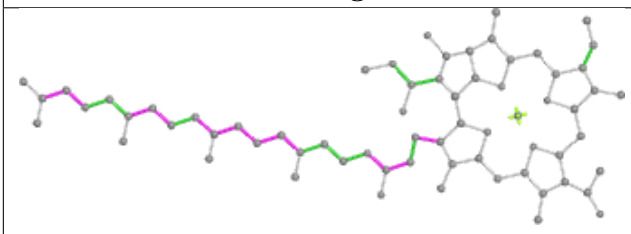
Ligand BCL W 101



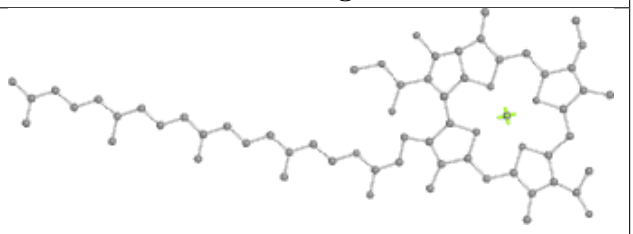
Bond lengths



Bond angles

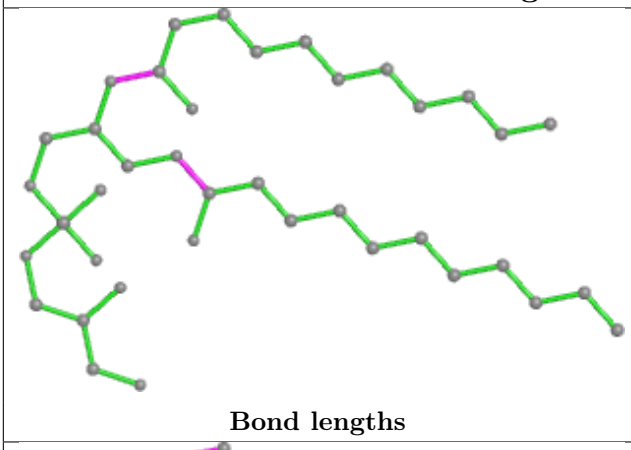


Torsions

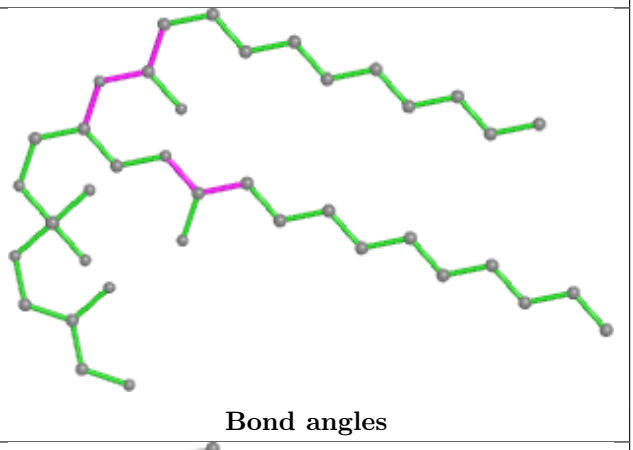


Rings

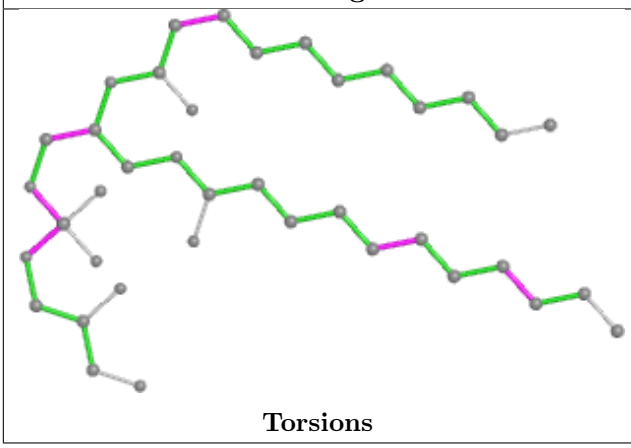
Ligand PGV X 101



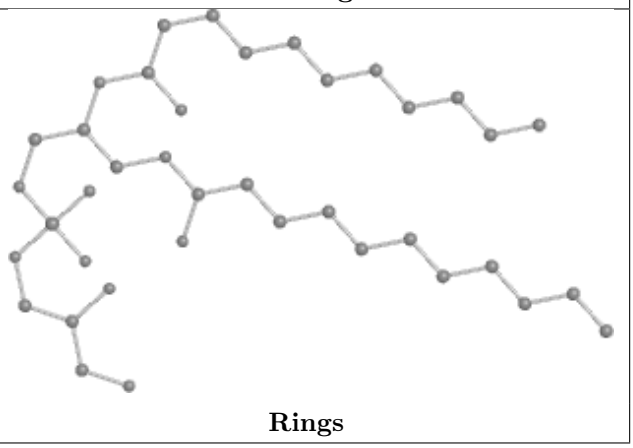
Bond lengths



Bond angles

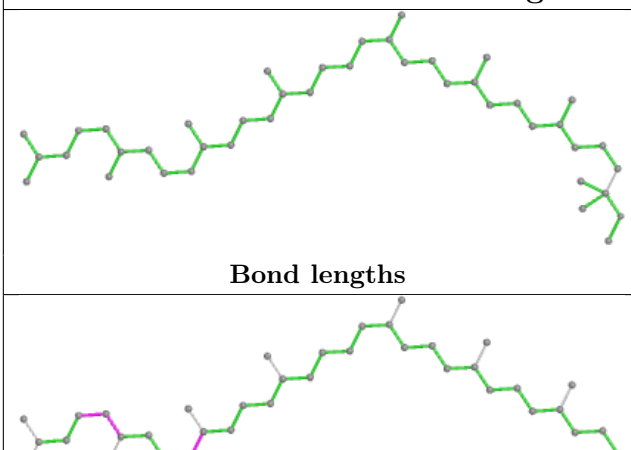


Torsions

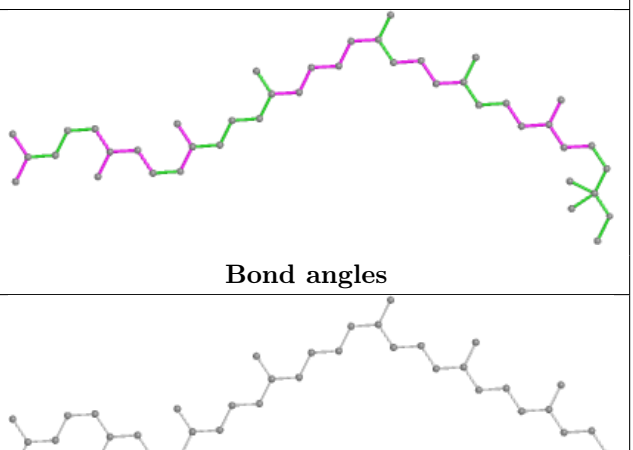


Rings

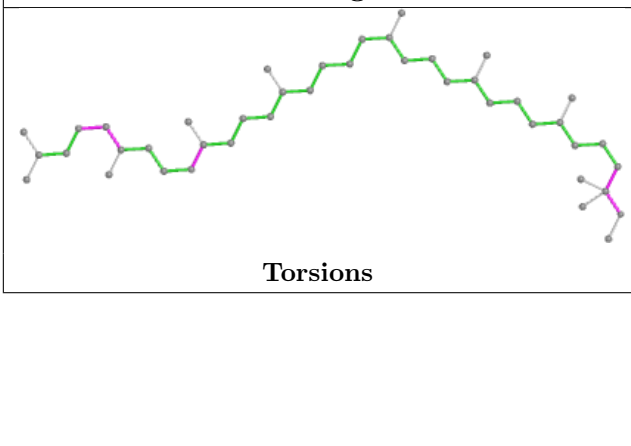
Ligand SPO T 102



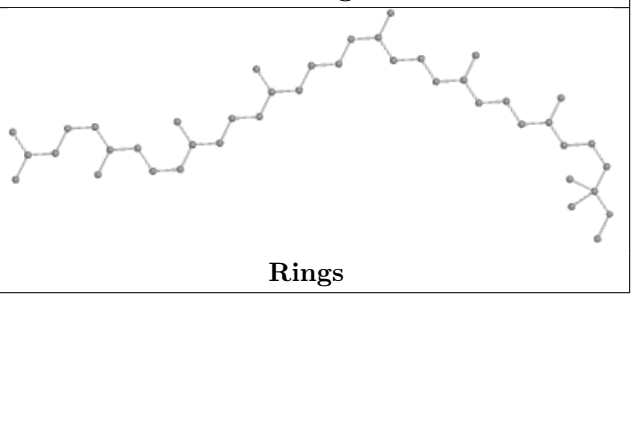
Bond lengths



Bond angles

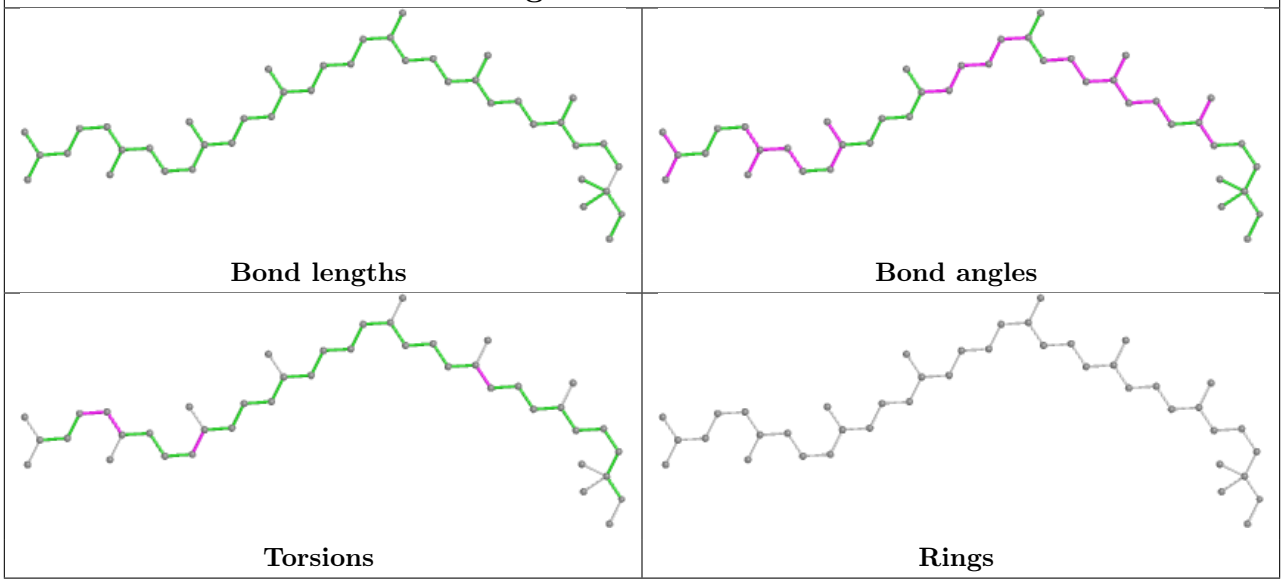


Torsions

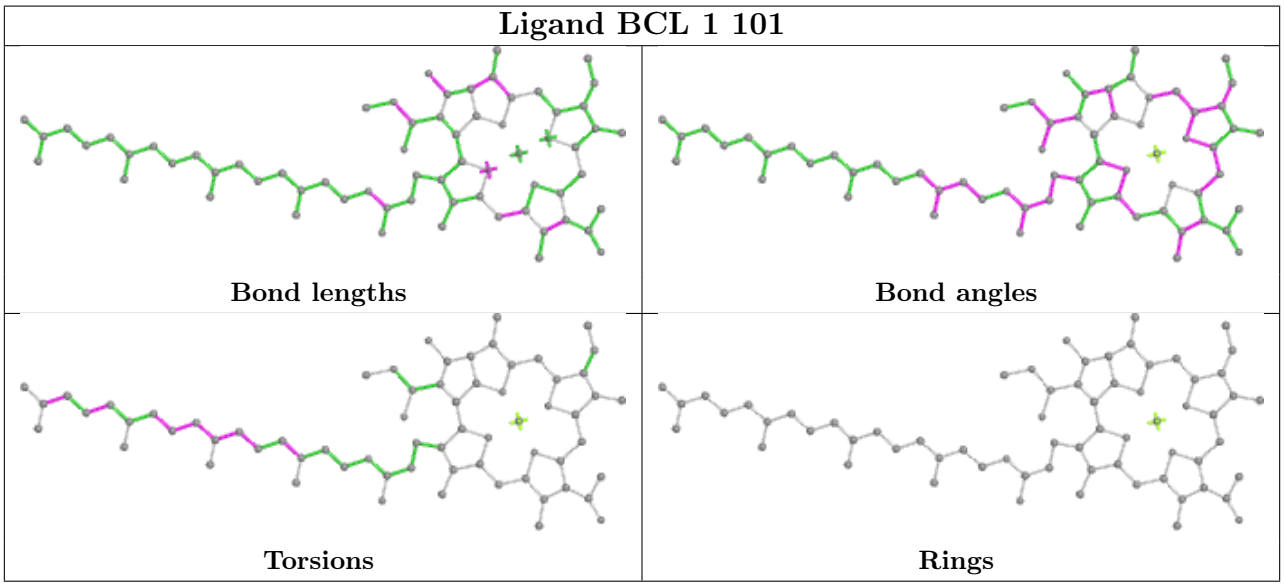


Rings

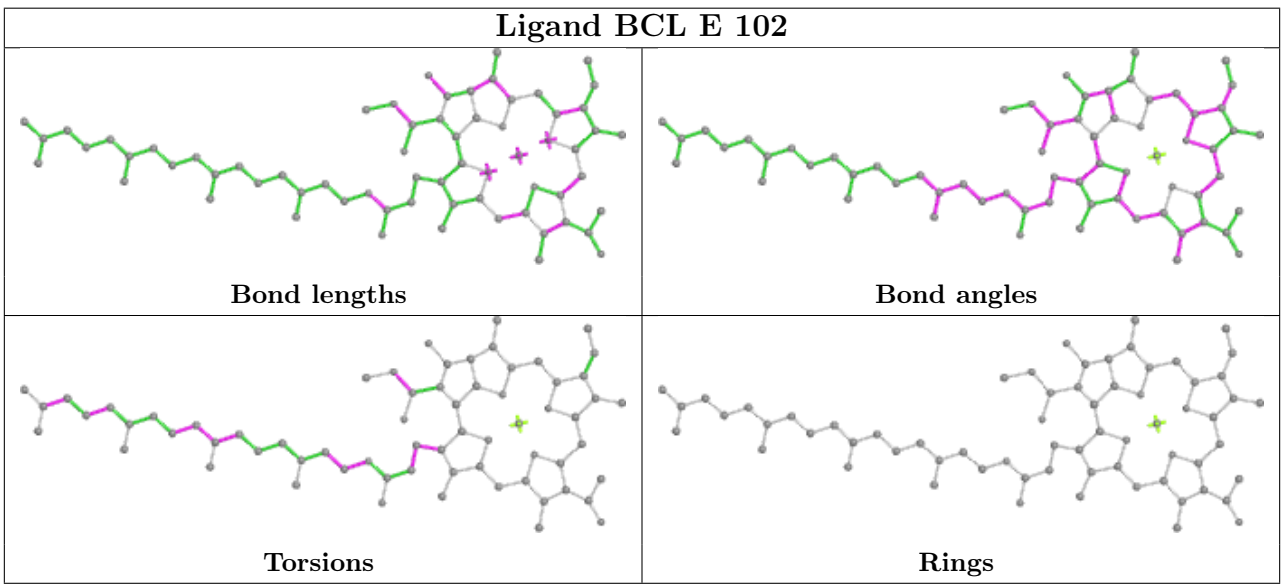
Ligand SPO G 102



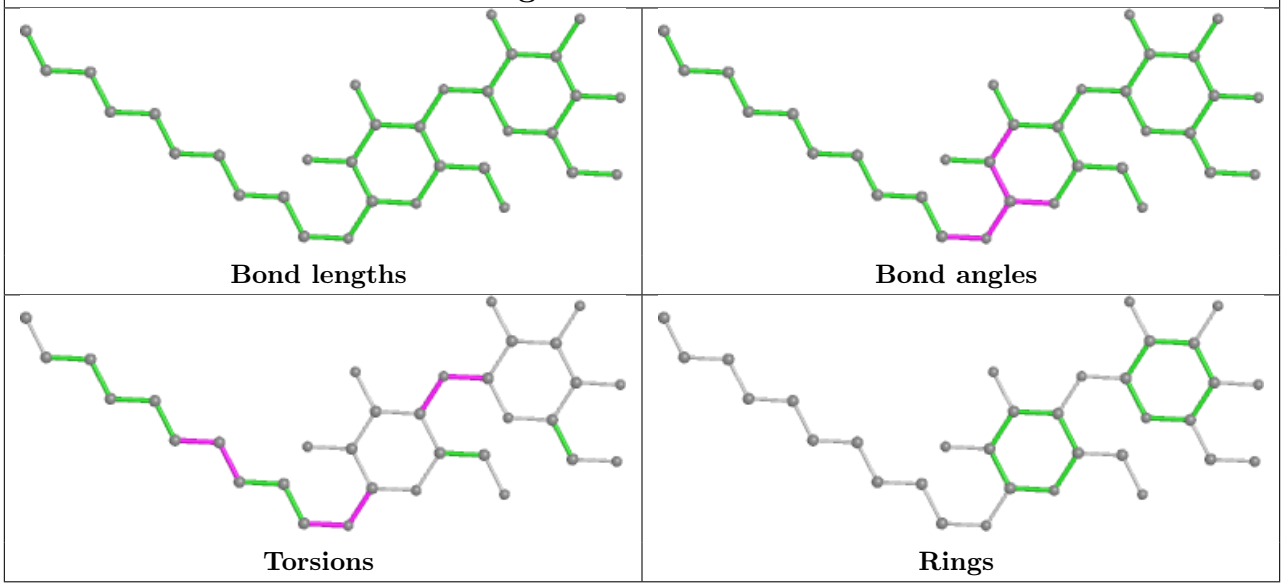
Ligand BCL 1 101



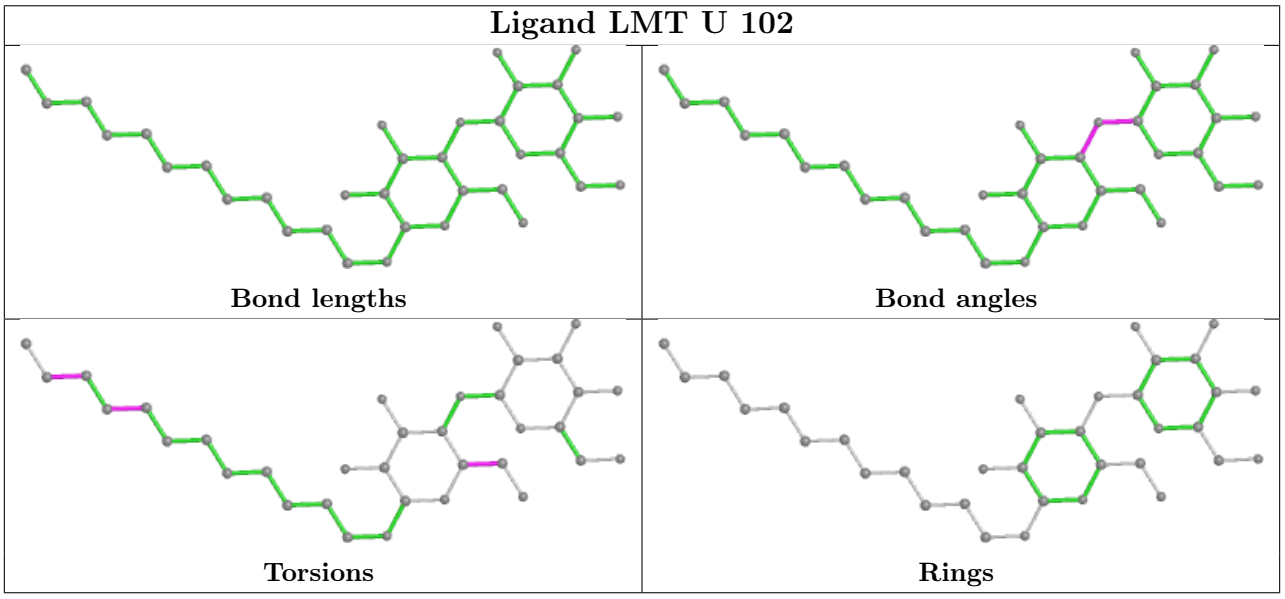
Ligand BCL E 102



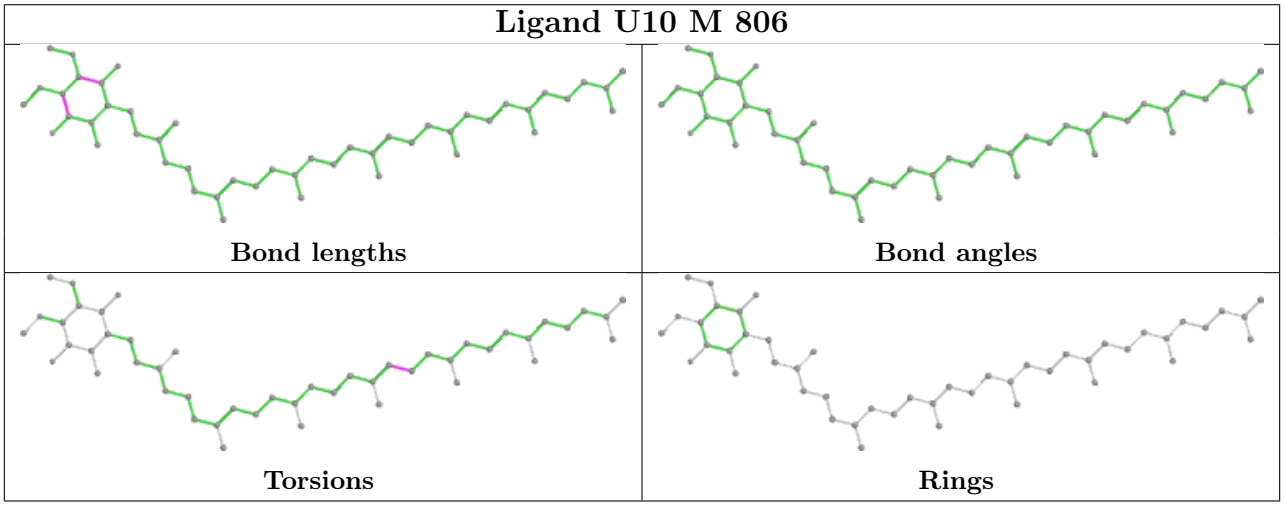
Ligand LMT M 810



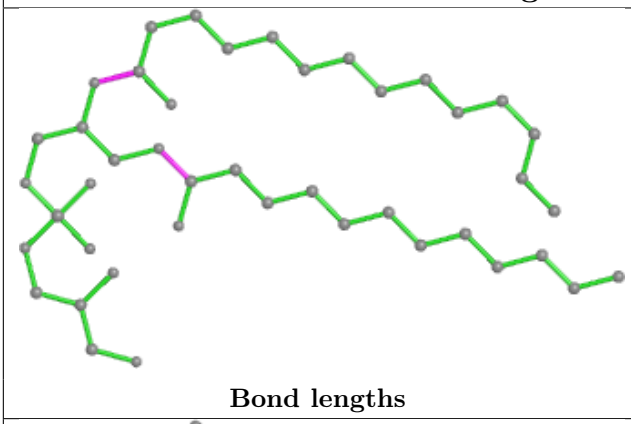
Ligand LMT U 102



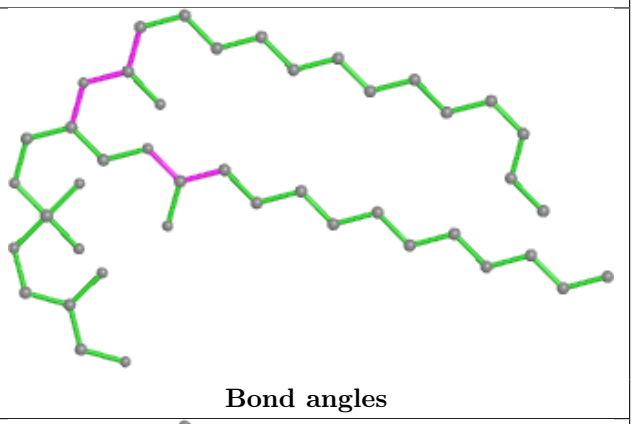
Ligand U10 M 806



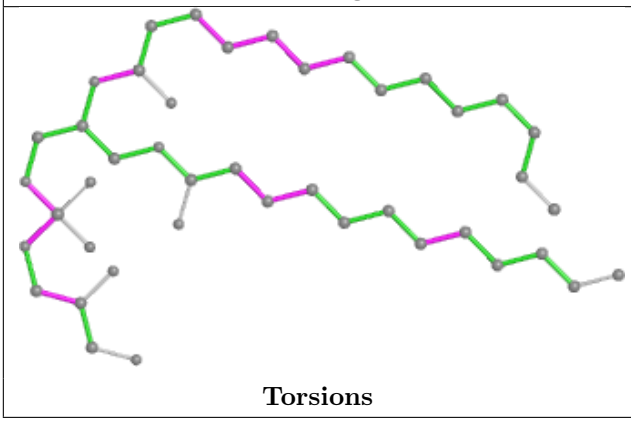
Ligand PGV Y 104



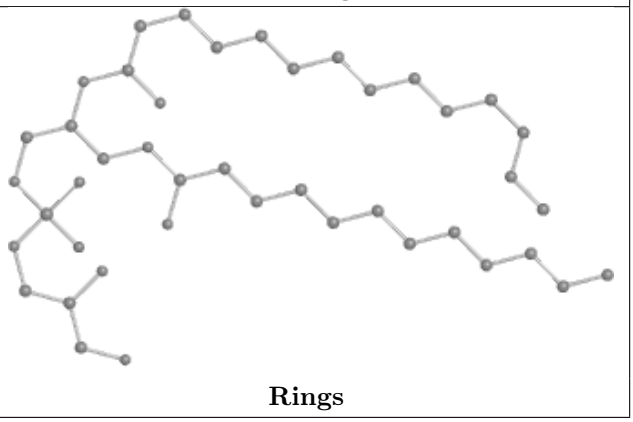
Bond lengths



Bond angles

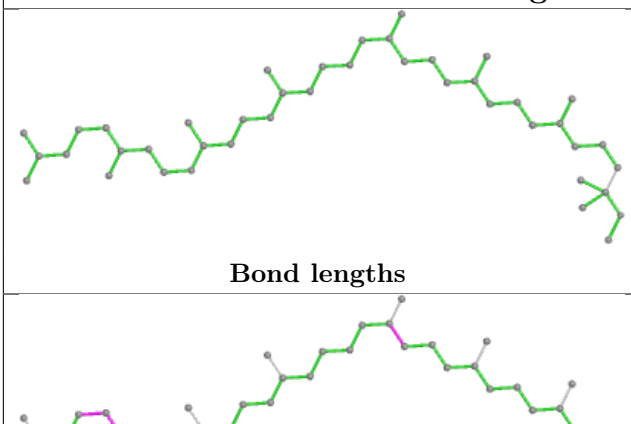


Torsions

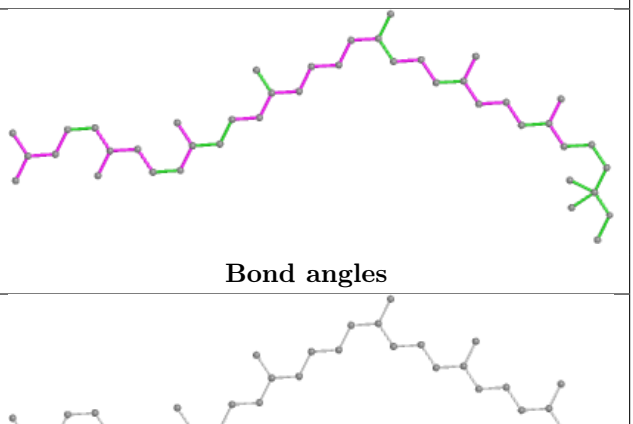


Rings

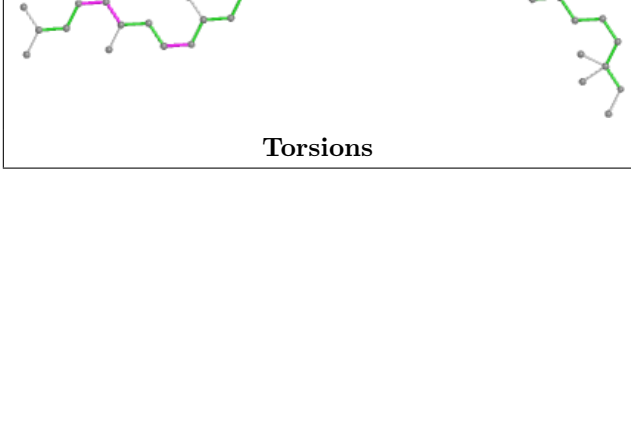
Ligand SPO 1 105



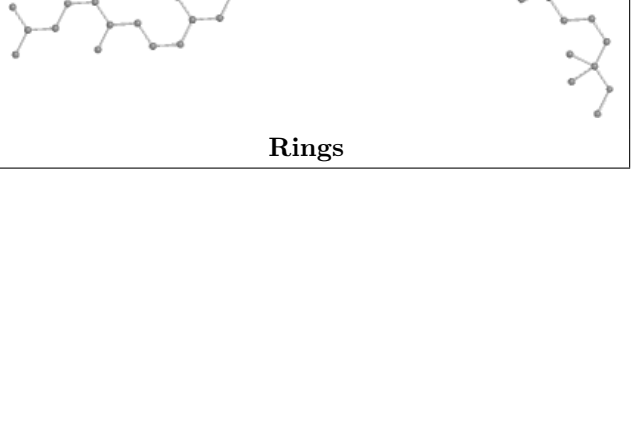
Bond lengths



Bond angles

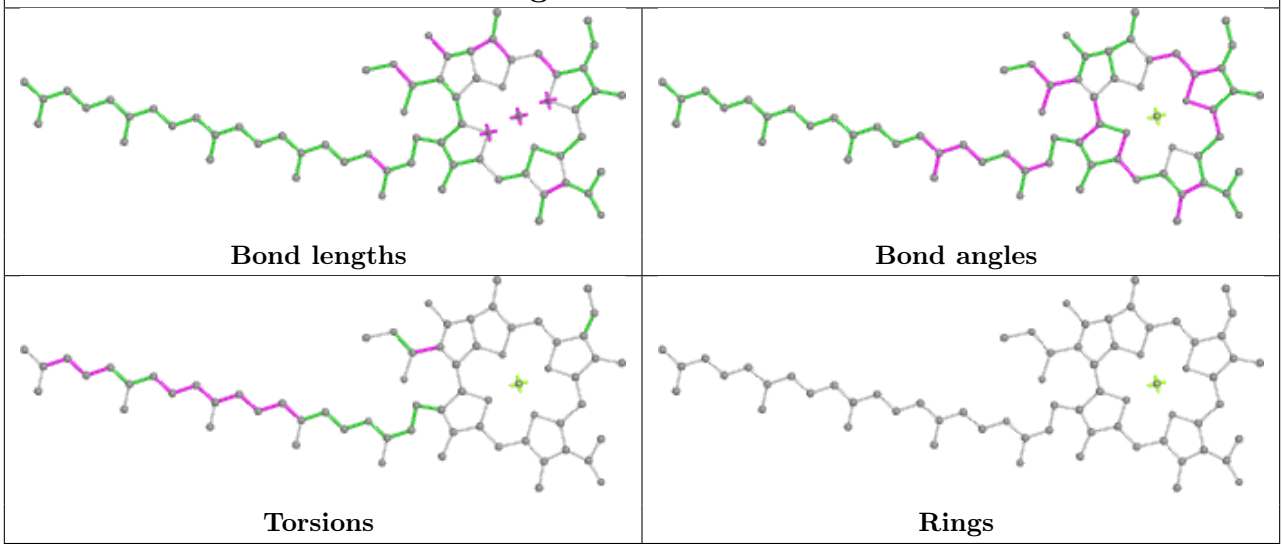


Torsions

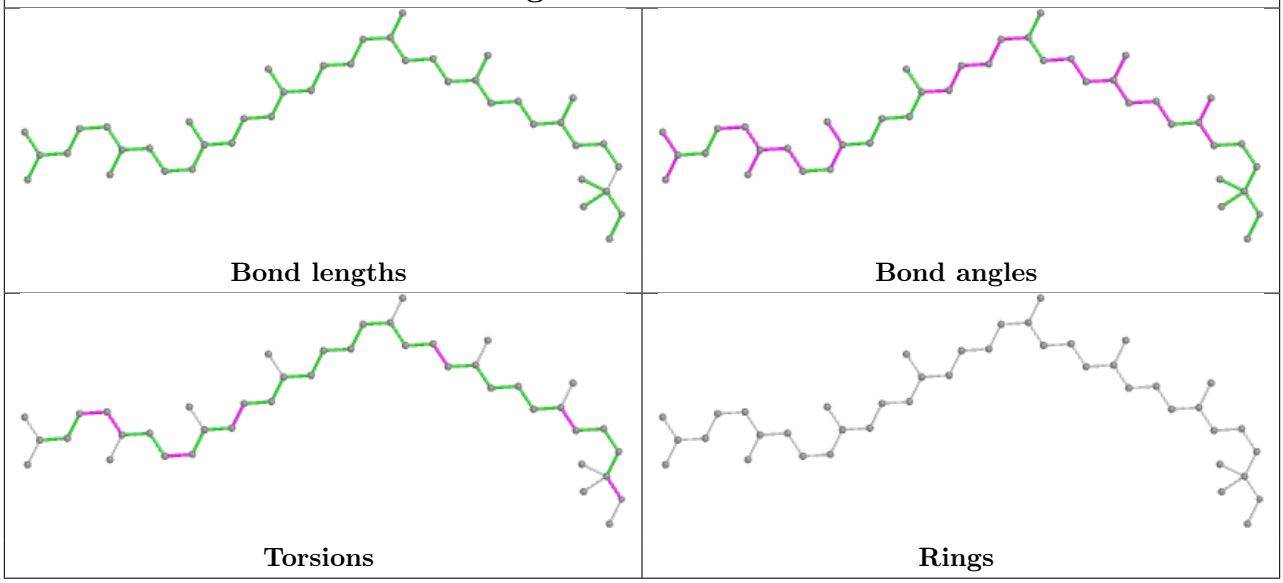


Rings

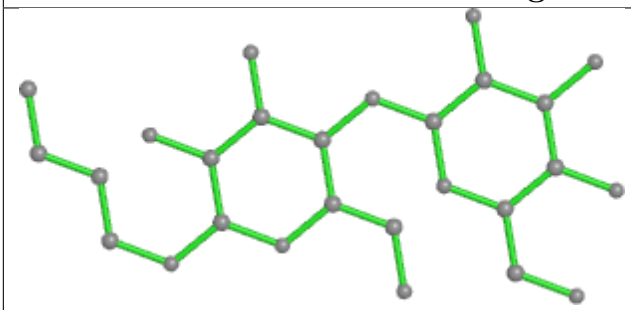
Ligand BCL 7 101



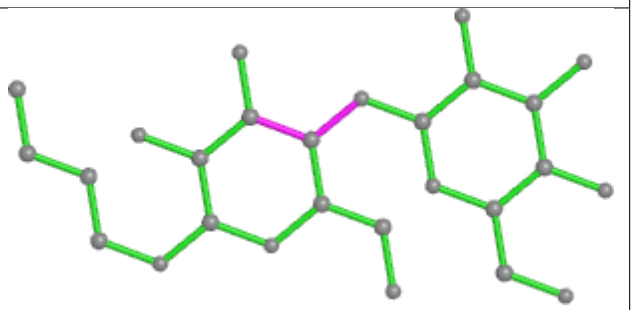
Ligand SPO O 103



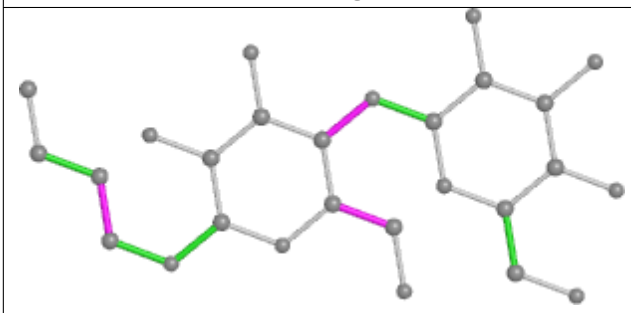
Ligand LMT I 102



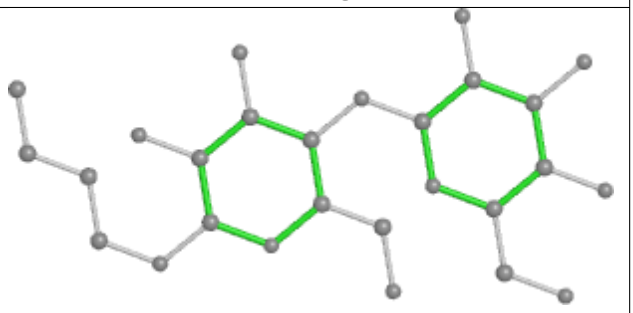
