Full wwPDB EM Validation Report ⓘ

Feb 19, 2023 – 12:25 AM JST

PDB ID	:	7YML
EMDB ID	:	EMD-33931
Title	:	Structure of photosynthetic LH1-RC super-complex of Rhodobacter capsulatus
Authors	:	Tani, K.; Kanno, R.; Ji, X.-C.; Satoh, I.; Kobayashi, Y.; Nagashima, K.V.P.; Hall, M.; Yu, L.-J.; Kimura, Y.; Mizoguchi, A.; Humbel, B.M.; Madigan, M.T.; Wang-Otomo, Z.-Y.
Deposited on	:	2022-07-28
Resolution	:	2.60 Å(reported)
Based on initial model	:	7F0L

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

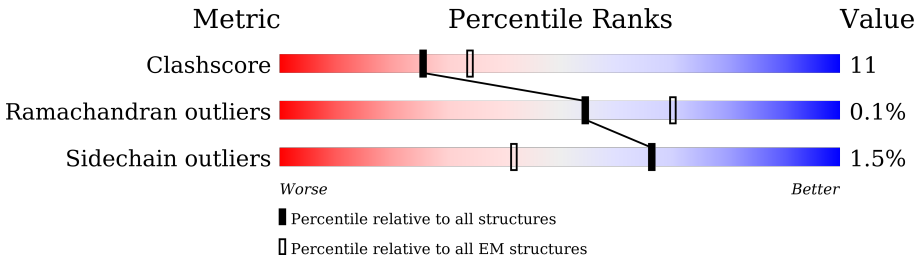
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.60 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	87% 12%
2	M	307	81% 18%
3	H	253	81% 17%
4	A	58	53% 21% 24%
4	D	58	5% 76% 21%
4	F	58	67% 24% 7%
4	I	58	78% 19%
4	K	58	66% 29% 5%

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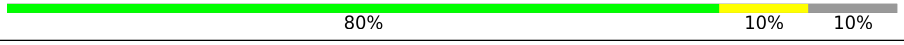
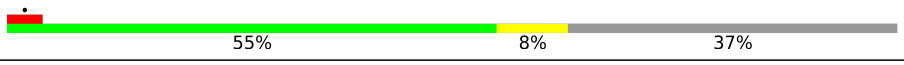
Mol	Chain	Length	Quality of chain
4	O	58	
4	Q	58	
4	S	58	
4	V	58	
4	Y	58	
5	B	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	P	49	
5	R	49	
5	T	49	
5	W	49	
5	Z	49	
6	X	78	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 18554 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	1	0
			2239	1501	356	365	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	304	Total	C	N	O	S	0	0
			2417	1608	392	404	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	248	Total	C	N	O	S	0	0
			1956	1246	329	371	10		

- Molecule 4 is a protein called Light-harvesting protein B-870 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	44	Total	C	N	O	S	0	0
			374	262	58	53	1		
4	D	56	Total	C	N	O	S	0	0
			457	315	73	68	1		
4	F	54	Total	C	N	O	S	0	0
			447	309	71	66	1		
4	I	56	Total	C	N	O	S	0	0
			457	315	73	68	1		
4	K	55	Total	C	N	O	S	0	0
			452	312	72	67	1		
4	O	56	Total	C	N	O	S	0	0
			453	312	72	68	1		
4	Q	56	Total	C	N	O	S	0	0
			457	315	73	68	1		

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Mol	Chain	Residues	Atoms	AltConf	Trace
4	S	56	Total C N O 462 318 76 68	1	0
4	V	56	Total C N O S 457 315 73 68 1	0	0
4	Y	42	Total C N O 335 228 56 51	0	0