Bond lengths



Bond angles

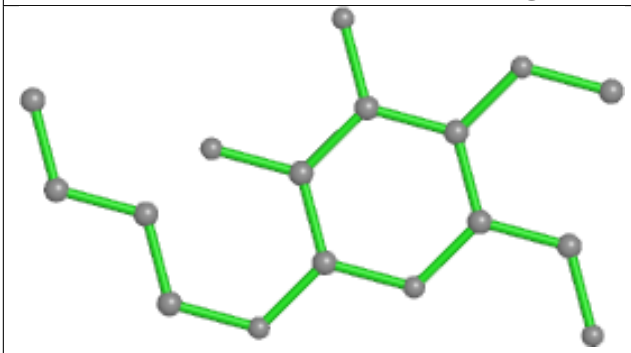


Torsions

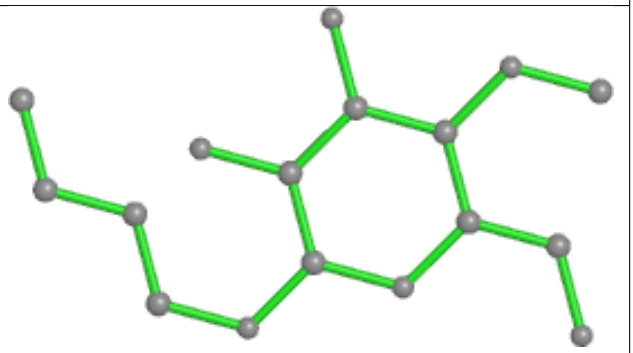


Rings

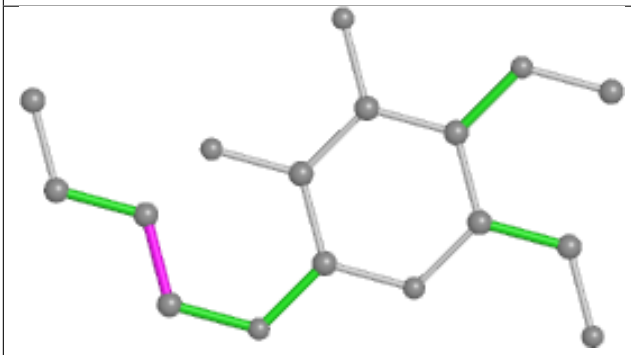
Ligand LMT F 105



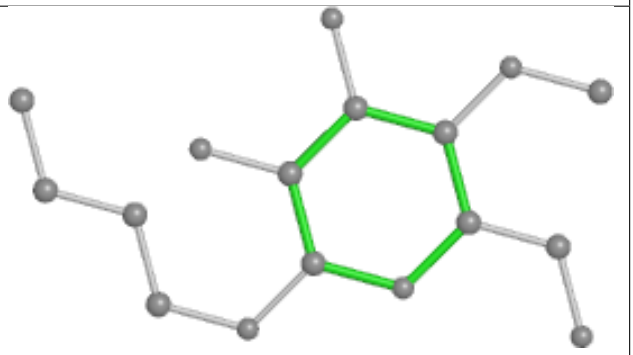
Bond lengths



Bond angles

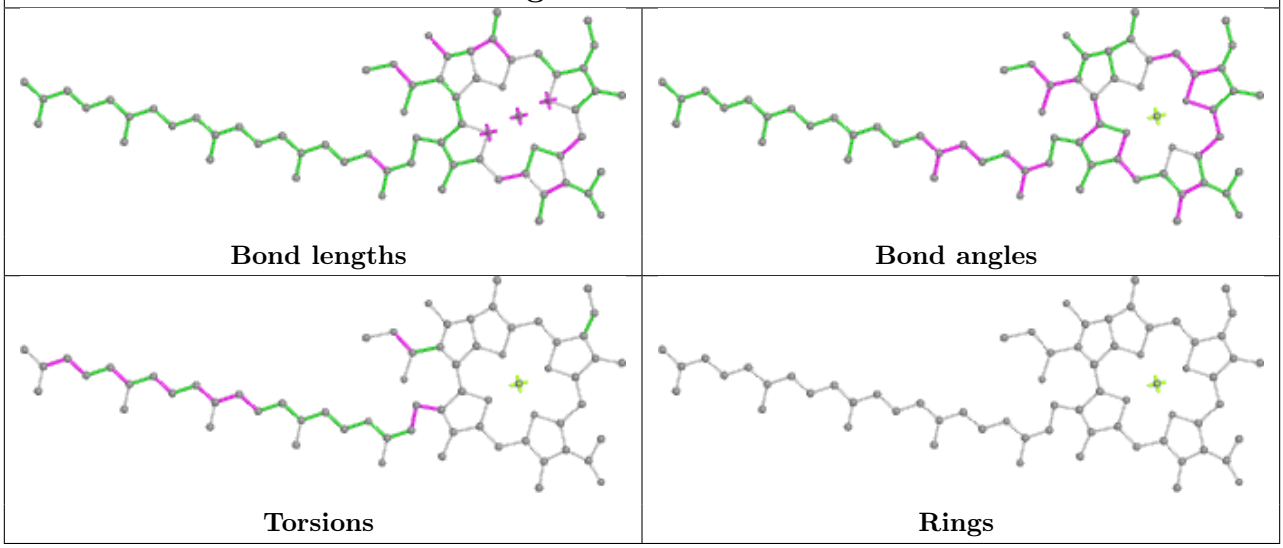


Torsions

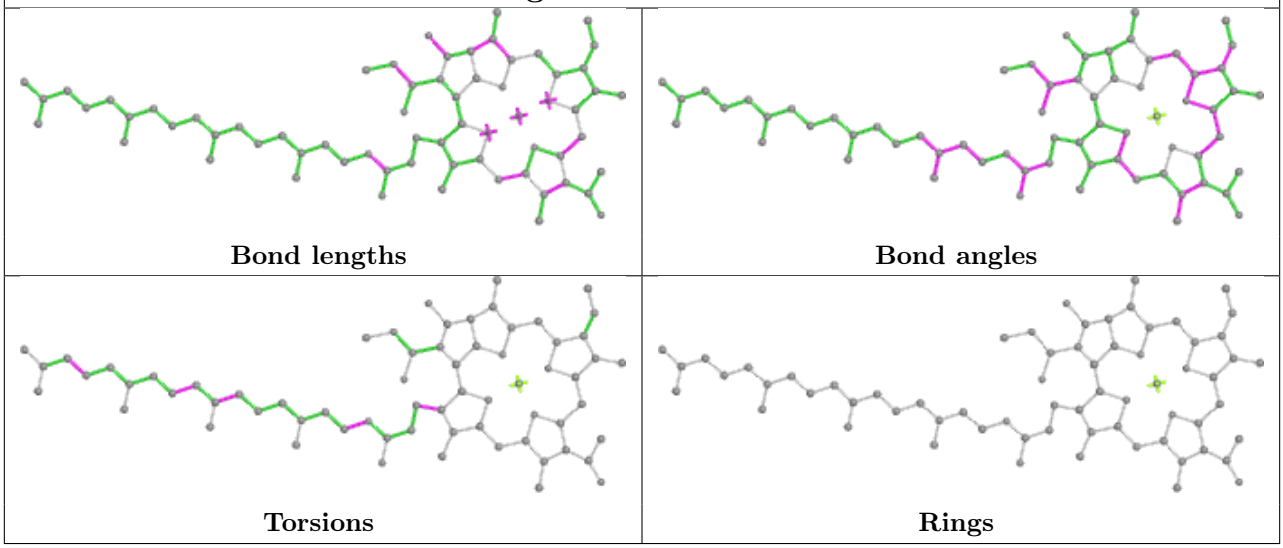


Rings

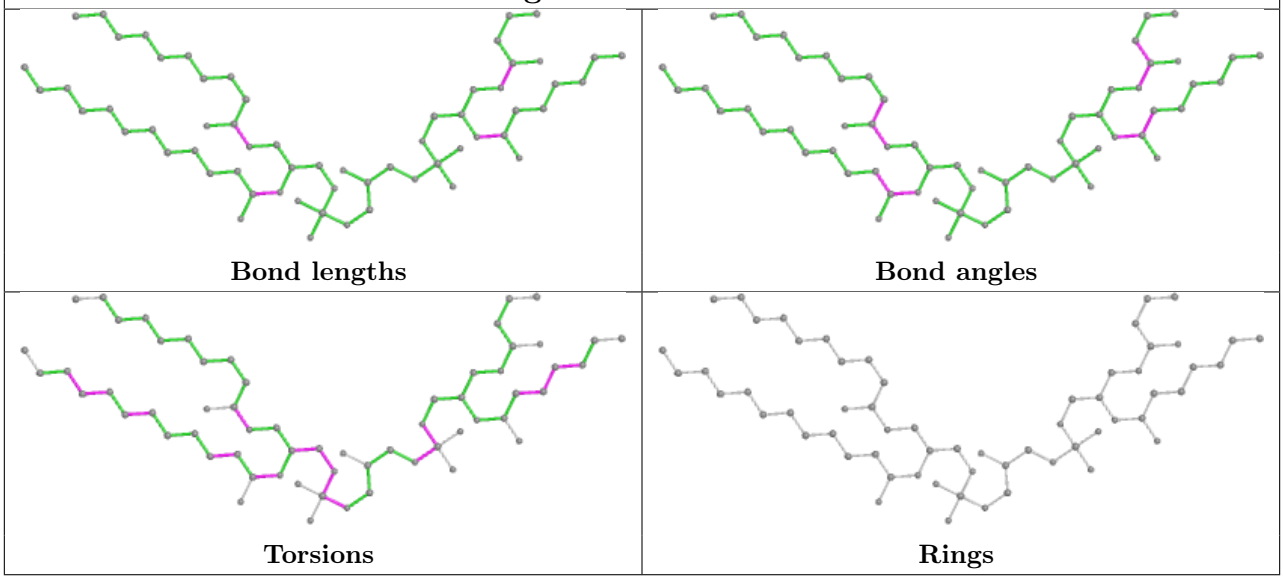
Ligand BCL P 102



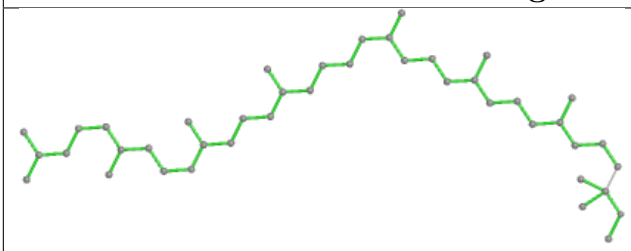
Ligand BCL B 101



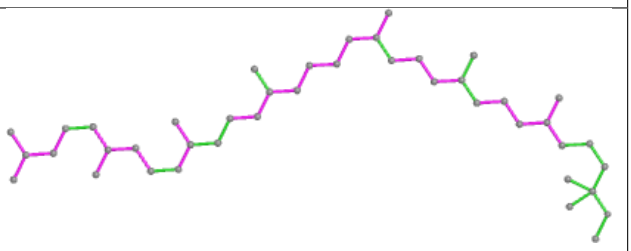
Ligand CDL H 304



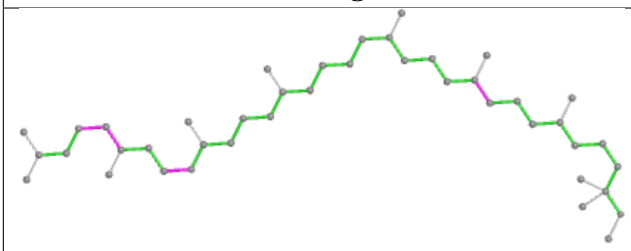
Ligand SPO S 103



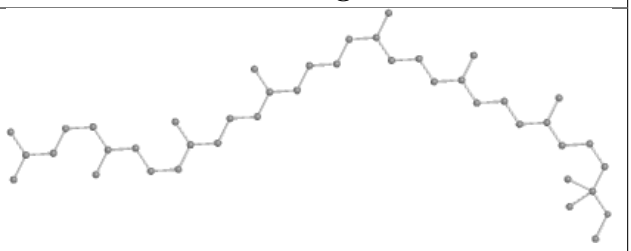
Bond lengths



Bond angles

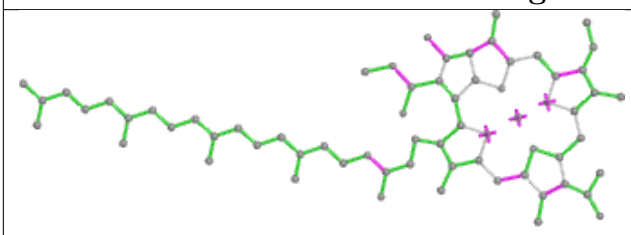


Torsions

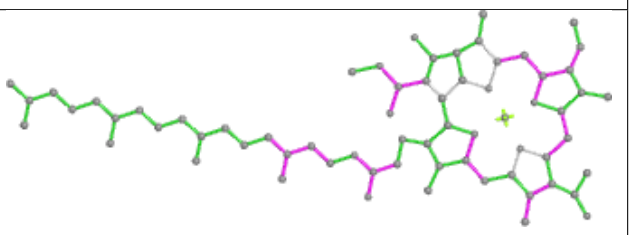


Rings

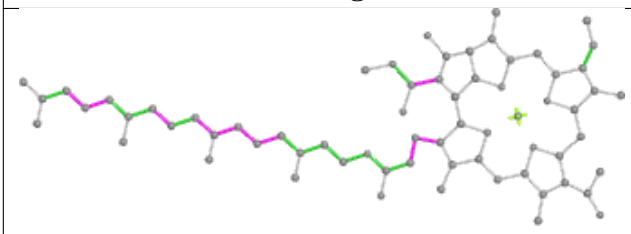
Ligand BCL J 101



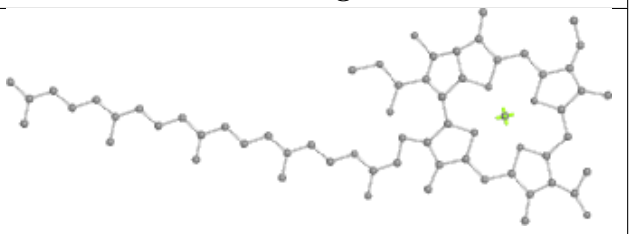
Bond lengths



Bond angles

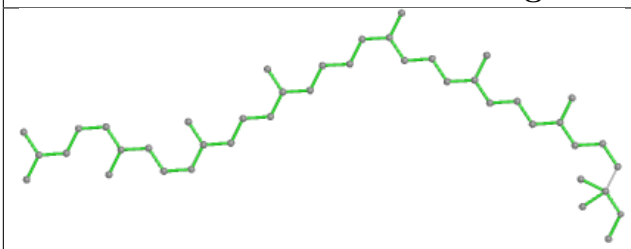


Torsions



Rings

Ligand SPO N 101



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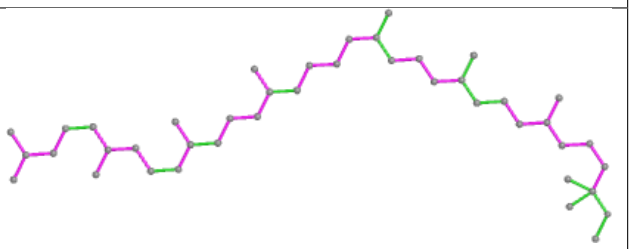
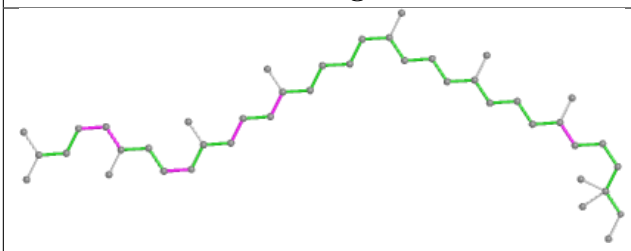
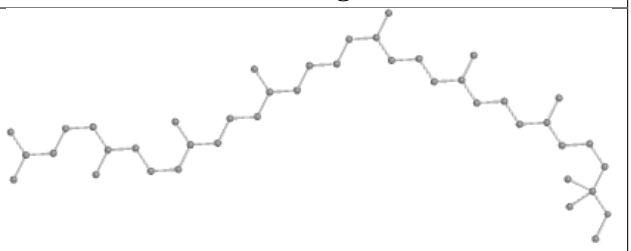


Bond angles

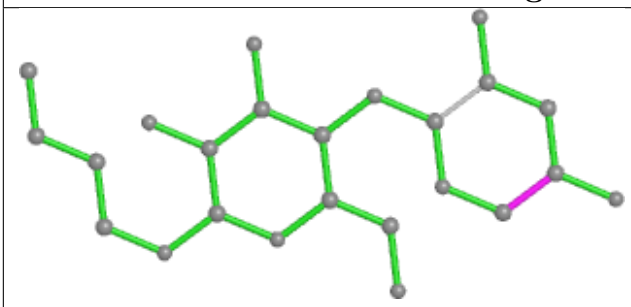


Torsions



Rings

Ligand LMT 1 104



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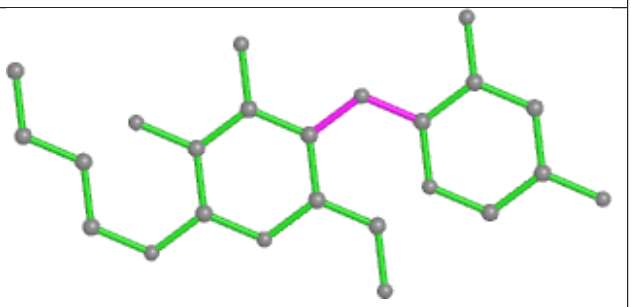
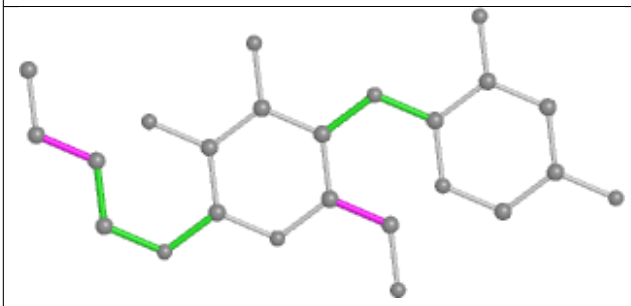


Bond angles



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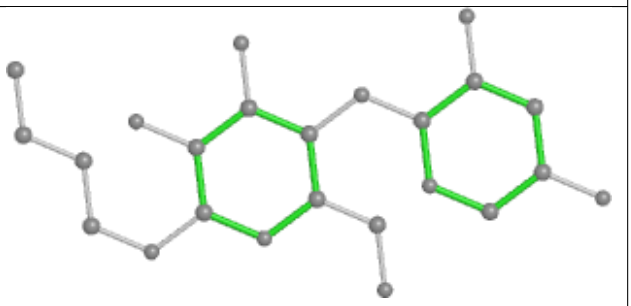
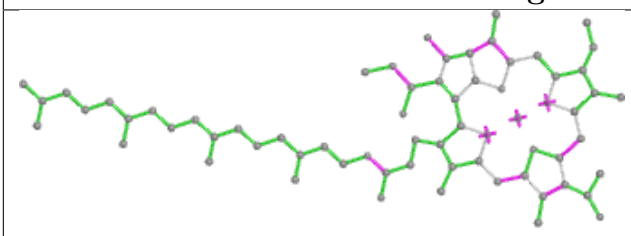


Rings

Ligand BCL L 309



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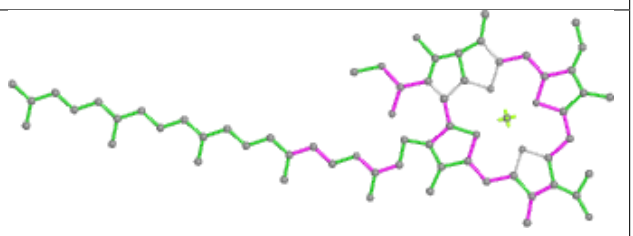
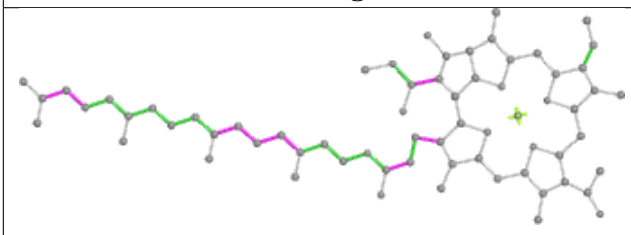
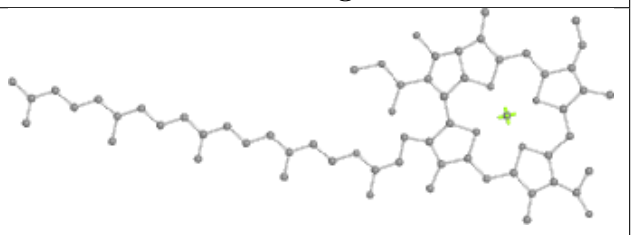


Bond angles

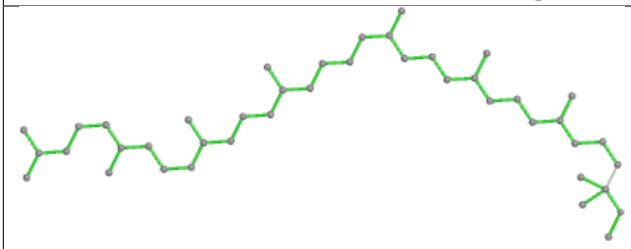


Torsions



Rings

Ligand SPO 1 103



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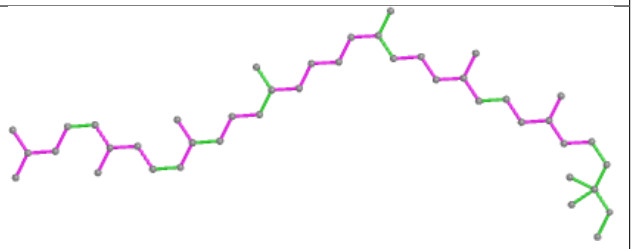
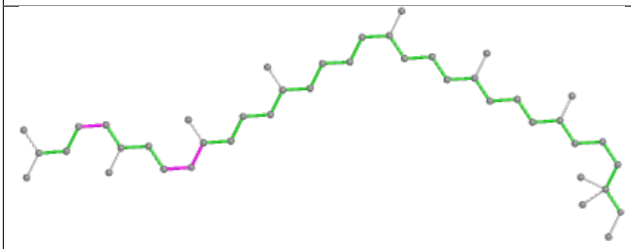
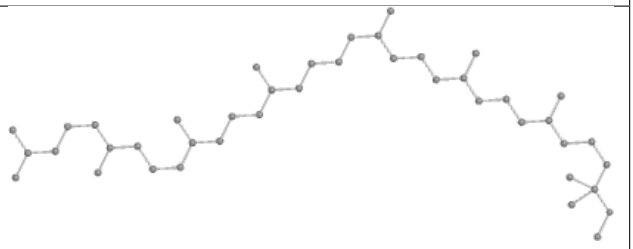


Bond angles

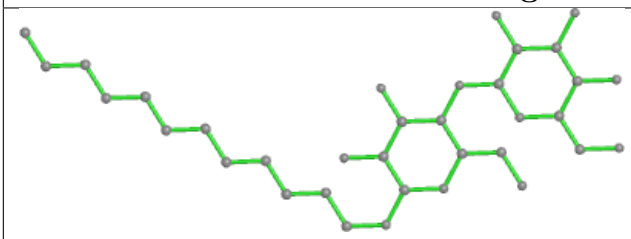


Torsions



Rings

Ligand LMT A 701



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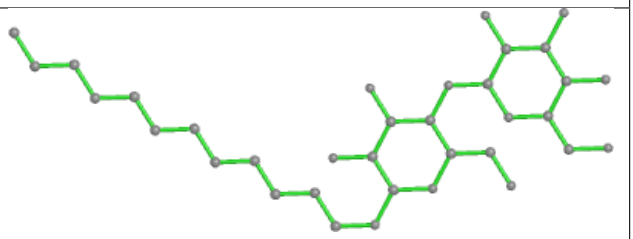
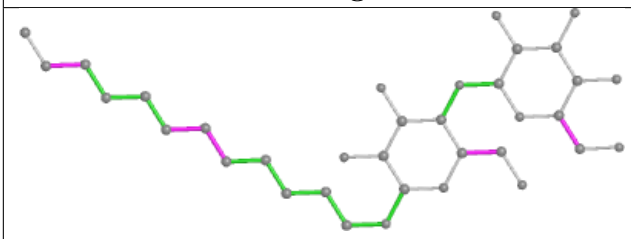
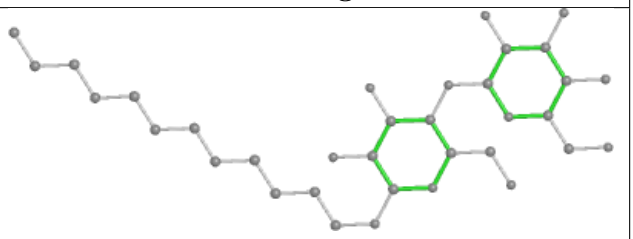


Bond angles

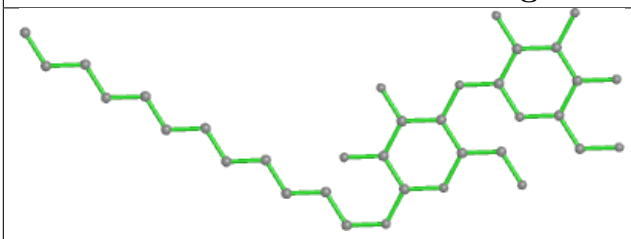


Torsions



Rings

Ligand LMT K 101



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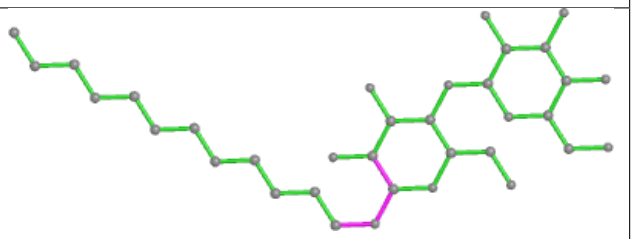
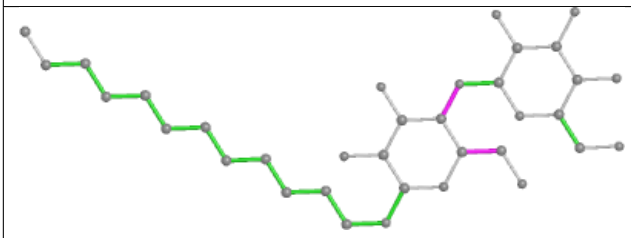
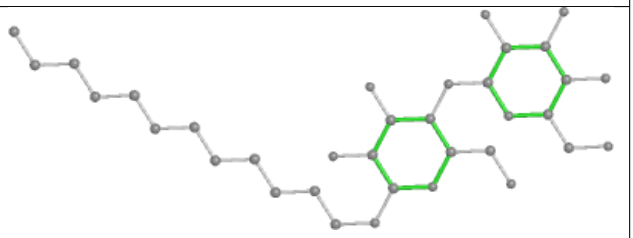


Bond angles

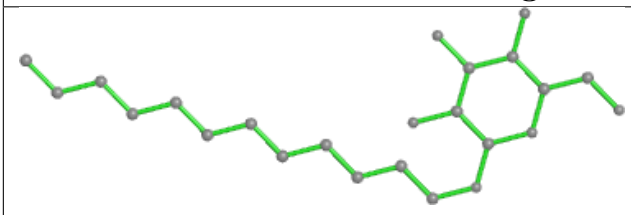


Torsions



Rings

Ligand LMT Q 101



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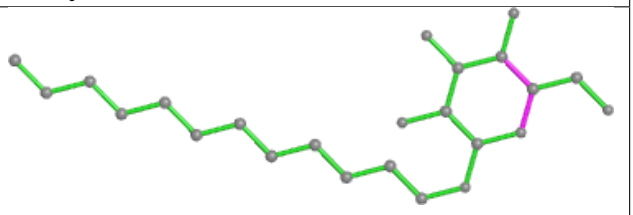
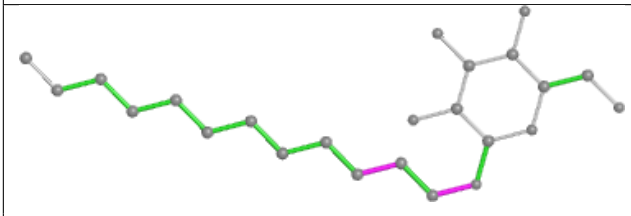


Bond angles



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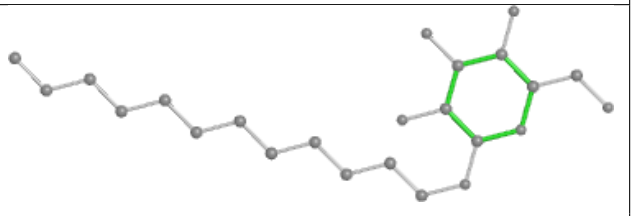
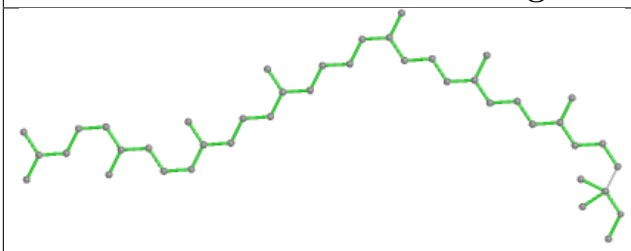


Rings

Ligand SPO F 103



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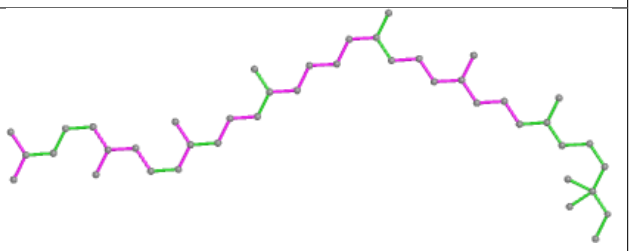
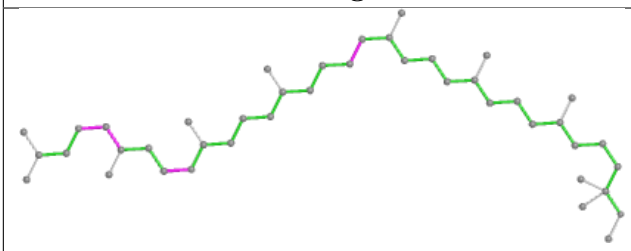


Bond angles



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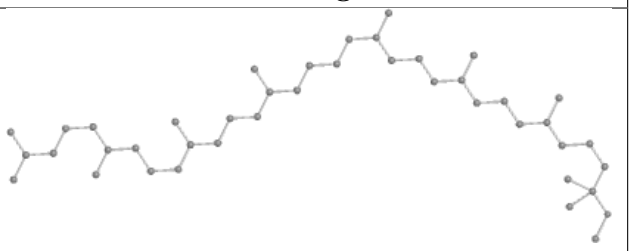
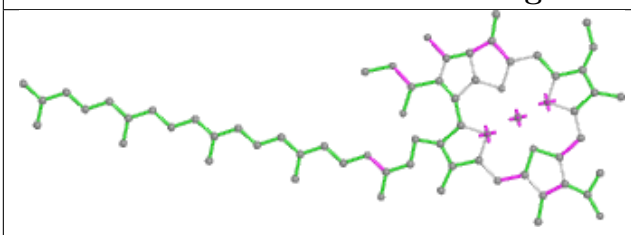


Rings

Ligand BCL R 102



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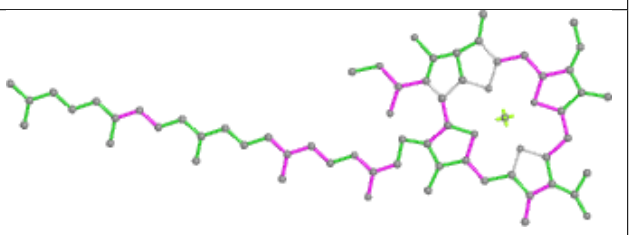
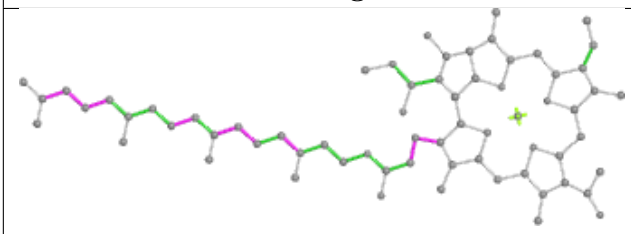
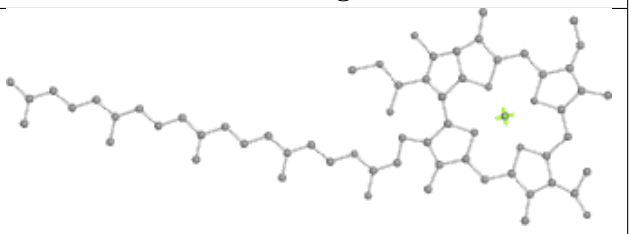