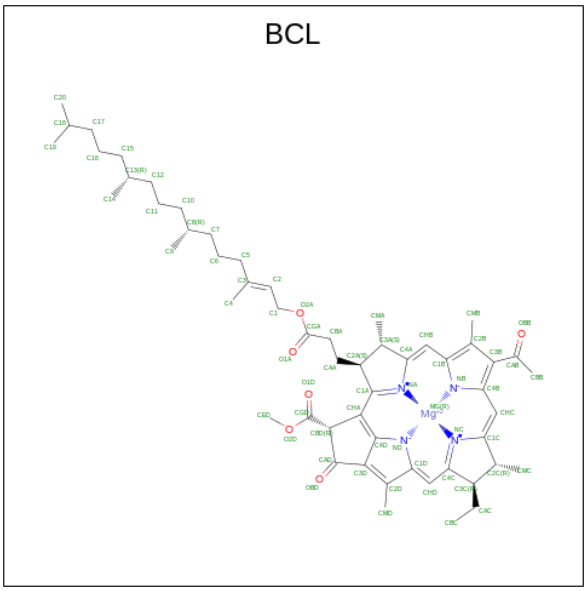
- Molecule 5 is a protein called Light-harvesting protein B-870 beta chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	B	44	Total C N O S 346 229 55 60 2	0	0
5	E	44	Total C N O S 346 229 55 60 2	0	0
5	G	43	Total C N O S 338 225 54 57 2	0	0
5	J	44	Total C N O S 346 229 55 60 2	0	0
5	N	43	Total C N O S 338 225 54 57 2	0	0
5	P	43	Total C N O S 338 225 54 57 2	0	0
5	R	43	Total C N O S 334 223 54 55 2	0	0
5	T	43	Total C N O S 338 225 54 57 2	0	0
5	W	41	Total C N O S 309 204 52 51 2	0	0
5	Z	31	Total C N O S 224 150 36 36 2	0	0

- Molecule 6 is a protein called Photosynthetic reaction center PufX protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	X	65	Total C N O S 502 333 79 86 4	0	0

- Molecule 7 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
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 61	C 50	Mg 1	N 4	O 6	0
7	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0

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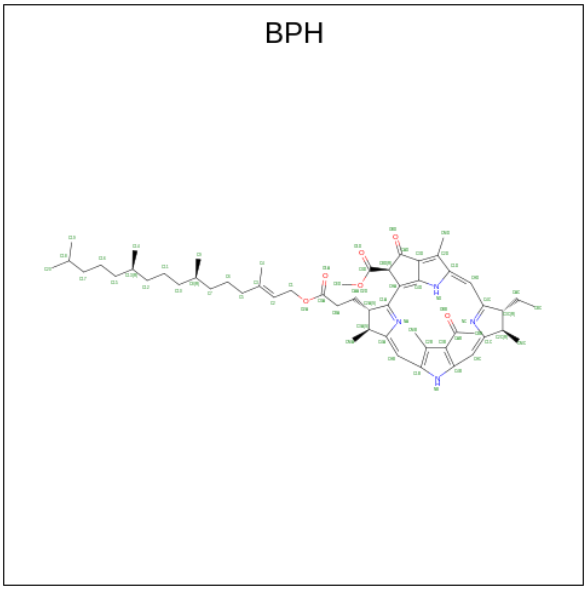
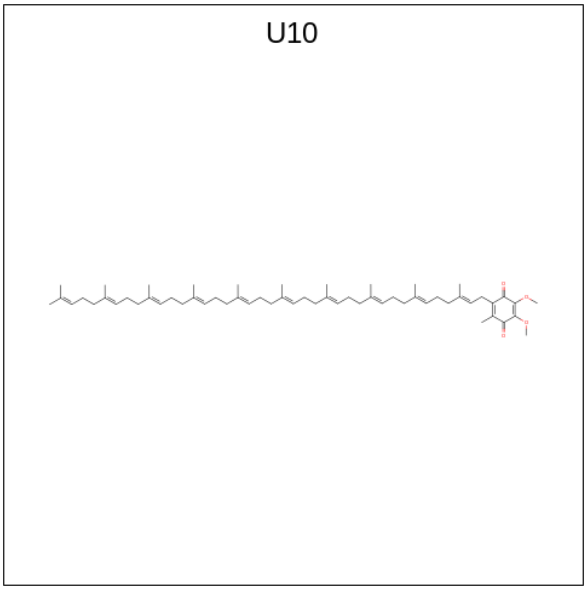
Mol	Chain	Residues	Atoms					AltConf
7	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