Bond angles

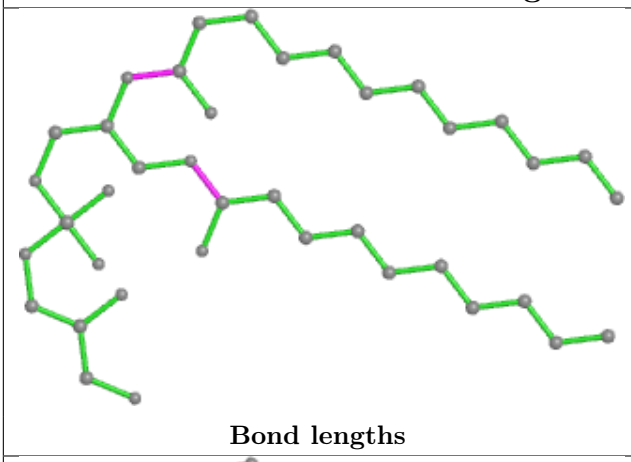


Torsions



Rings

Ligand PGV L 305



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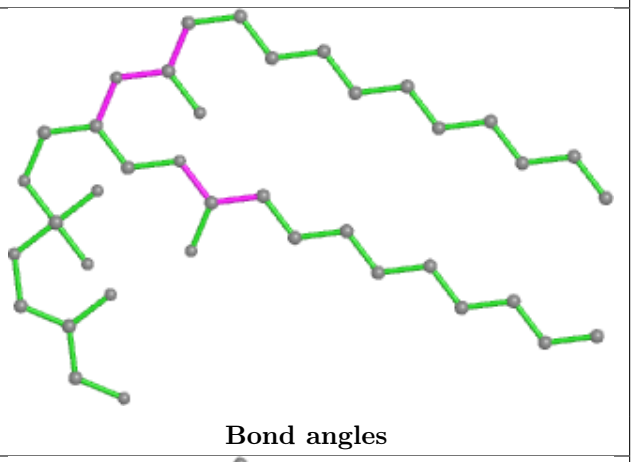
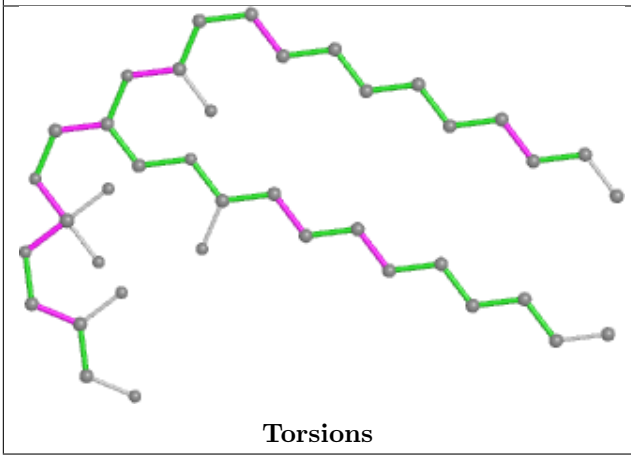
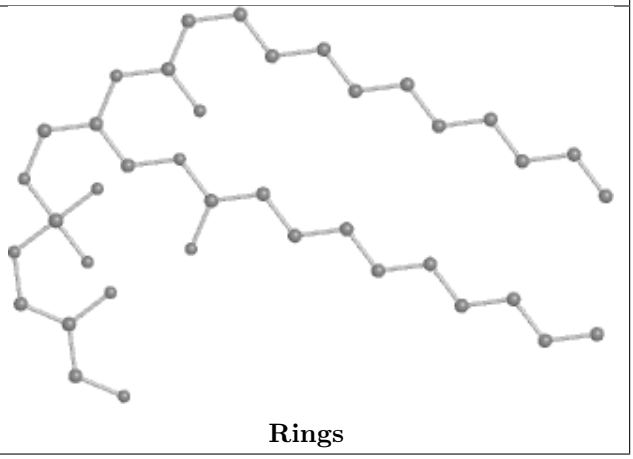


Bond angles

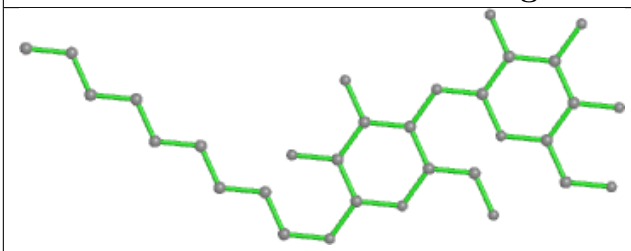


Torsions

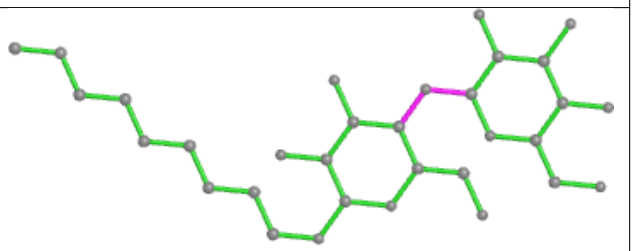


Rings

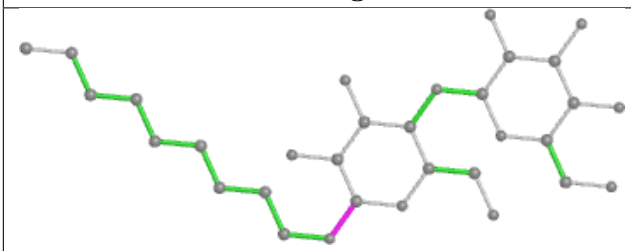
Ligand LMT U 101



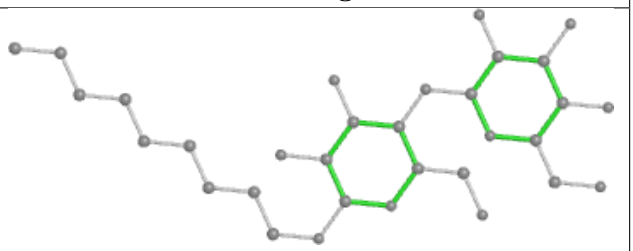
Bond lengths



Bond angles

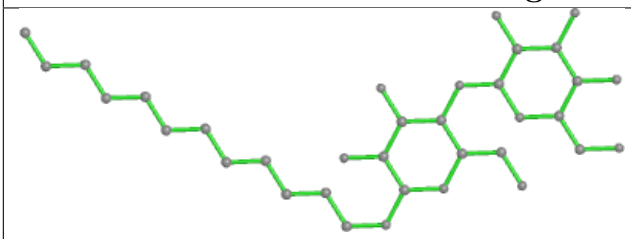


Torsions

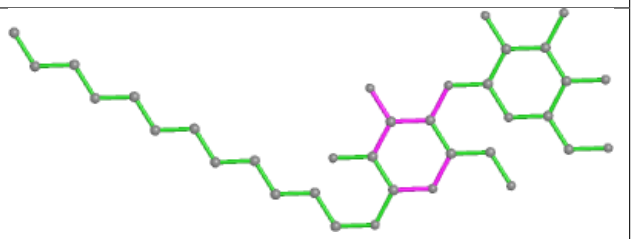


Rings

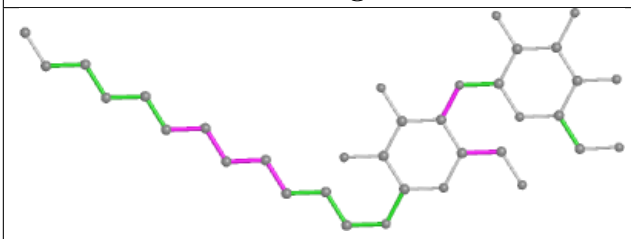
Ligand LMT 3 101



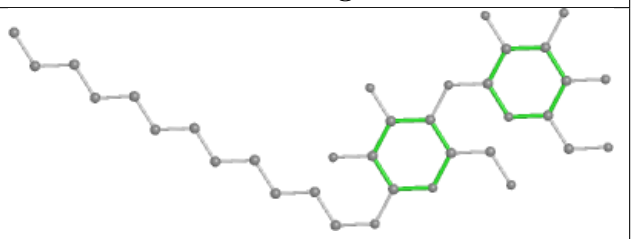
Bond lengths



Bond angles

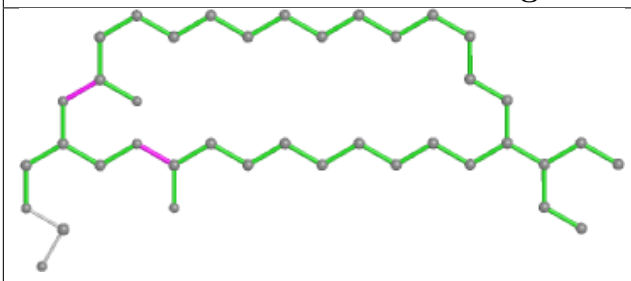


Torsions

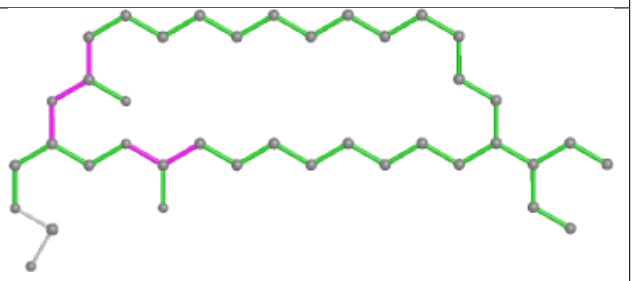


Rings

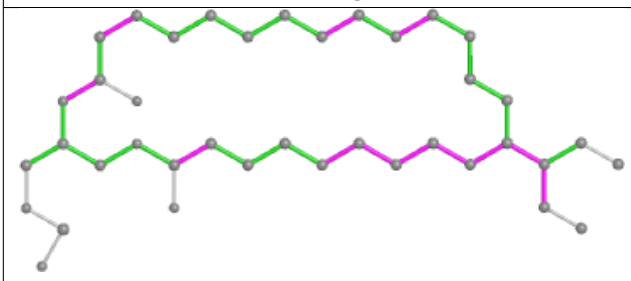
Ligand PGV K 104



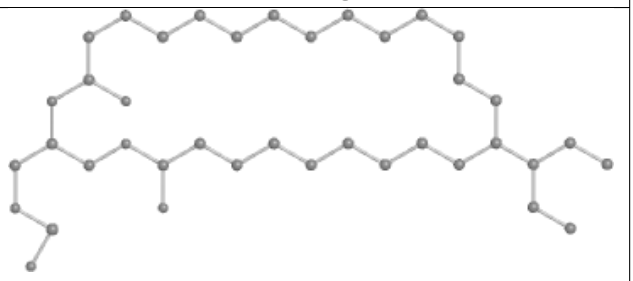
Bond lengths



Bond angles

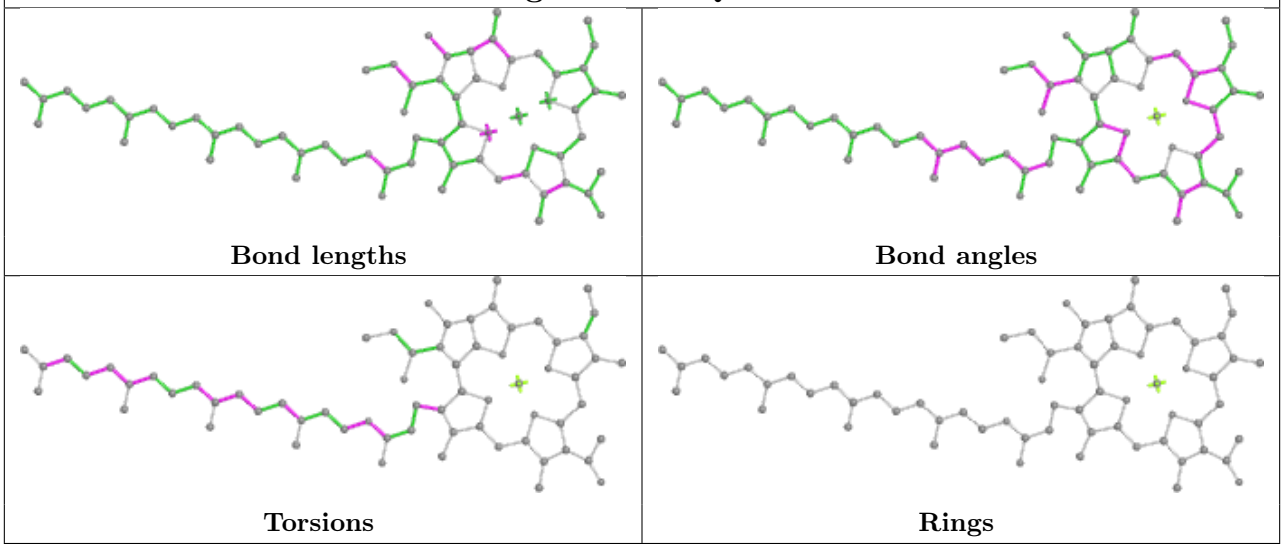


Torsions

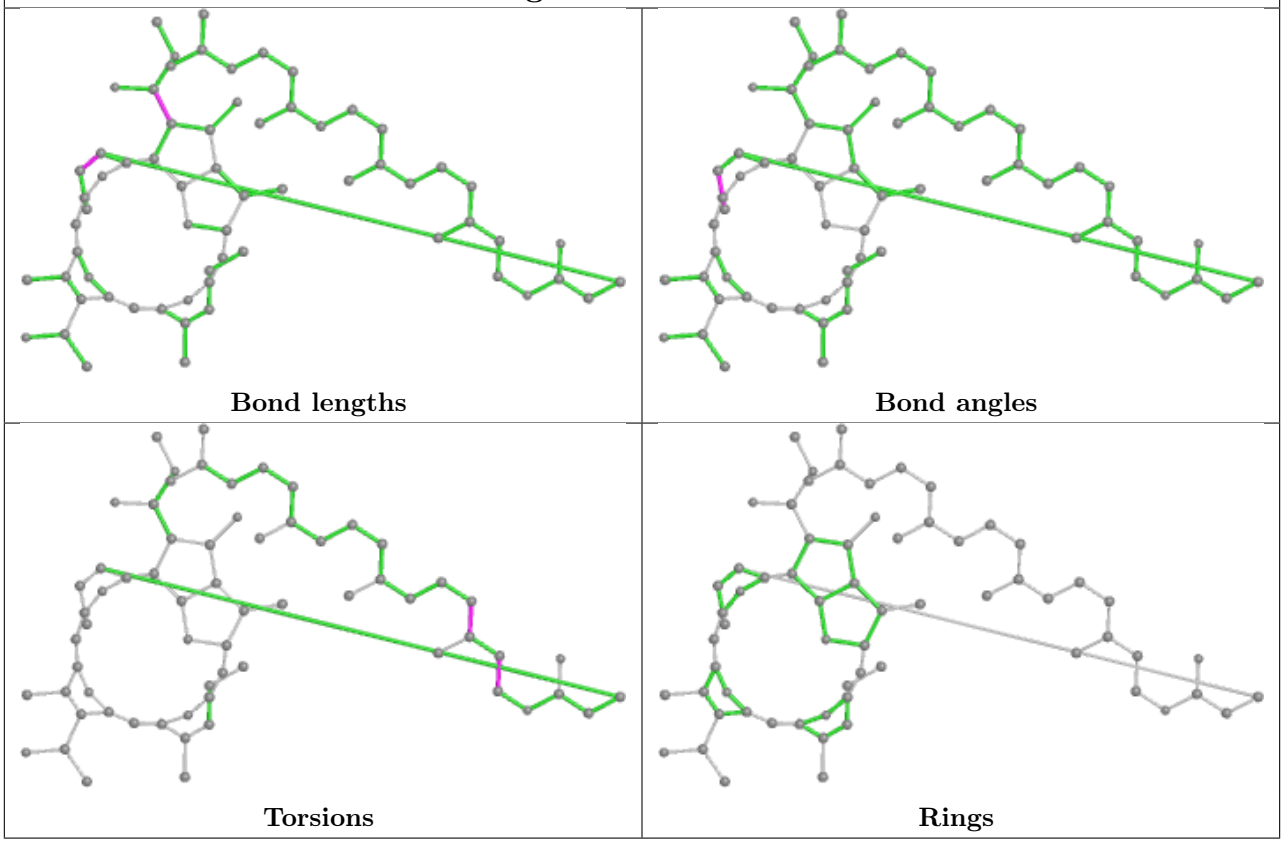


Rings

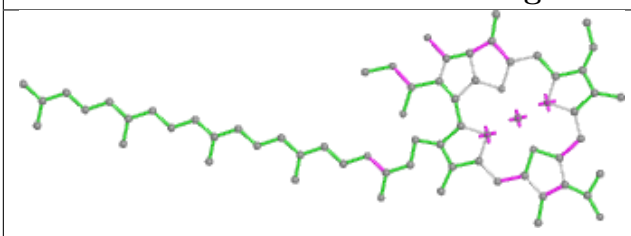
Ligand BCL Q 104



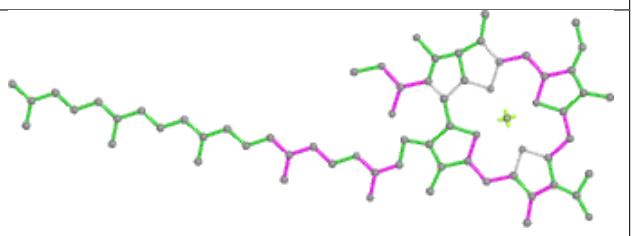
Ligand BPH L 302



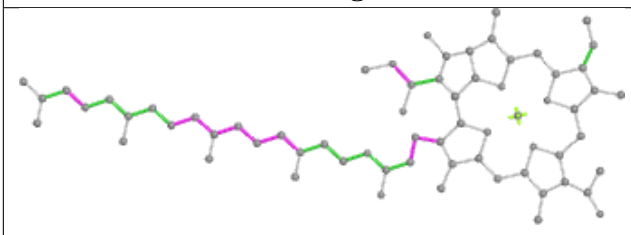
Ligand BCL G 101



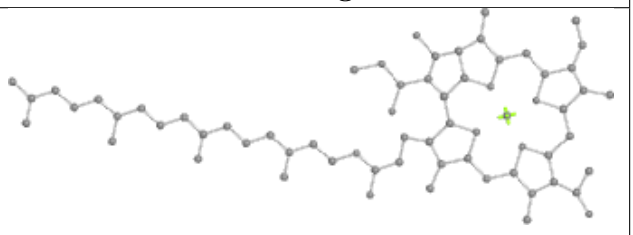
Bond lengths



Bond angles

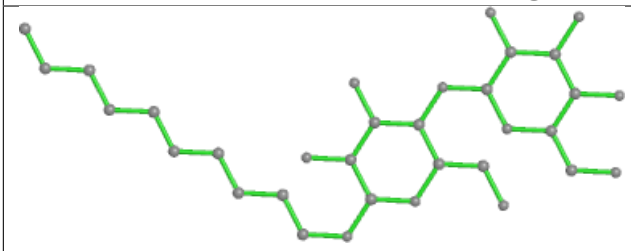


Torsions

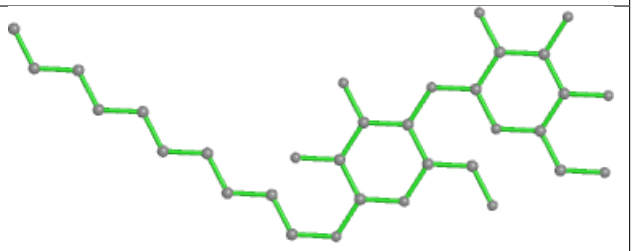


Rings

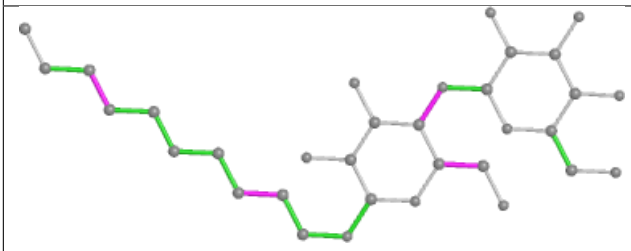
Ligand LMT 5 101



Bond lengths



Bond angles



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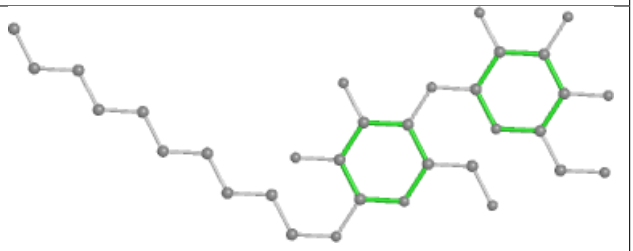
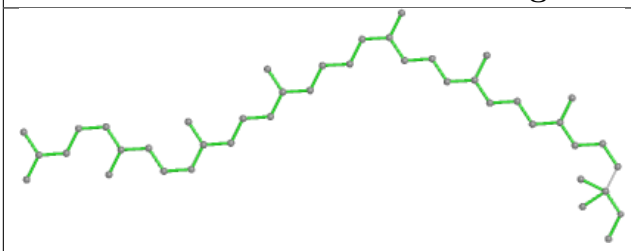


Rings

Ligand SPO 8 101



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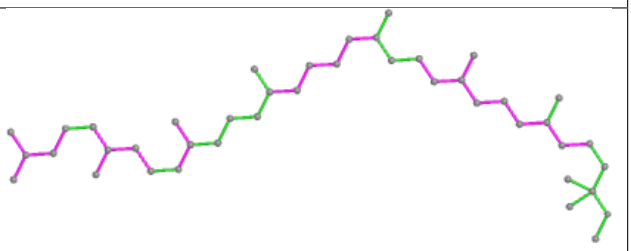
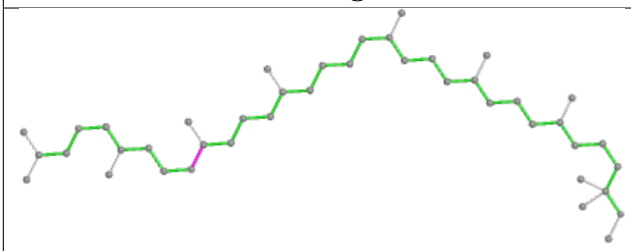


Bond angles



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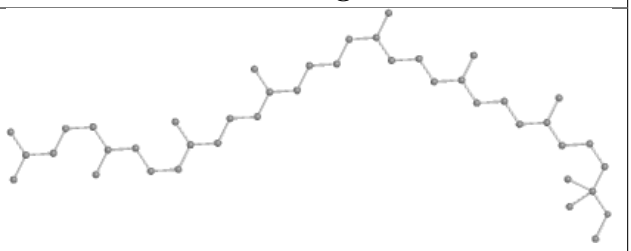
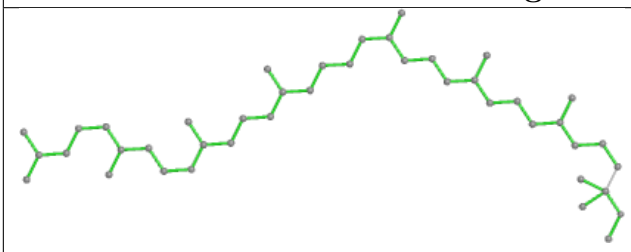


Rings

Ligand SPO G 103



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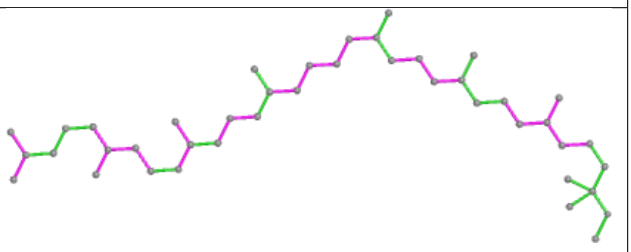
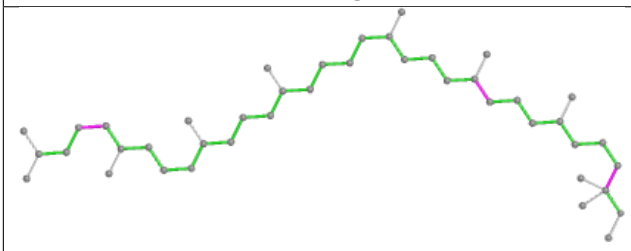


Bond angles



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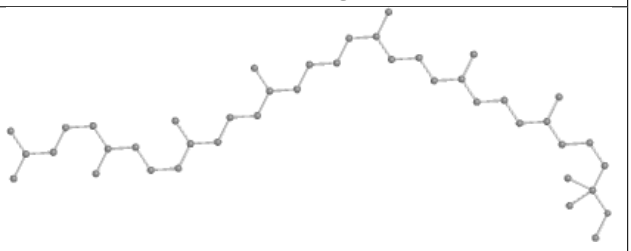
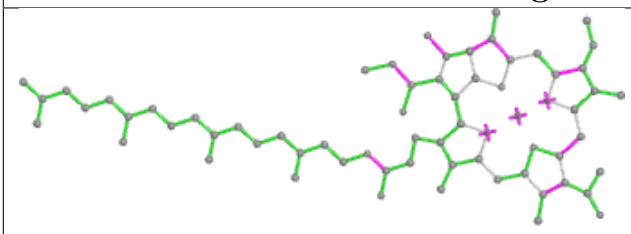


Rings

Ligand BCL I 101



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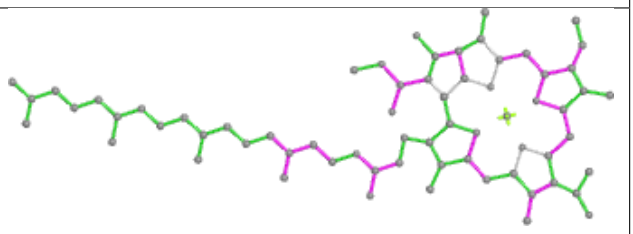
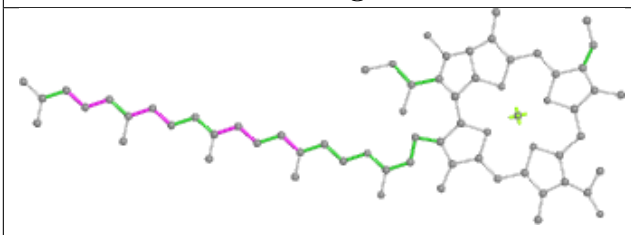


Bond angles



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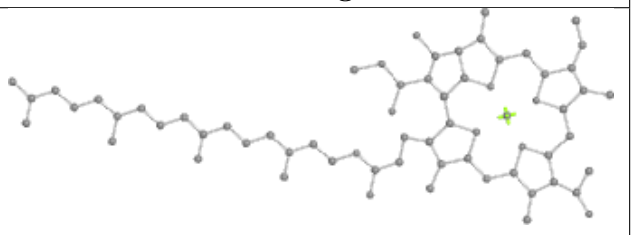
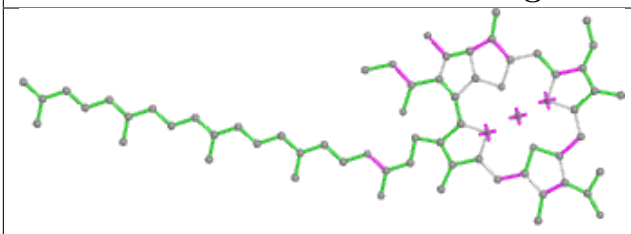
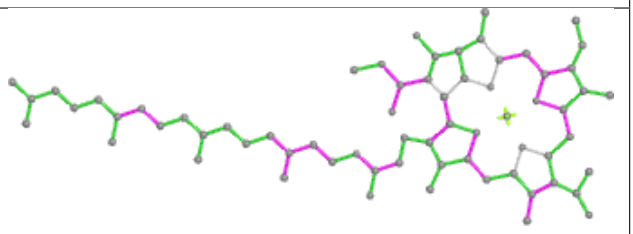


Rings

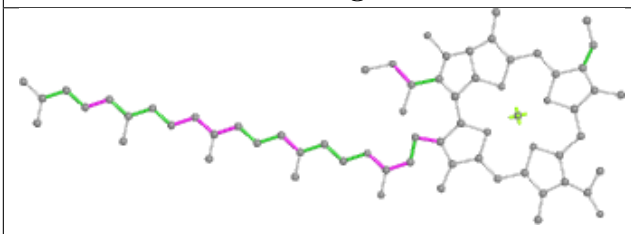
Ligand BCL N 102



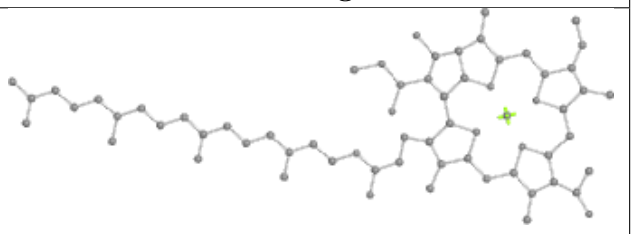
Bond lengths



Bond angles

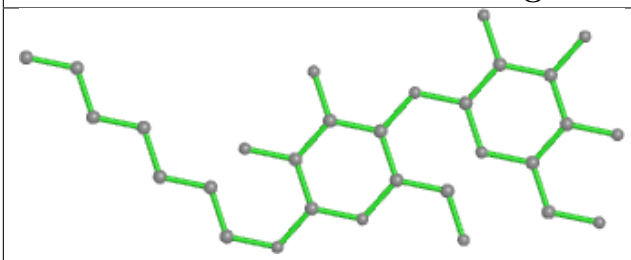


Torsions

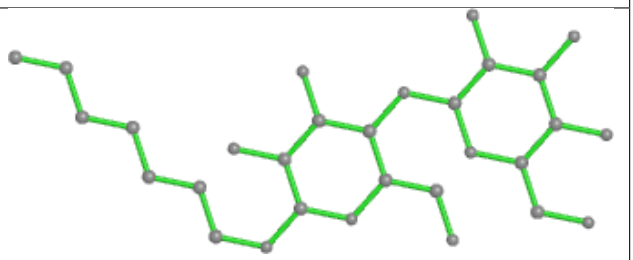


Rings

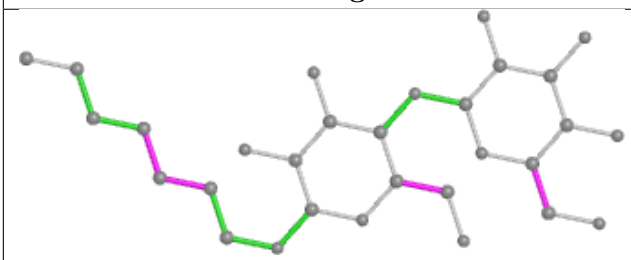
Ligand LMT S 105



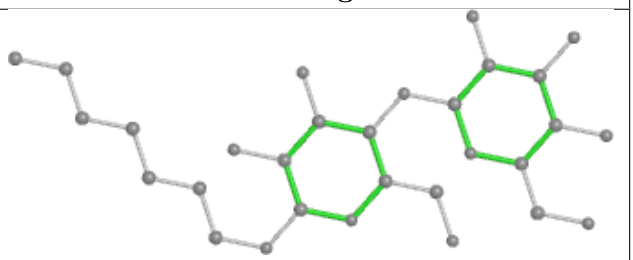
Bond lengths



Bond angles

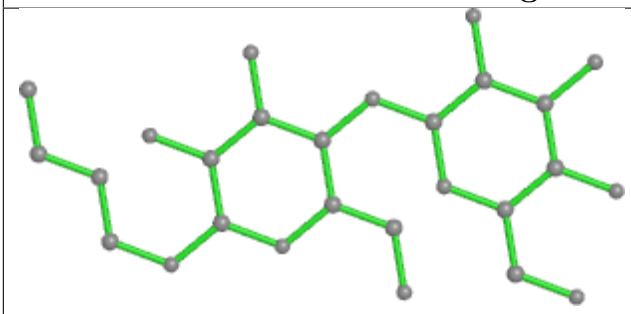


Torsions

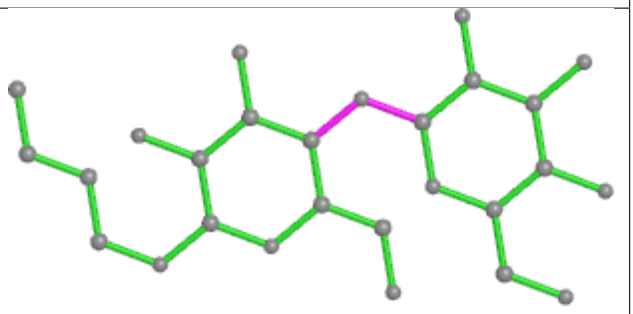


Rings

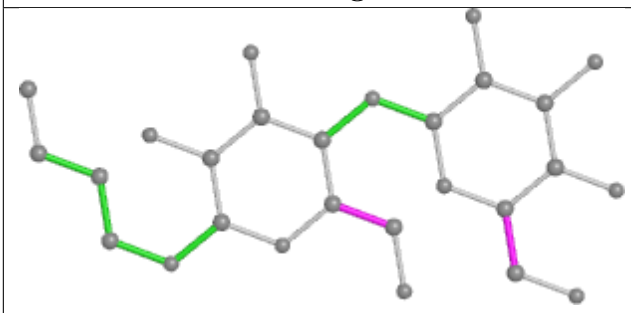
Ligand LMT D 103



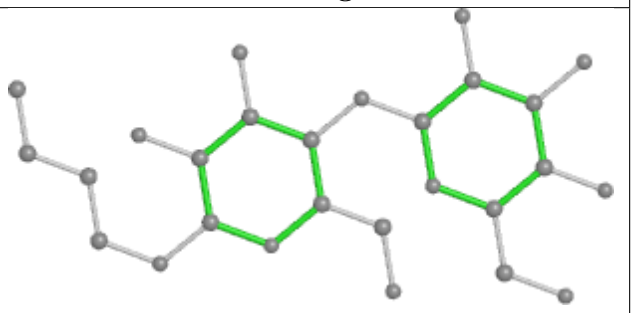
Bond lengths



Bond angles

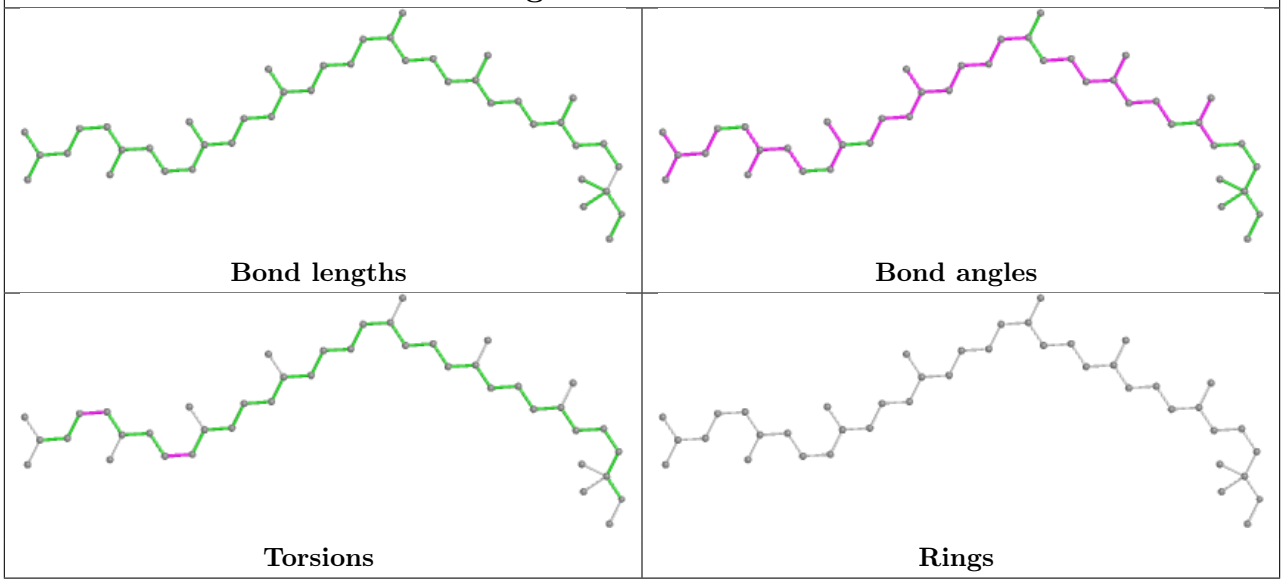


Torsions

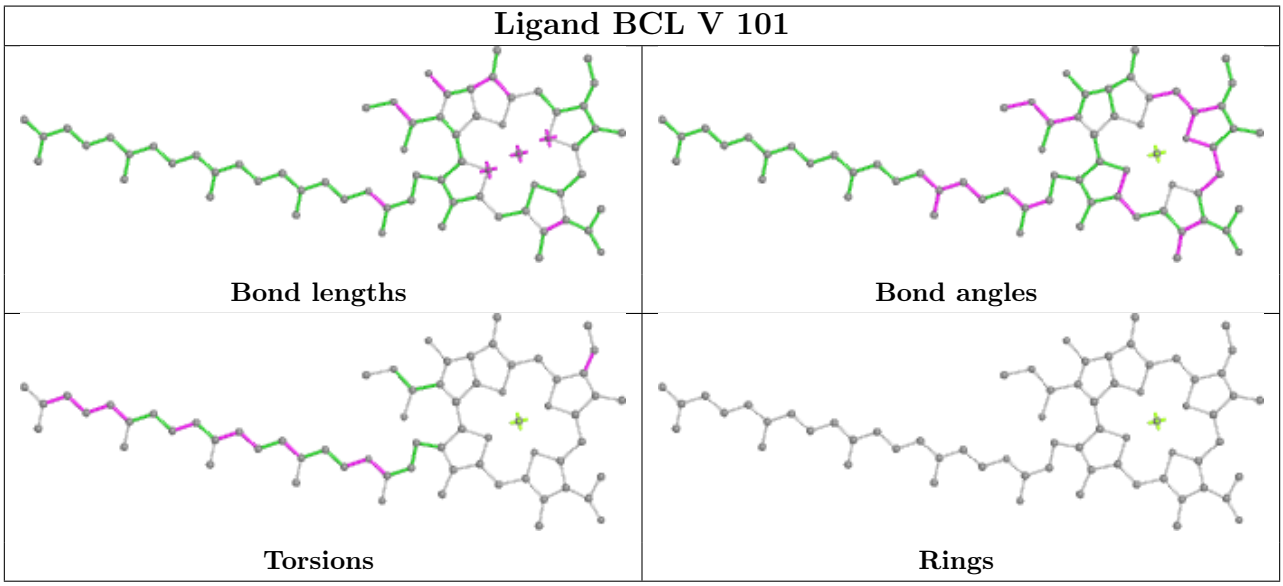


Rings

Ligand SPO D 102



Ligand BCL V 101



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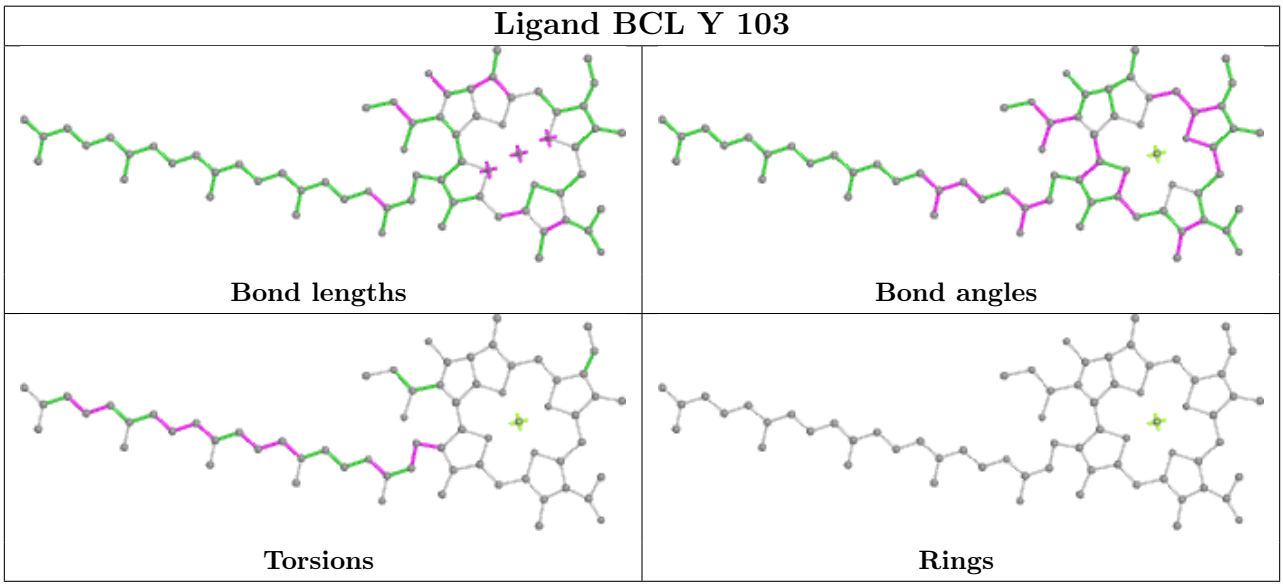
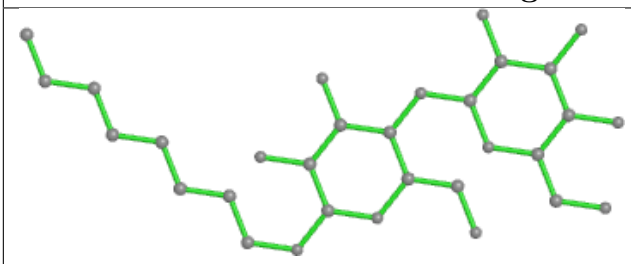
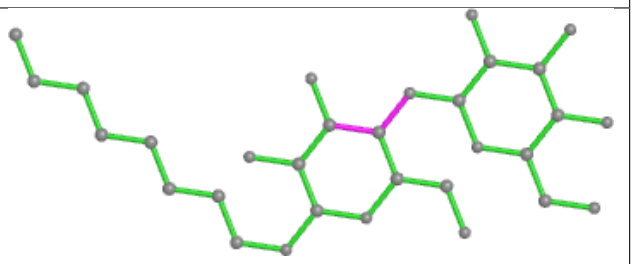


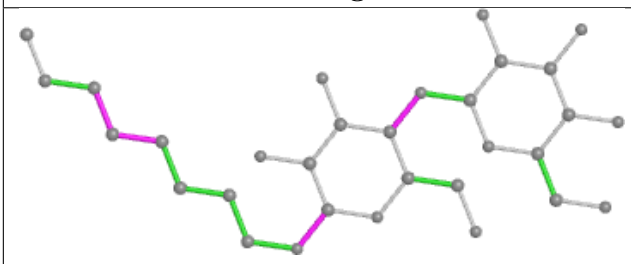
Ligand LMT X 105



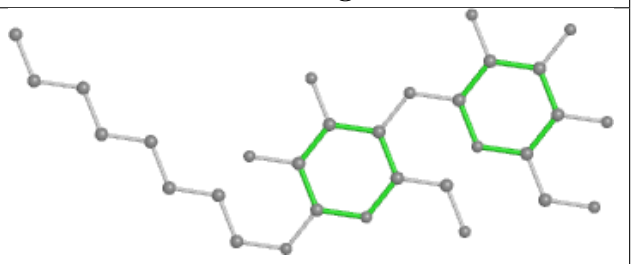
Bond lengths



Bond angles

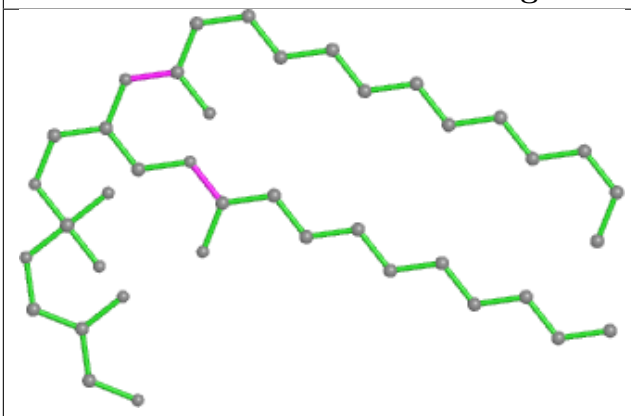


Torsions

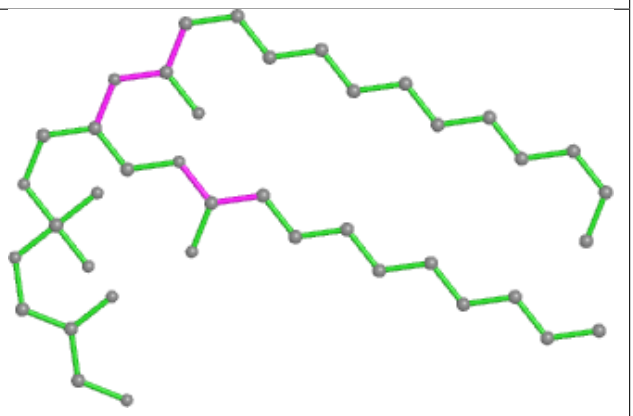


Rings

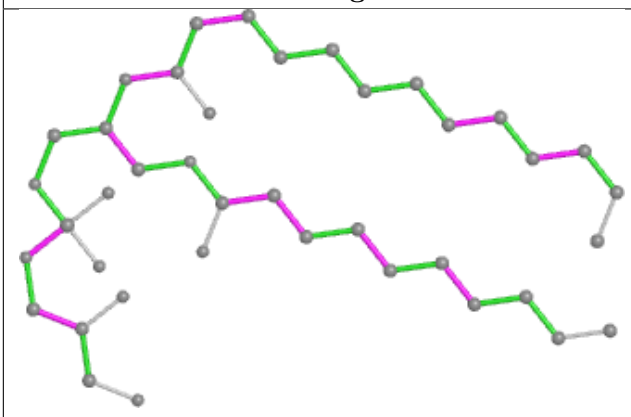
Ligand PGV H 306



Bond lengths



Bond angles



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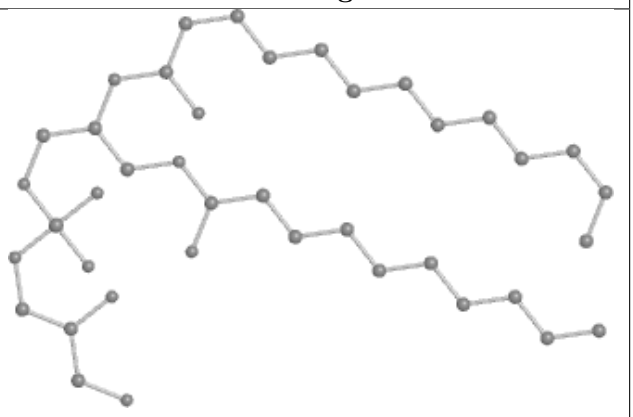
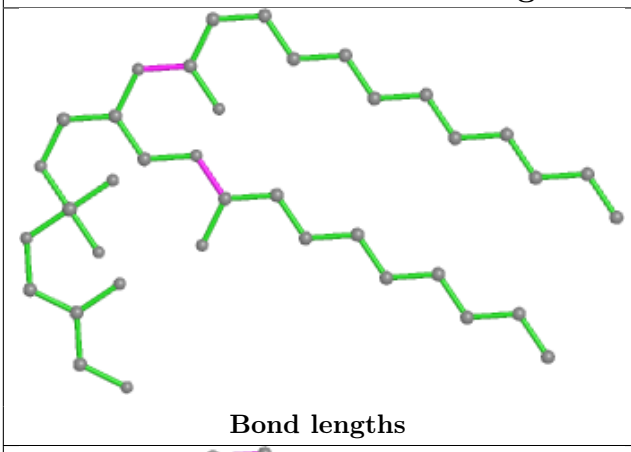
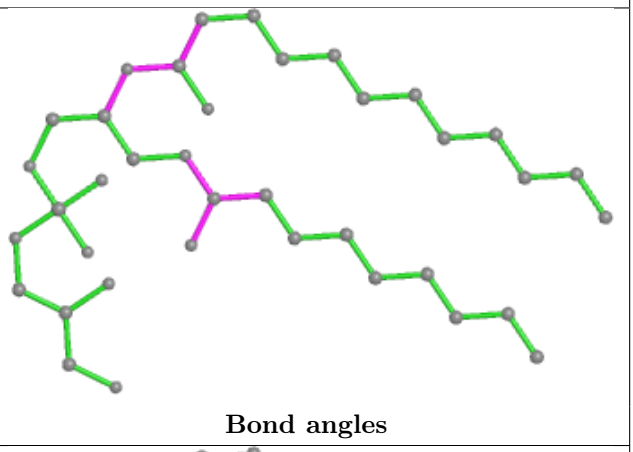