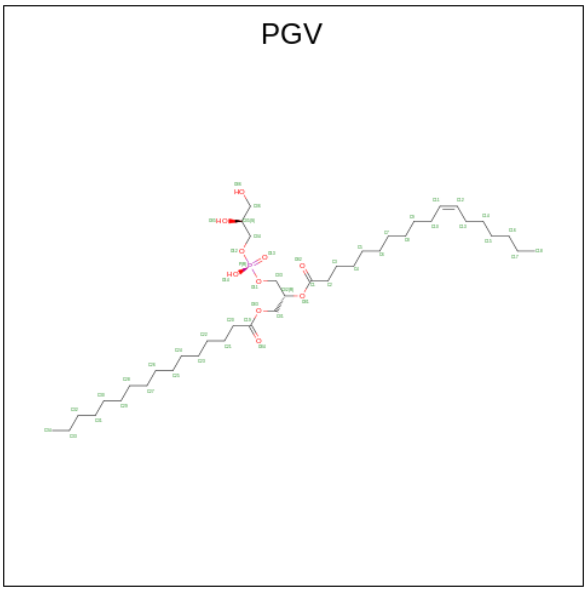
Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total	C	N	O	0
			65	55	4	6	
8	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



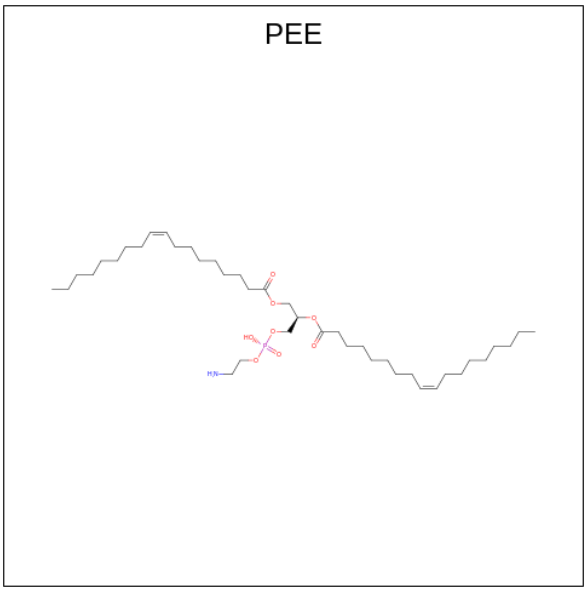
Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total	C	O	0
			48	44	4	
9	L	1	Total	C	O	0
			63	59	4	
9	M	1	Total	C	O	0
			20	16	4	
9	M	1	Total	C	O	0
			48	44	4	

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



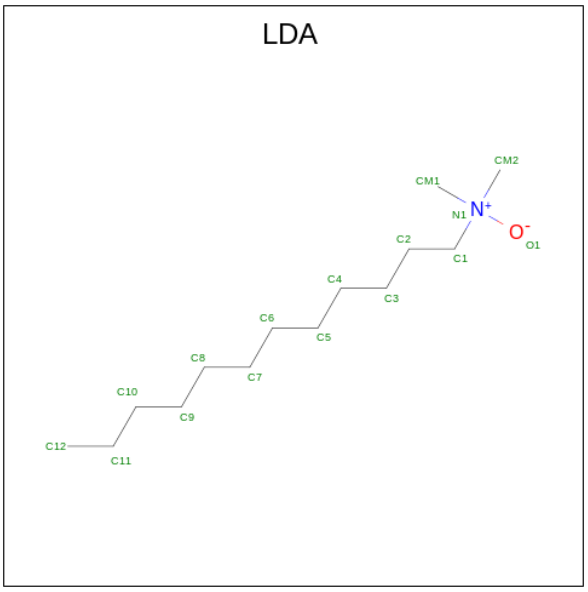
Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	O	P	0
			39	28	10	1	
10	M	1	Total	C	O	P	0
			36	25	10	1	
10	M	1	Total	C	O	P	0
			45	34	10	1	
10	M	1	Total	C	O	P	0
			35	24	10	1	
10	M	1	Total	C	O	P	0
			38	27	10	1	
10	H	1	Total	C	O	P	0
			43	32	10	1	
10	H	1	Total	C	O	P	0
			34	23	10	1	
10	Q	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	N	O	0
			16	14	1	1	
12	M	1	Total	C	N	O	0
			16	14	1	1	