Rings

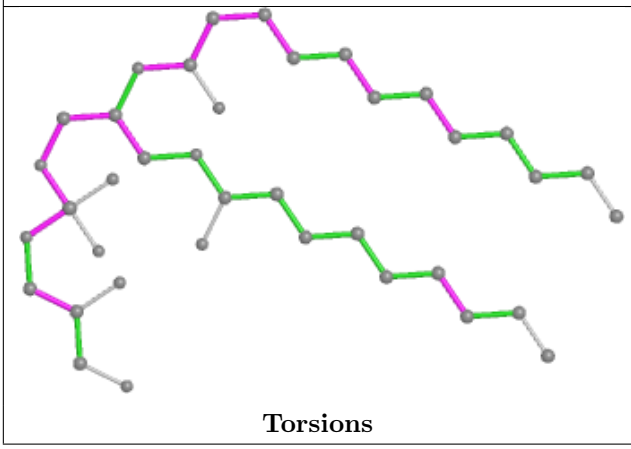
Ligand PGV M 812



Bond lengths



Bond angles



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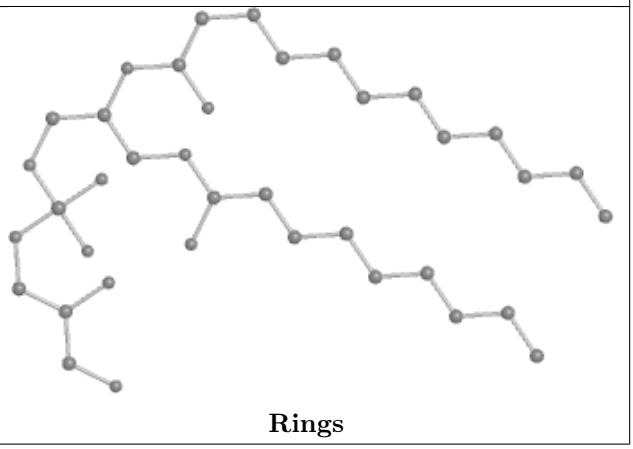
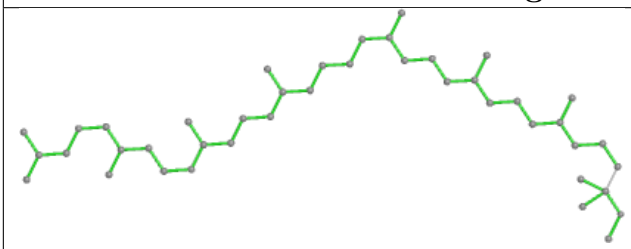
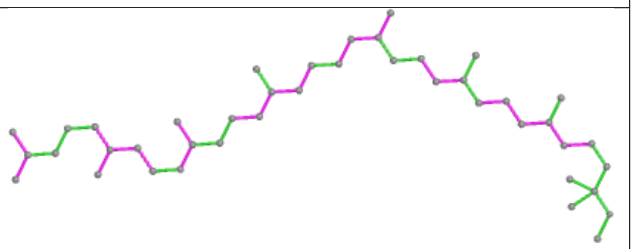


Rings

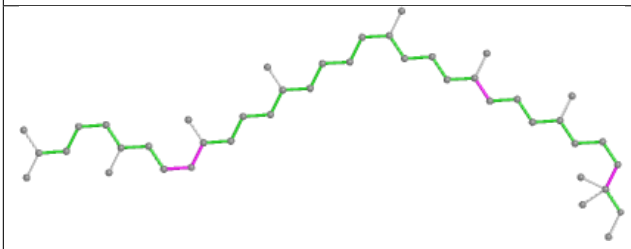
Ligand SPO O 102



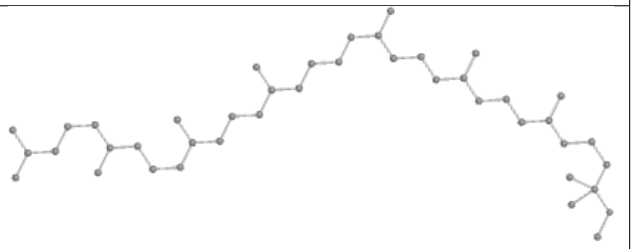
Bond lengths



Bond angles

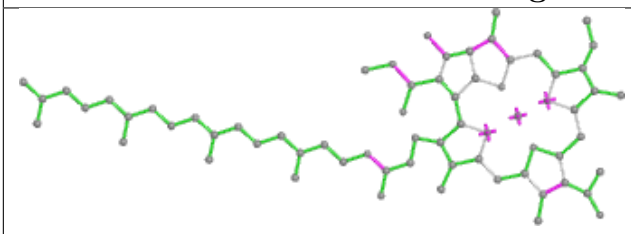


Torsions



Rings

Ligand BCL 5 102



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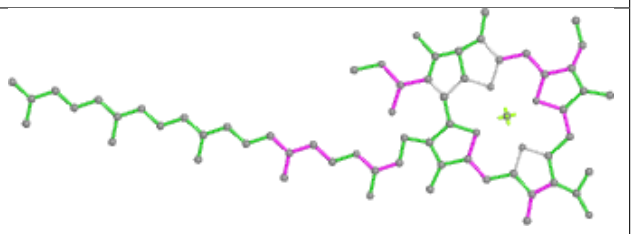
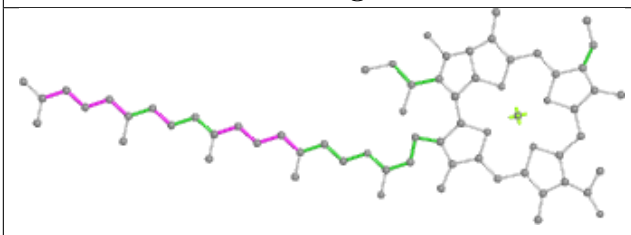
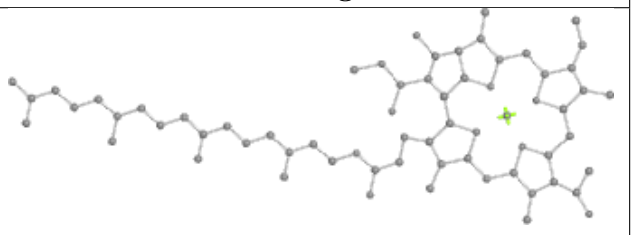


Bond angles

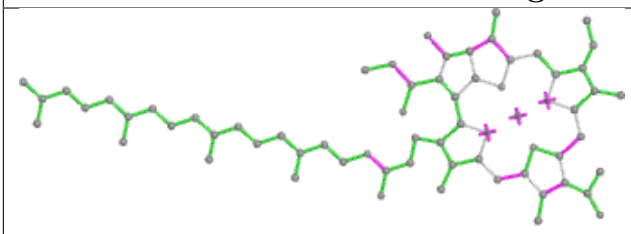


Torsions



Rings

Ligand BCL L 301



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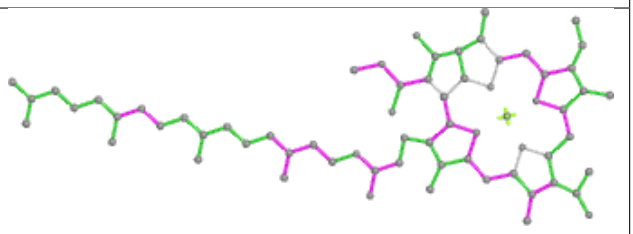
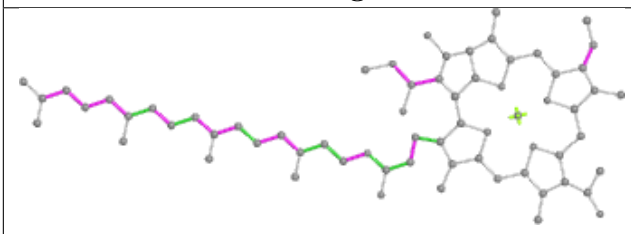
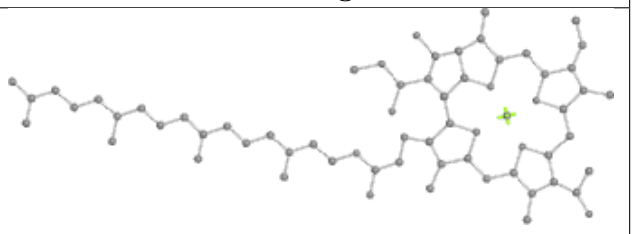


Bond angles

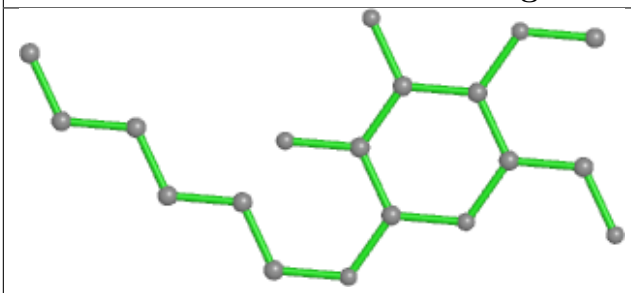


Torsions



Rings

Ligand LMT Q 102



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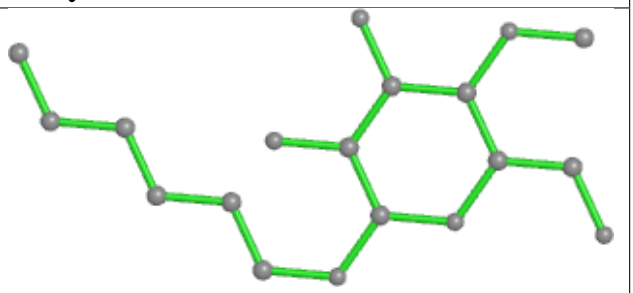
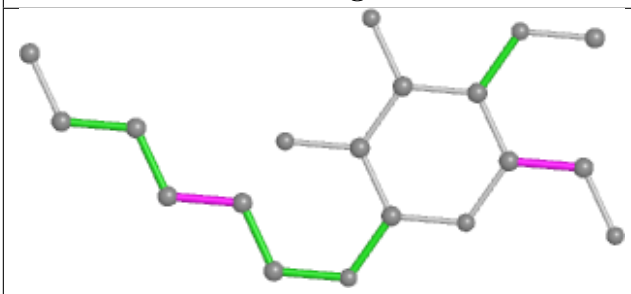
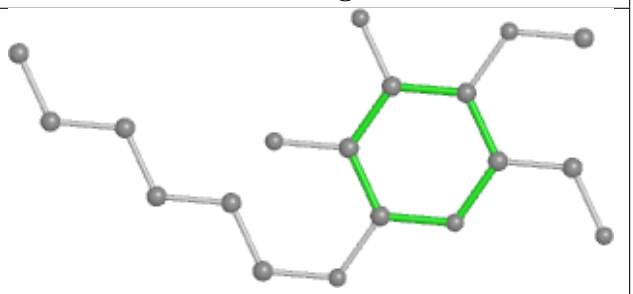


Bond angles

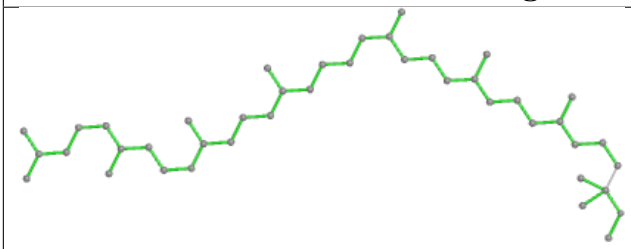


Torsions

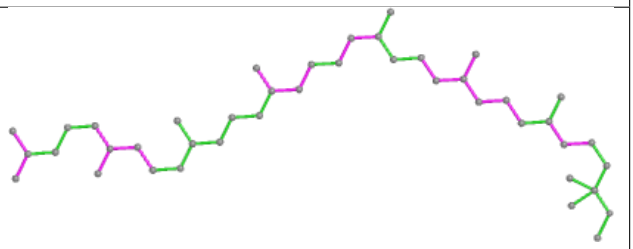


Rings

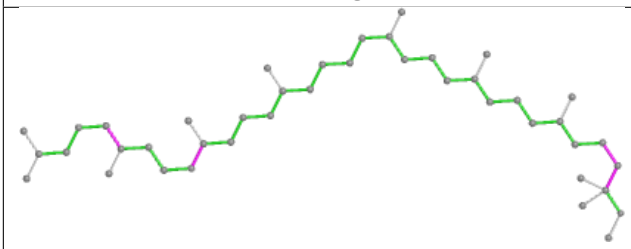
Ligand SPO M 807



Bond lengths



Bond angles



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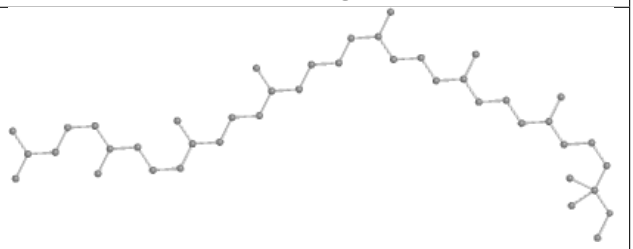
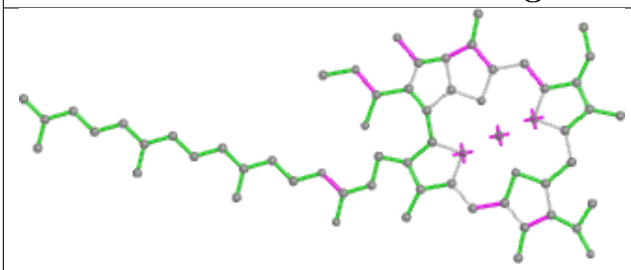


Rings

Ligand BCL A 703



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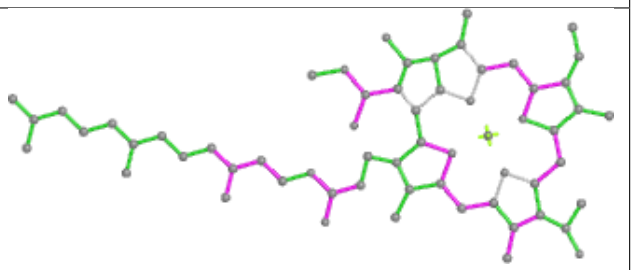
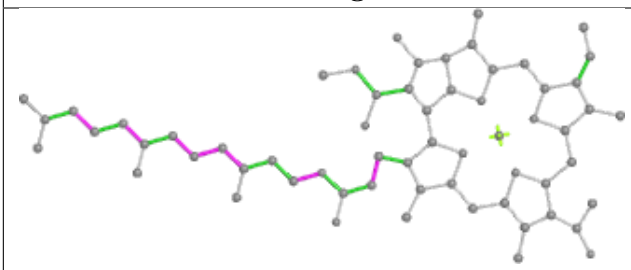
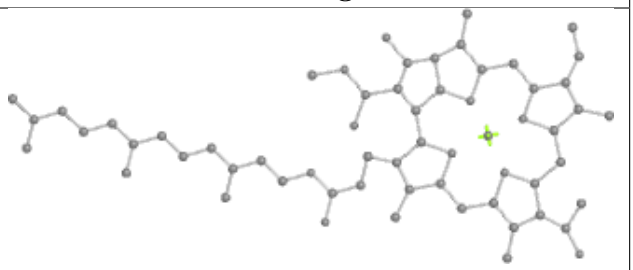


Bond angles

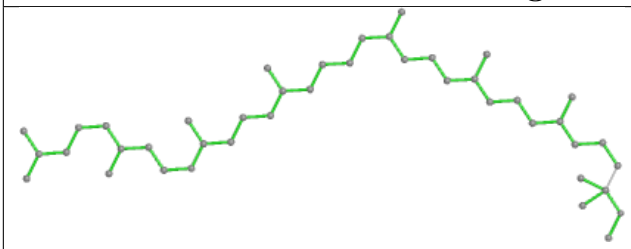


Torsions



Rings

Ligand SPO P 101



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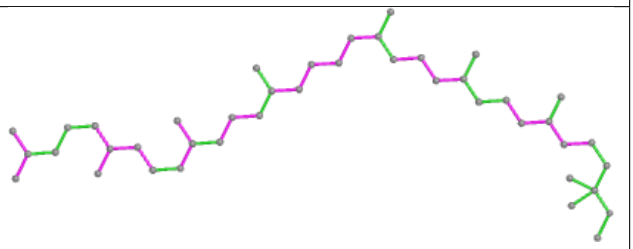
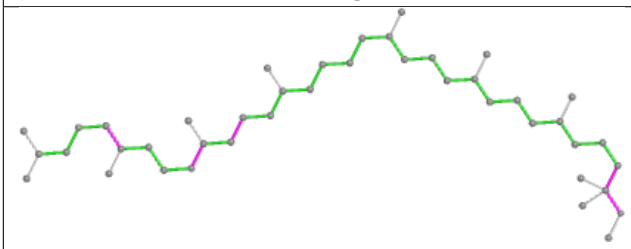
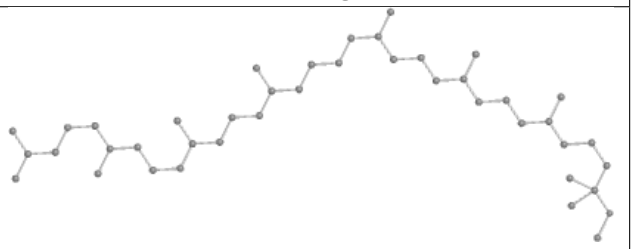


Bond angles

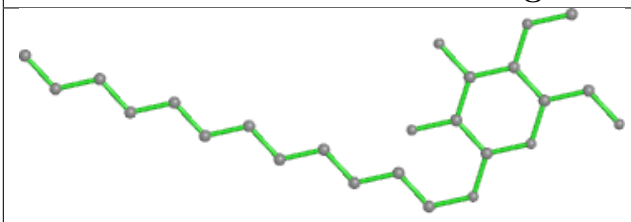


Torsions

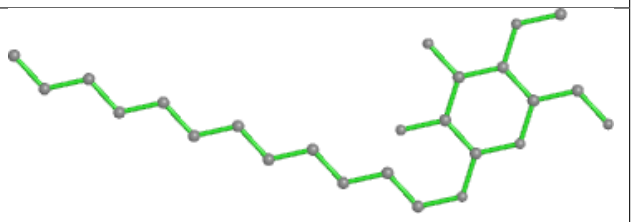


Rings

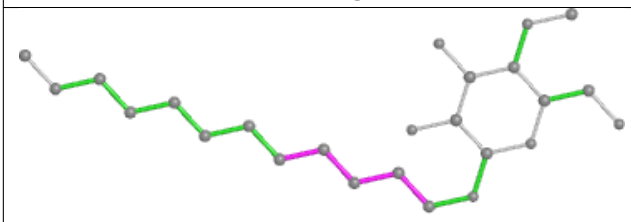
Ligand LMT S 101



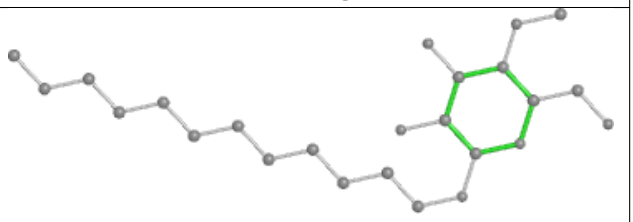
Bond lengths



Bond angles

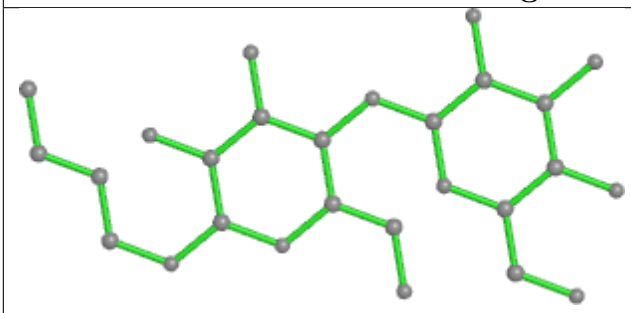


Torsions

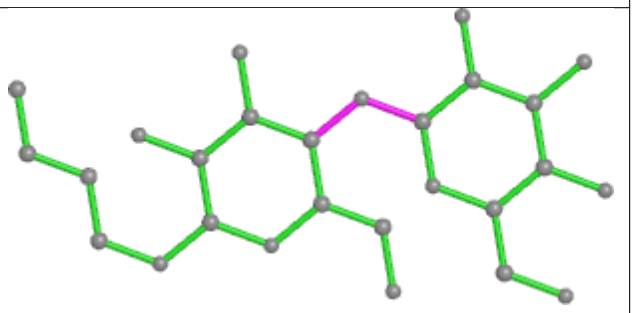


Rings

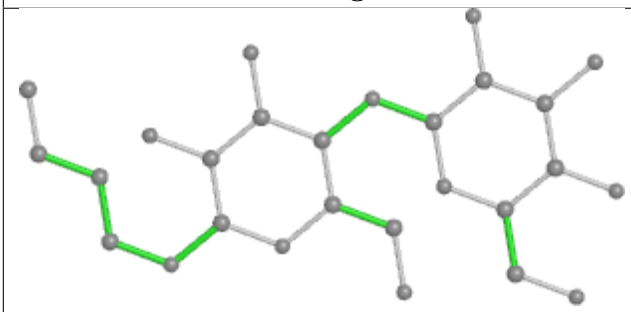
Ligand LMT A 704



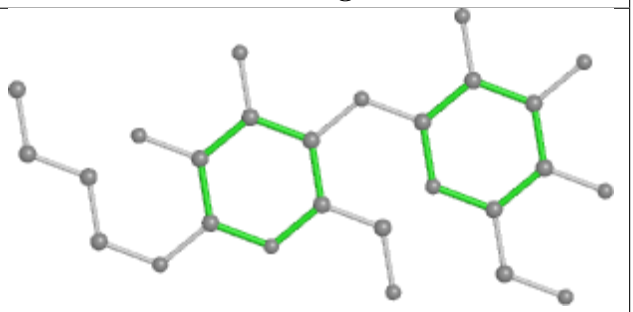
Bond lengths



Bond angles

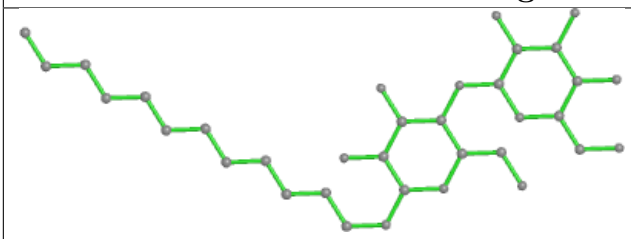


Torsions

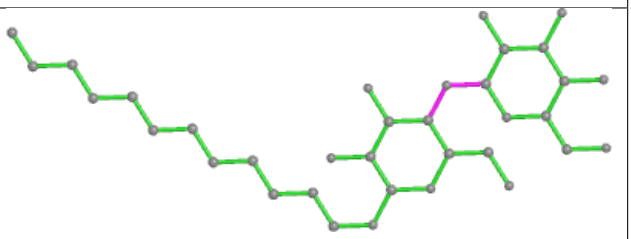


Rings

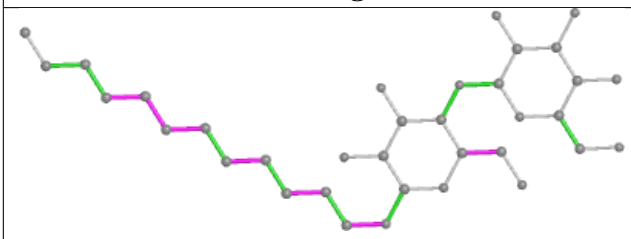
Ligand LMT M 809



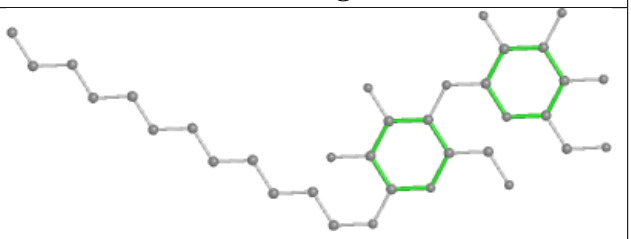
Bond lengths



Bond angles

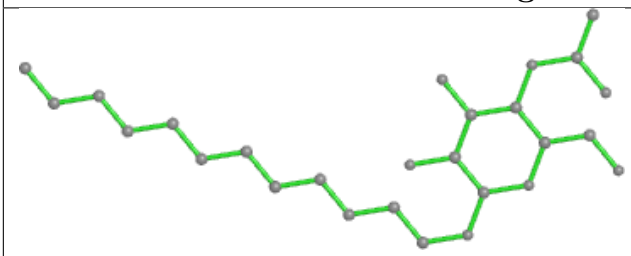


Torsions



Rings

Ligand LMT M 808



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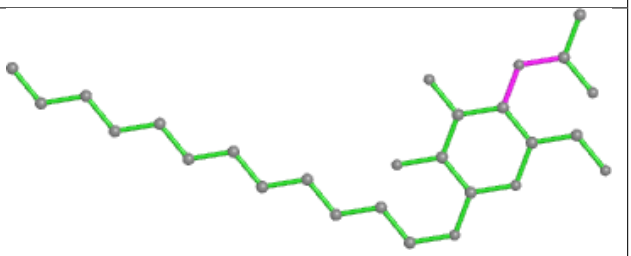
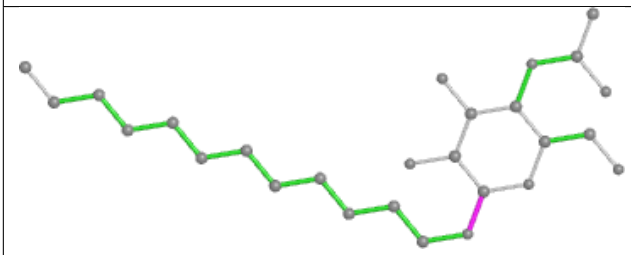
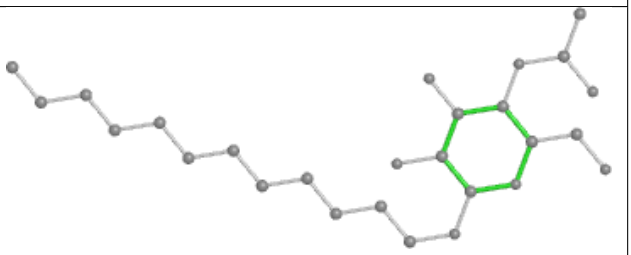


Bond angles

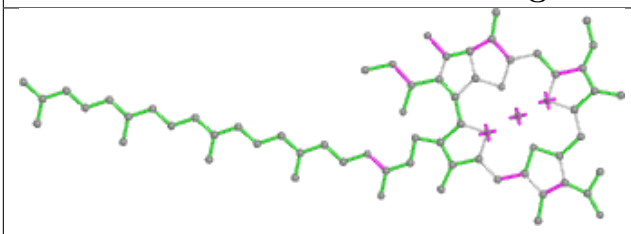


Torsions



Rings

Ligand BCL 2 101



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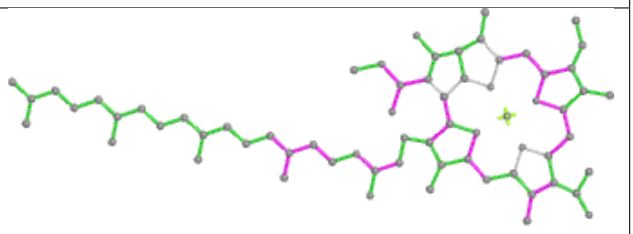
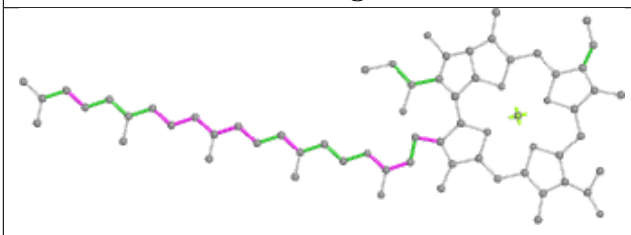
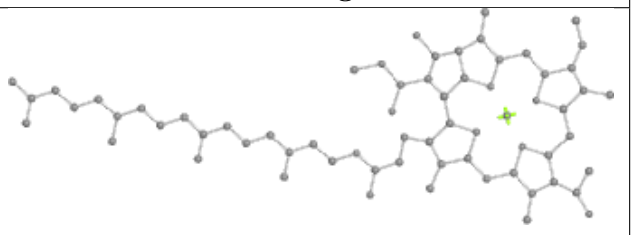


Bond angles

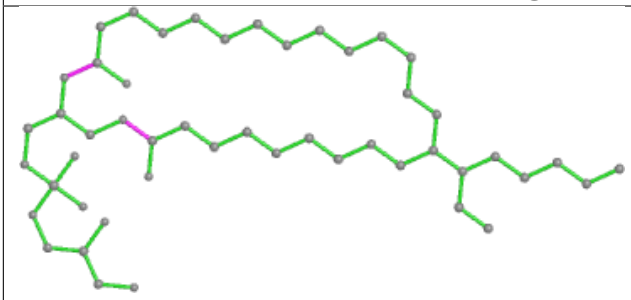


Torsions



Rings

Ligand PGV 3 102



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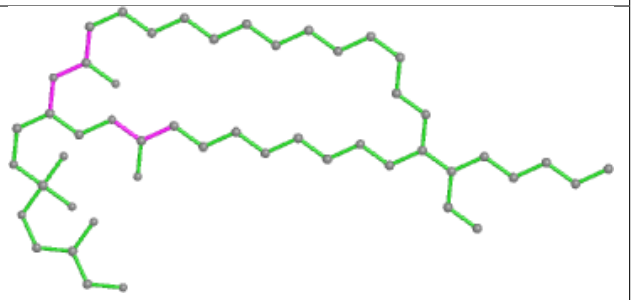
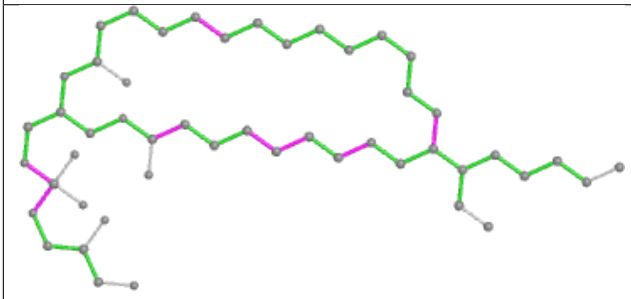
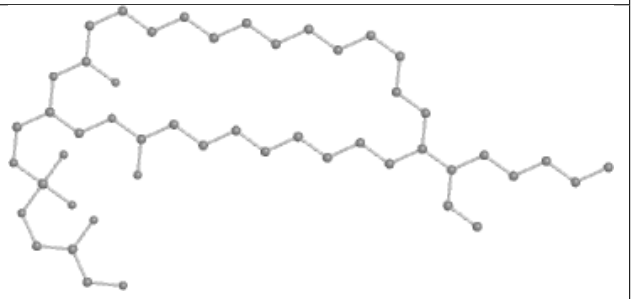


Bond angles

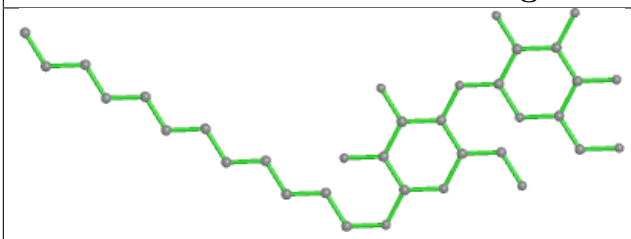


Torsions

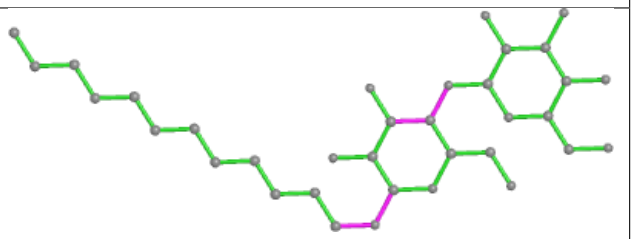


Rings

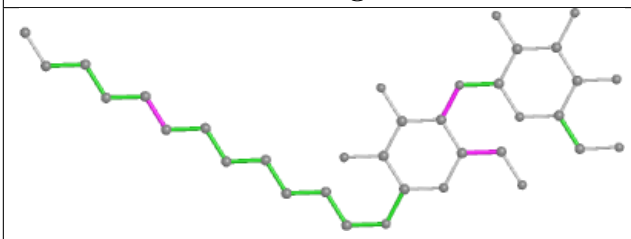
Ligand LMT H 301



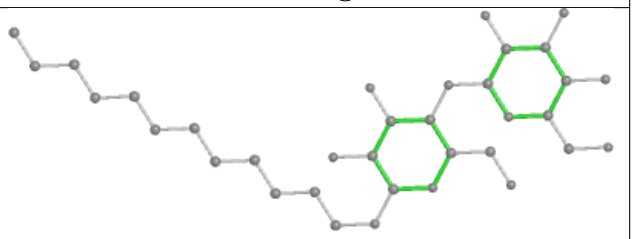
Bond lengths



Bond angles

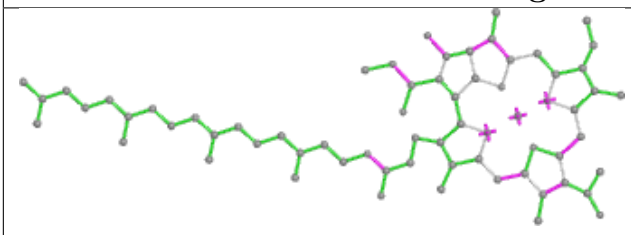


Torsions

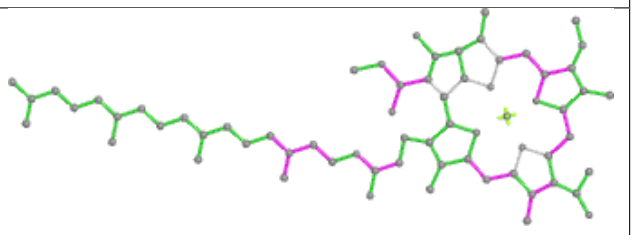


Rings

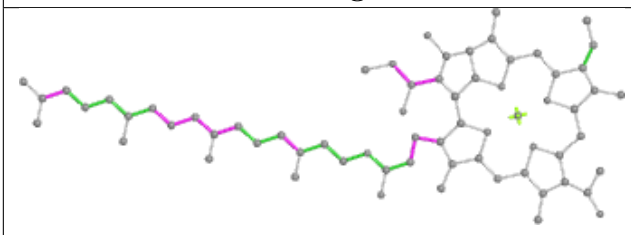
Ligand BCL 6 101



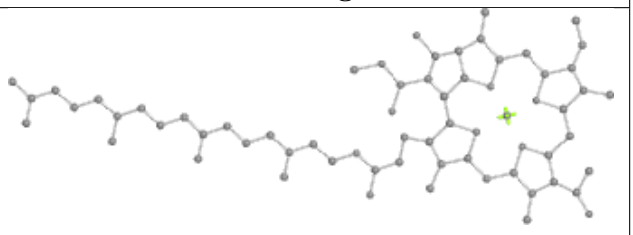
Bond lengths



Bond angles

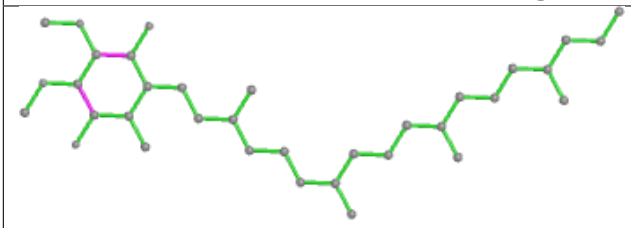


Torsions

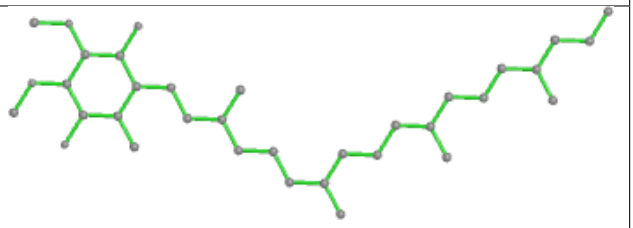


Rings

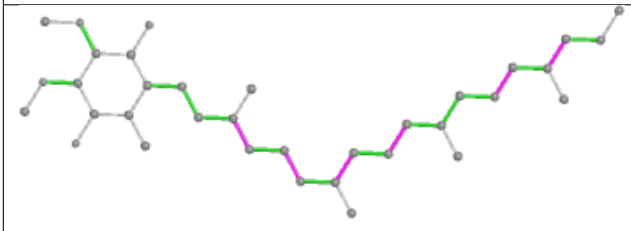
Ligand U10 L 303



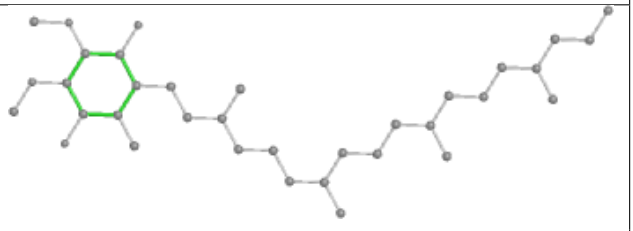
Bond lengths



Bond angles

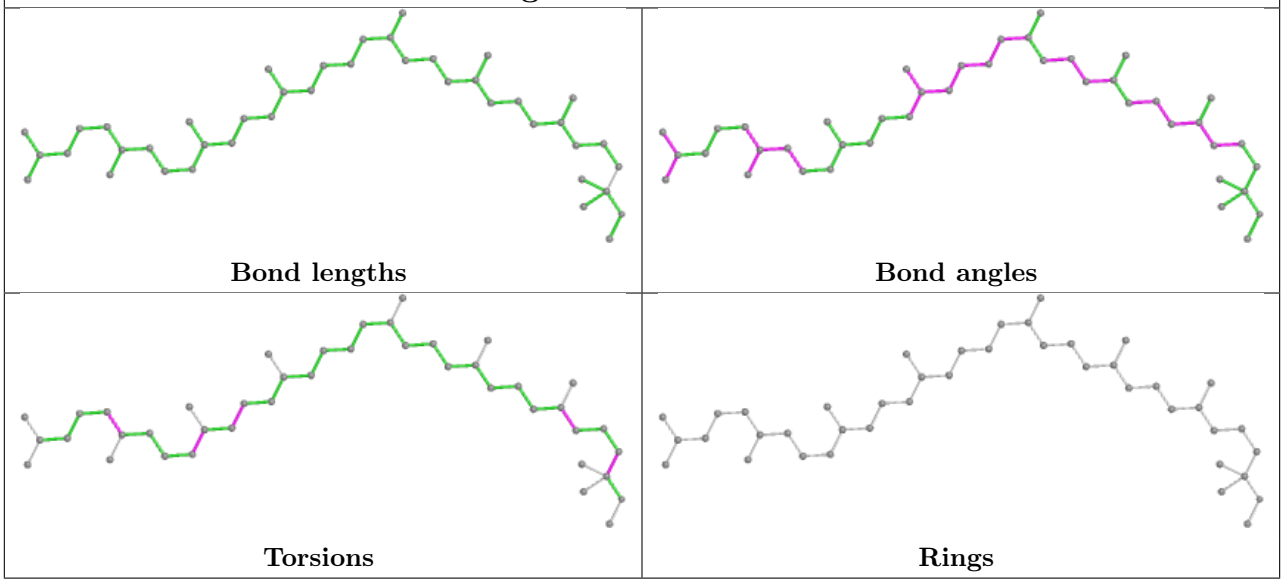


Torsions

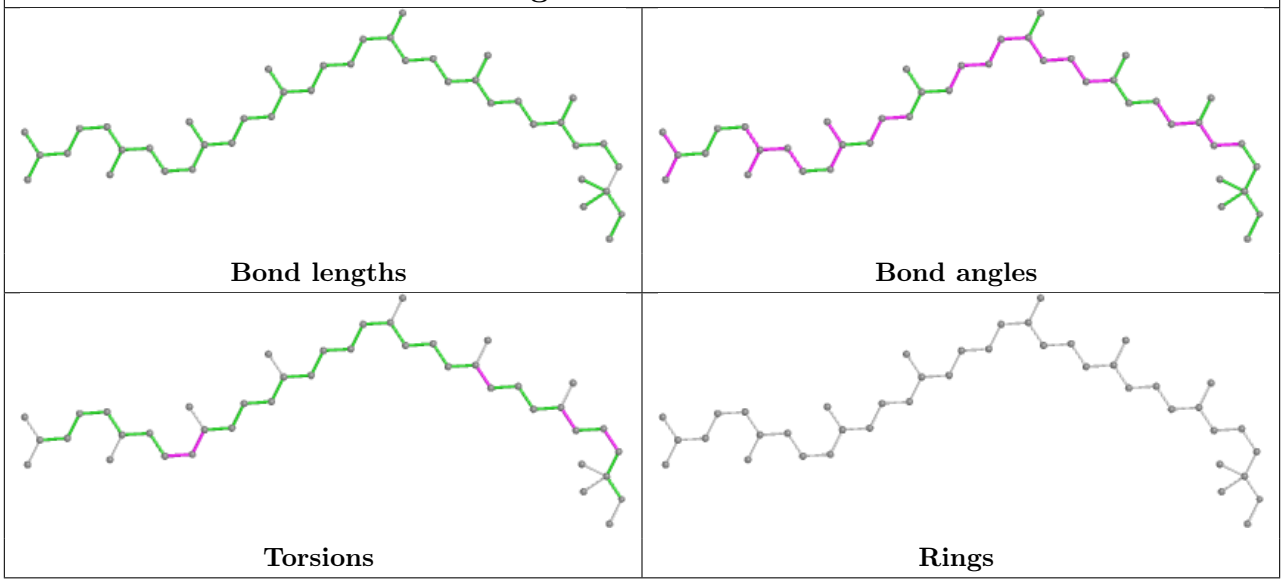


Rings

Ligand SPO W 102



Ligand SPO 5 104



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

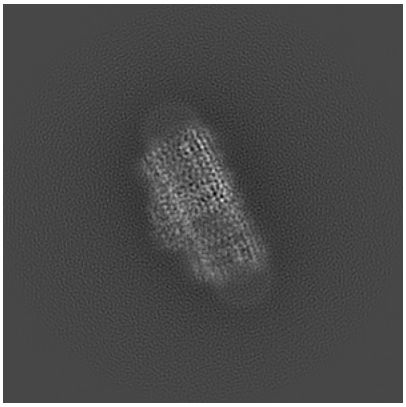
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31400. These allow visual inspection of the internal detail of the map and identification of artifacts.

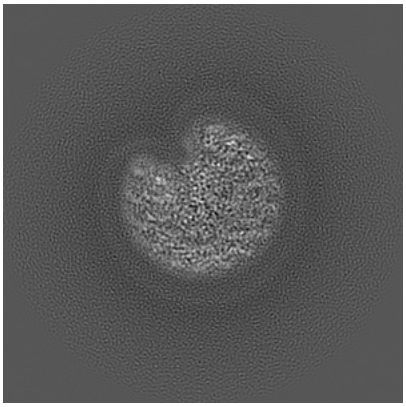
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

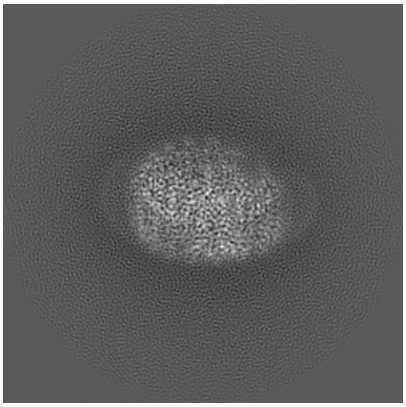
6.1.1 Primary map



X



Y

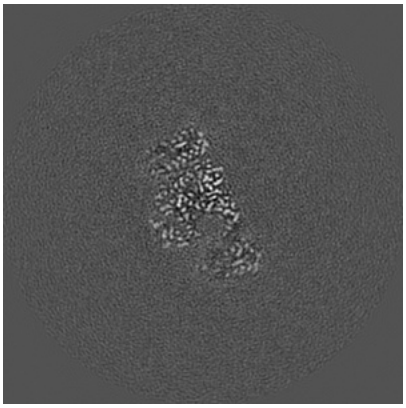


Z

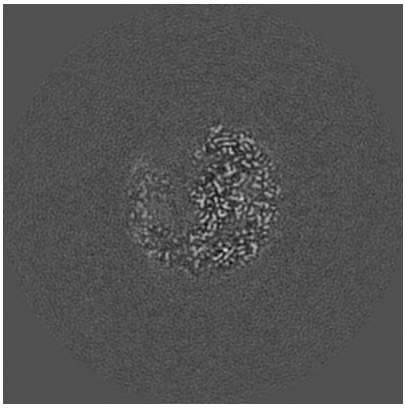
The images above show the map projected in three orthogonal directions.