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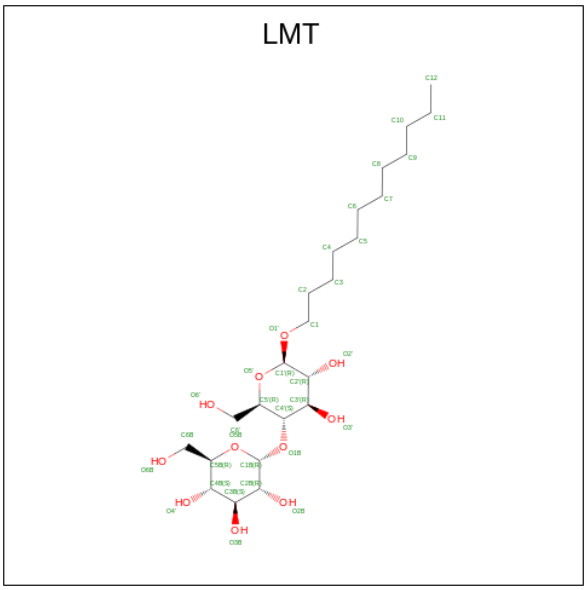
Mol	Chain	Residues	Atoms				AltConf
12	M	1	Total	C	N	O	0
			16	14	1	1	
12	M	1	Total	C	N	O	0
			16	14	1	1	
12	M	1	Total	C	N	O	0
			16	14	1	1	
12	H	1	Total	C	N	O	0
			16	14	1	1	
12	H	1	Total	C	N	O	0
			14	12	1	1	
12	D	1	Total	C	N	O	0
			16	14	1	1	
12	O	1	Total	C	N	O	0
			16	14	1	1	
12	Q	1	Total	C	N	O	0
			9	7	1	1	
12	Q	1	Total	C	N	O	0
			12	10	1	1	

- Molecule 13 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			35	24	11	
13	L	1	Total	C	O	0
			34	23	11	

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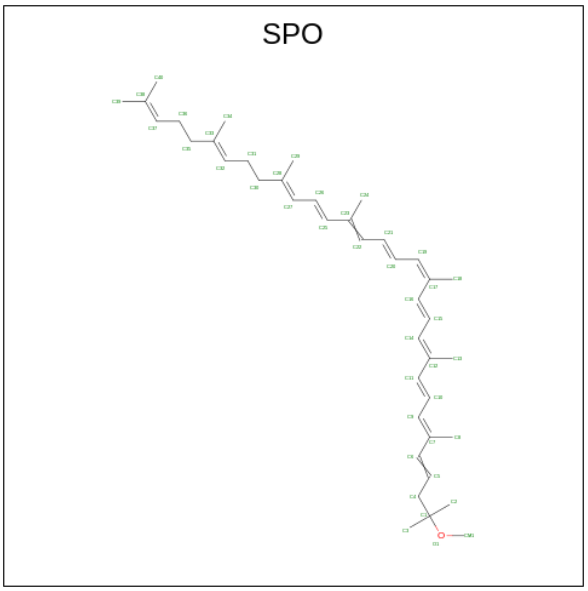
Mol	Chain	Residues	Atoms	AltConf
13	L	1	Total C O 35 24 11	0
13	M	1	Total C O 24 13 11	0
13	M	1	Total C O 35 24 11	0
13	M	1	Total C O 35 24 11	0
13	M	1	Total C O 32 21 11	0
13	M	1	Total C O 33 22 11	0
13	A	1	Total C O 32 21 11	0
13	I	1	Total C O 35 24 11	0
13	K	1	Total C O 35 24 11	0
13	Q	1	Total C O 35 24 11	0
13	S	1	Total C O 26 15 11	0
13	S	1	Total C O 33 22 11	0
13	Y	1	Total C O 28 17 11	0
13	Y	1	Total C O 27 16 11	0
13	X	1	Total C O 35 24 11	0
13	X	1	Total C O 35 24 11	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: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	D	1	Total	C	O	0
			42	41	1	
15	E	1	Total	C	O	0
			42	41	1	
15	F	1	Total	C	O	0
			42	41	1	
15	G	1	Total	C	O	0
			42	41	1	
15	I	1	Total	C	O	0
			42	41	1	
15	I	1	Total	C	O	0
			42	41	1	
15	N	1	Total	C	O	0
			42	41	1	
15	O	1	Total	C	O	0
			42	41	1	
15	O	1	Total	C	O	0
			42	41	1	
15	P	1	Total	C	O	0
			42	41	1	
15	R	1	Total	C	O	0
			42	41	1	