6.2 Central slices

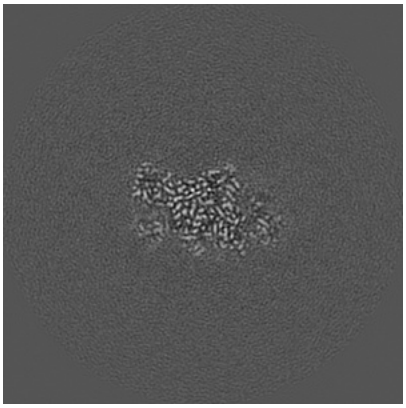
6.2.1 Primary map



X Index: 140



Y Index: 140

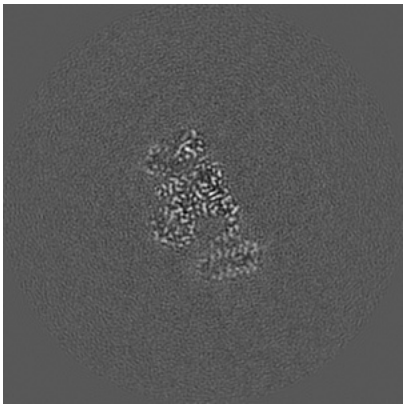


Z Index: 140

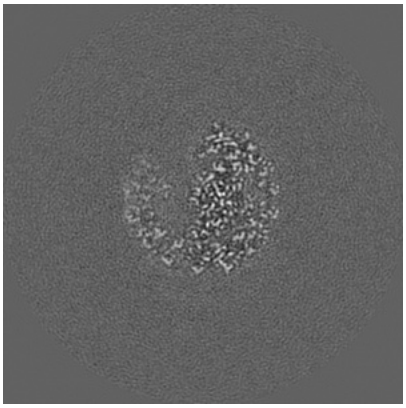
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

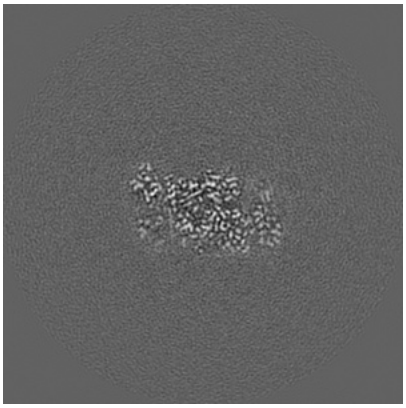
6.3.1 Primary map



X Index: 142



Y Index: 142



Z Index: 142

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 0.064. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

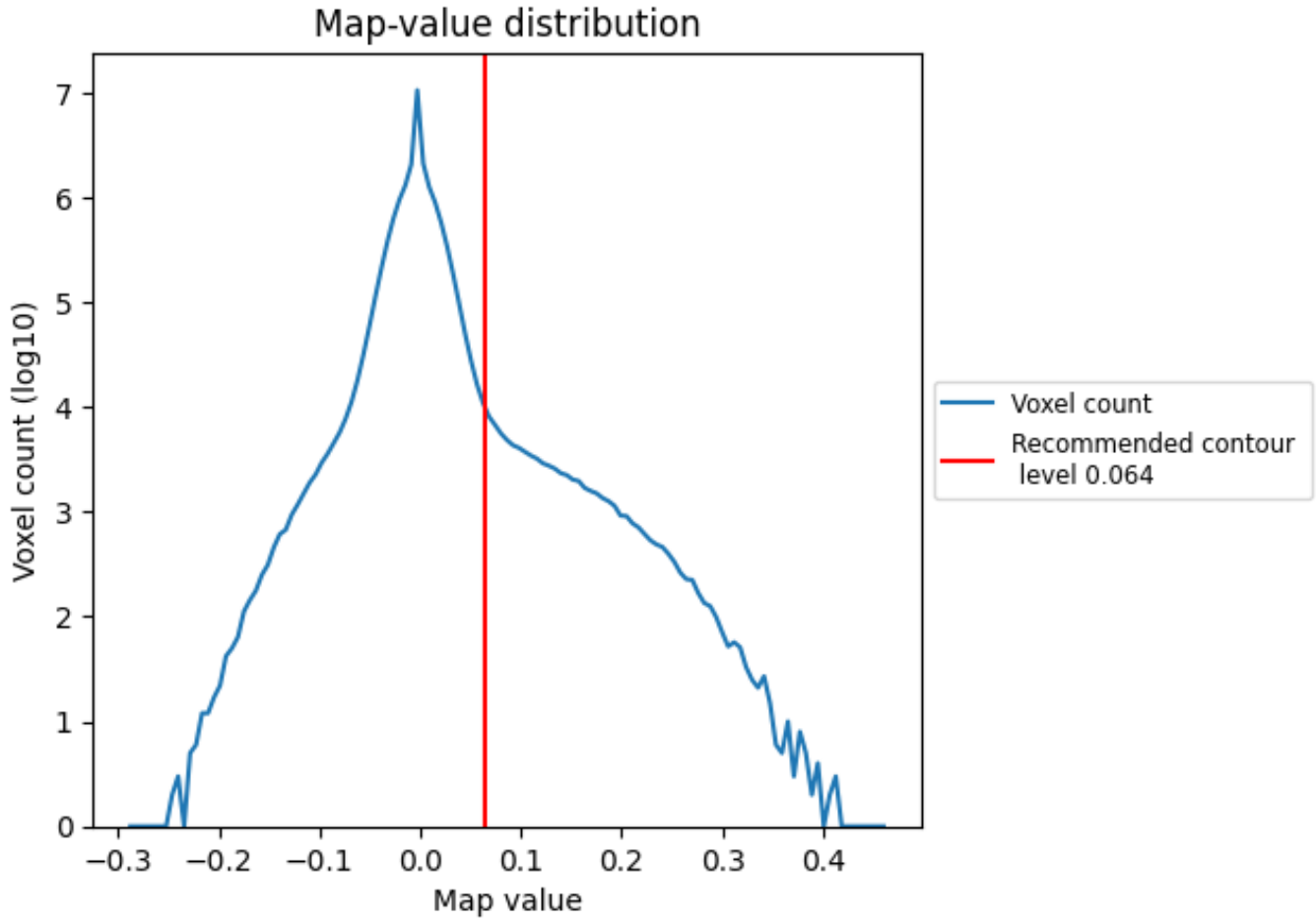
6.5 Mask visualisation (i)

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

7 Map analysis

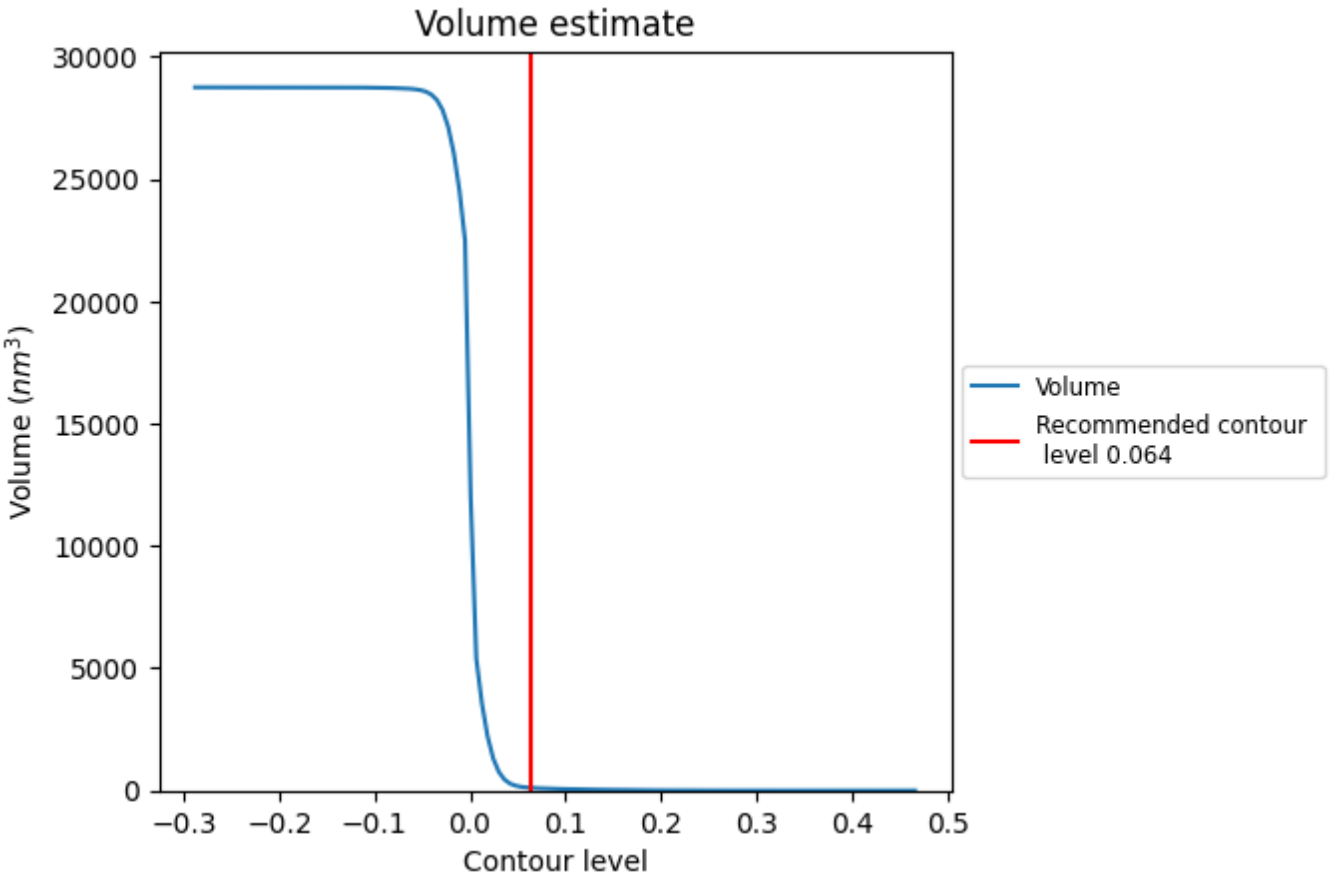
This section contains the results of statistical analysis of the map.

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.

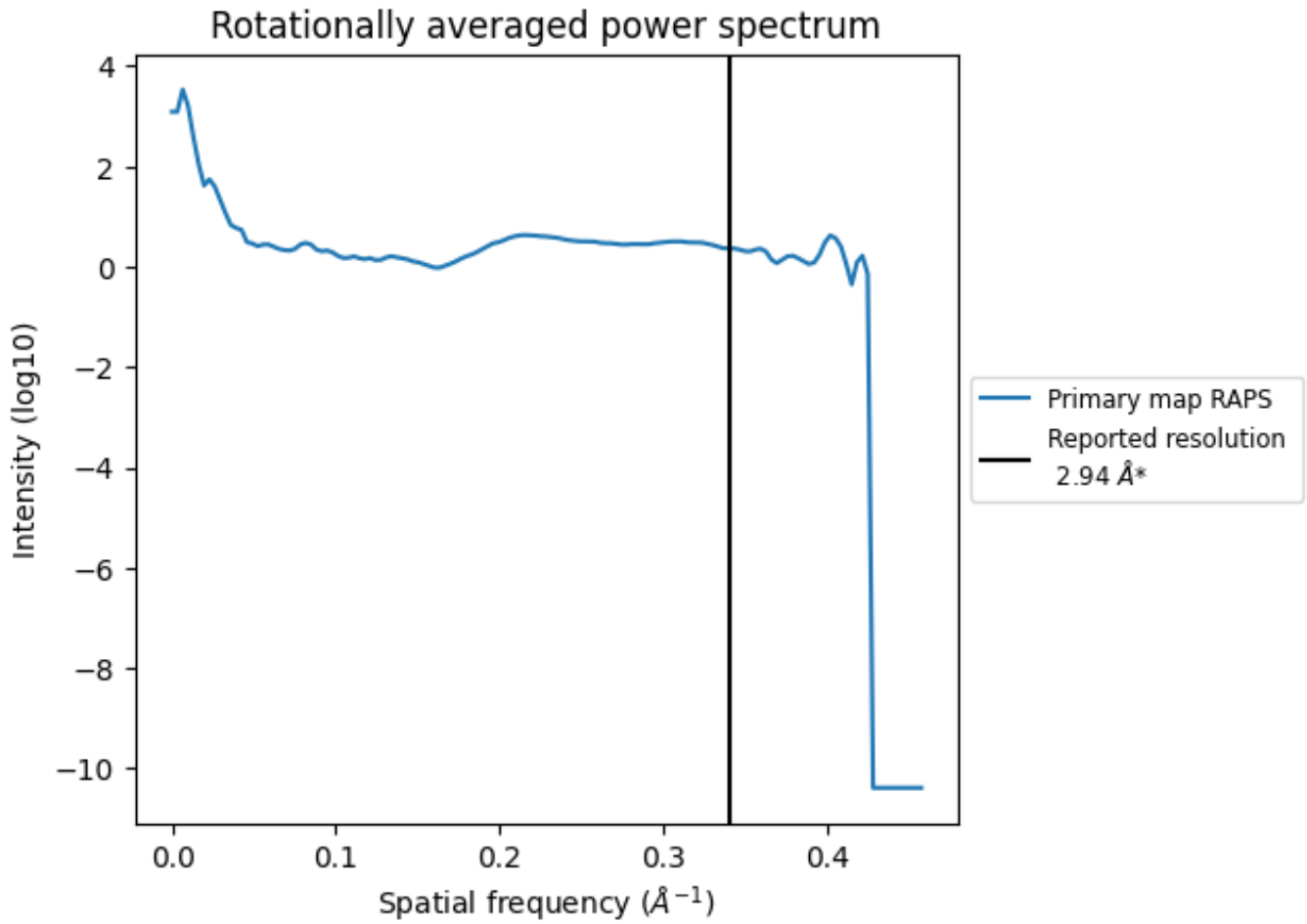
7.2 Volume estimate



The volume at the recommended contour level is 112 nm^3; this corresponds to an approximate mass of 101 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)

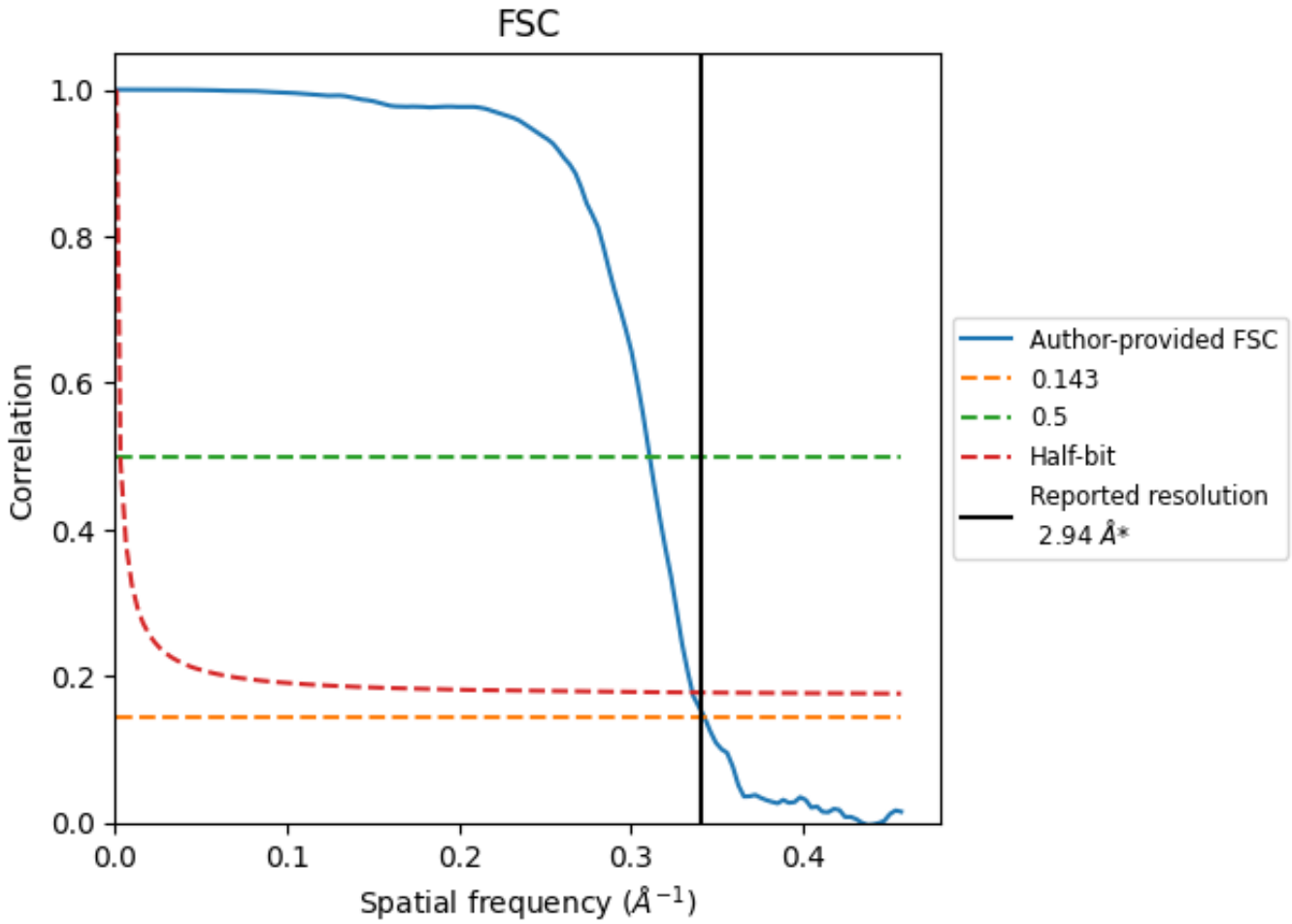


*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

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 0.340 Å^{-1}

8.2 Resolution estimates (i)

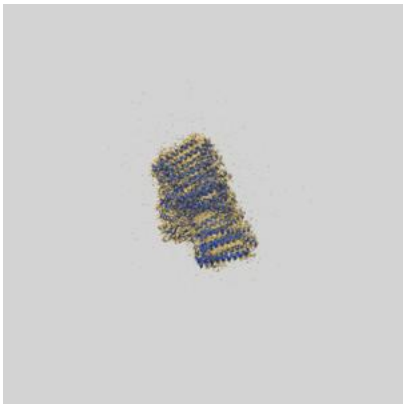
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.92	3.22	2.98
Unmasked-calculated*	-	-	-

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

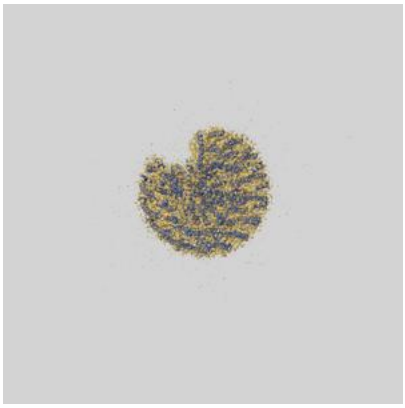
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31400 and PDB model 7F0L. Per-residue inclusion information can be found in section 3 on page 18.

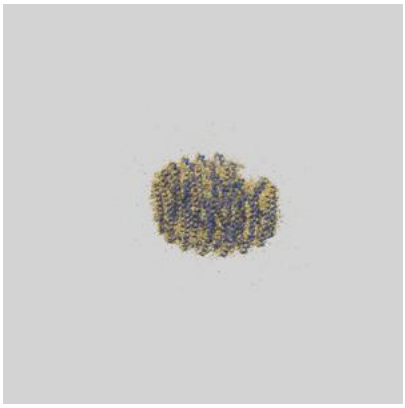
9.1 Map-model overlay



X



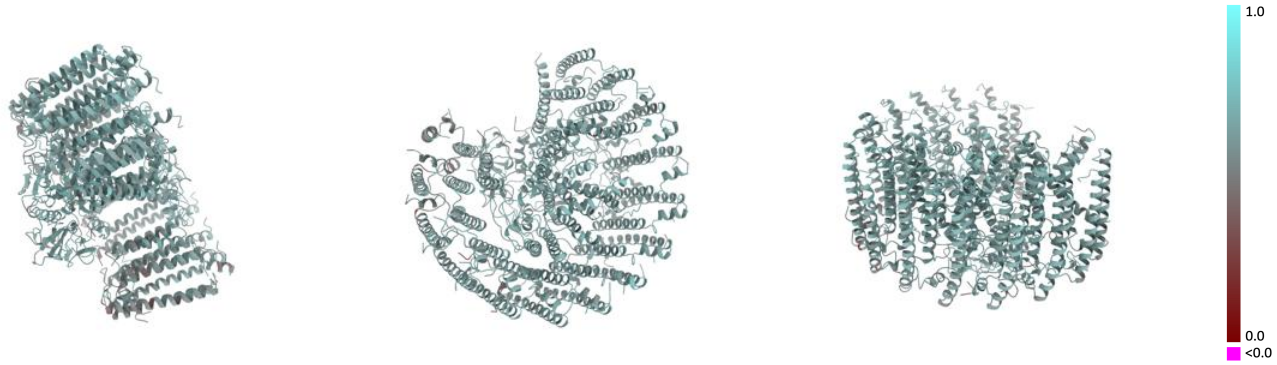
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.064 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

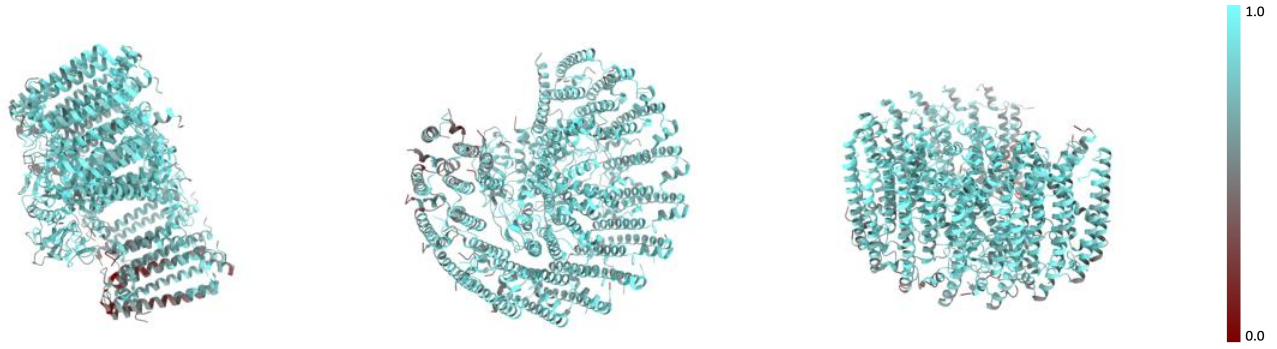
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

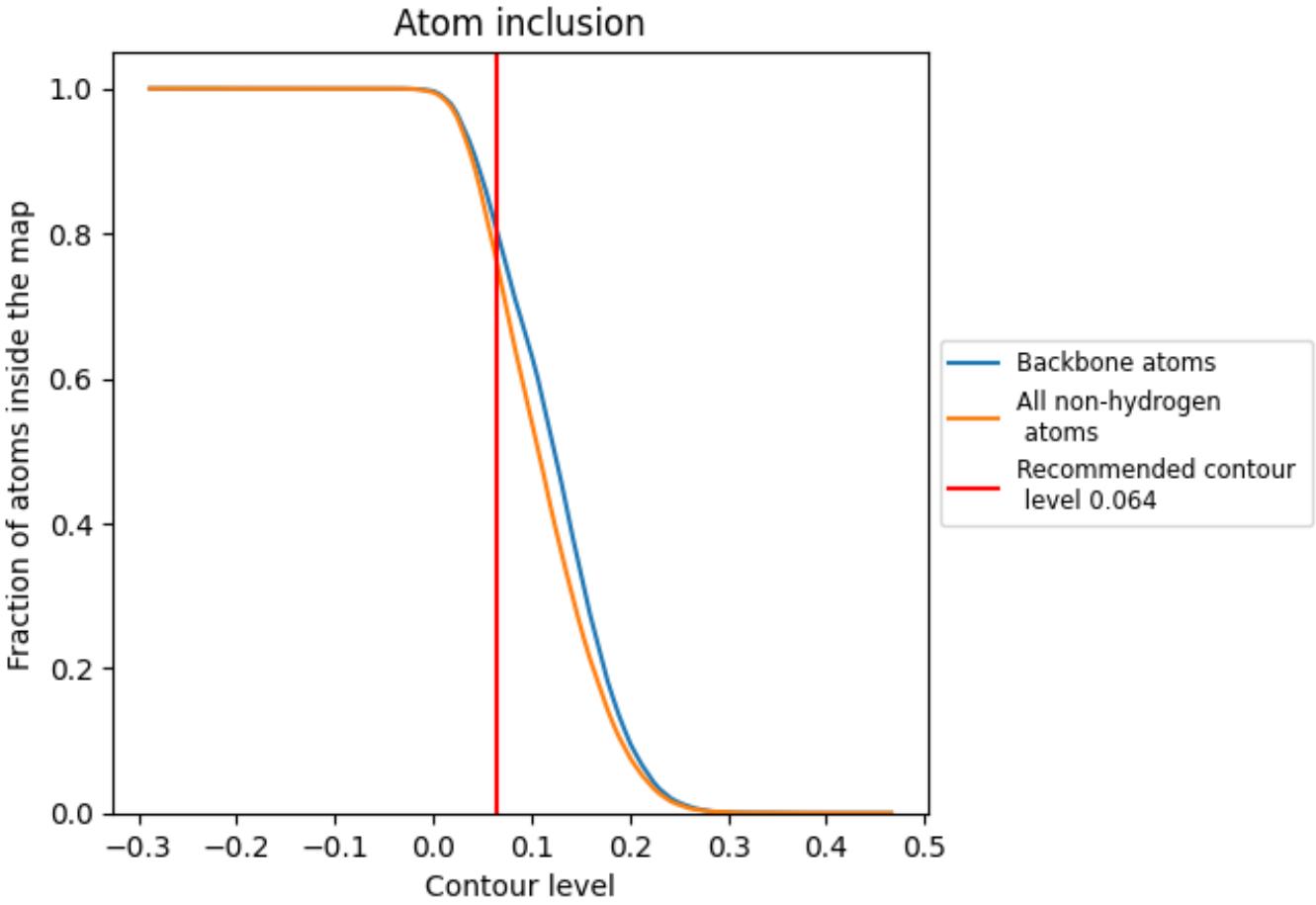
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.064).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.064) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7655	0.5970
1	0.7660	0.5980
2	0.7531	0.5810
3	0.6840	0.5720
4	0.6829	0.5670
5	0.6537	0.5810
6	0.6331	0.5530
7	0.5418	0.5360
8	0.4703	0.5080
A	0.7481	0.5780
B	0.7603	0.5800
D	0.8087	0.6140
E	0.8009	0.6060
F	0.7858	0.6070
G	0.7614	0.5920
H	0.7635	0.5980
I	0.8075	0.6070
J	0.8000	0.5950
K	0.7556	0.6060
L	0.8689	0.6310
M	0.8681	0.6330
N	0.7517	0.5950
O	0.7874	0.6020
P	0.7315	0.5920
Q	0.7220	0.5870
R	0.7517	0.5770
S	0.7764	0.5990
T	0.7315	0.5640
U	0.5912	0.5540
V	0.7618	0.5940
W	0.7540	0.5710
X	0.6691	0.5750
Y	0.7398	0.5960
Z	0.7531	0.5810