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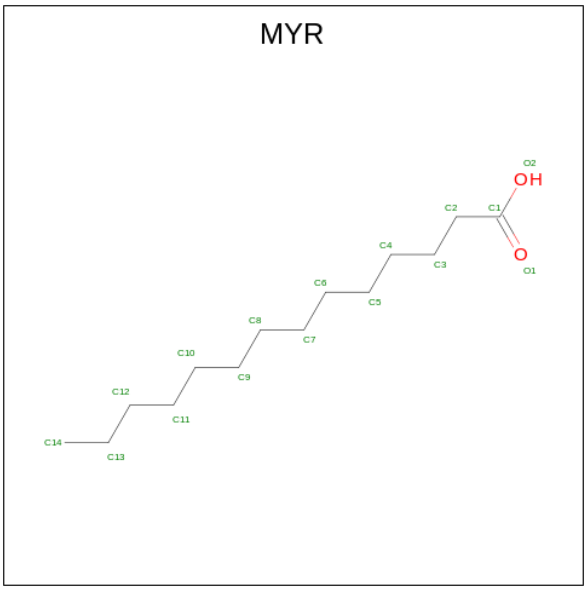
Mol	Chain	Residues	Atoms	AltConf
15	S	1	Total C O 42 41 1	0
15	S	1	Total C O 42 41 1	0
15	T	1	Total C O 42 41 1	0
15	W	1	Total C O 42 41 1	0

- Molecule 16 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	AltConf
16	F	1	Total C O 16 14 2	0

- Molecule 17 is water.

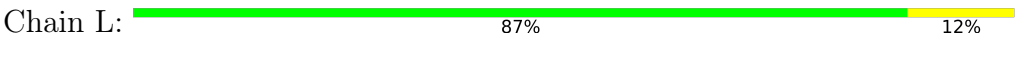
Mol	Chain	Residues	Atoms	AltConf
17	L	4	Total O 4 4	0
17	M	3	Total O 3 3	0

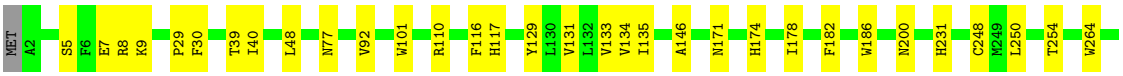
3 Residue-property plots (i)

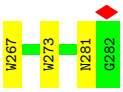
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Reaction center protein L chain

Chain L:





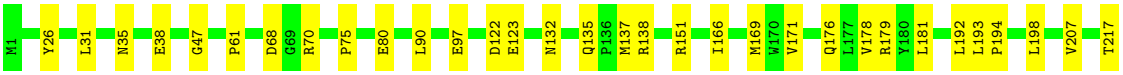


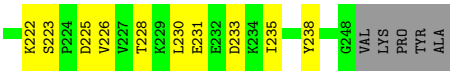
• Molecule 2: Reaction center protein M chain

Chain M:

• Molecule 3: Photosynthetic reaction center H subunit

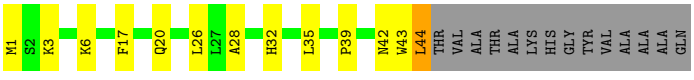
Chain H:





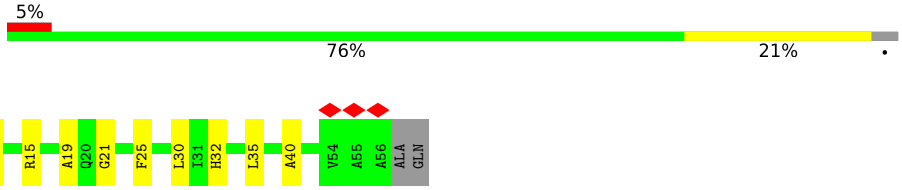
• Molecule 4: Light-harvesting protein B-870 alpha chain

Chain A:



• Molecule 4: Light-harvesting protein B-870 alpha chain

Chain D:

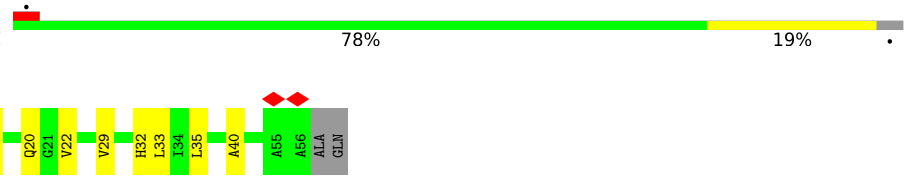


• Molecule 4: Light-harvesting protein B-870 alpha chain

Chain F:

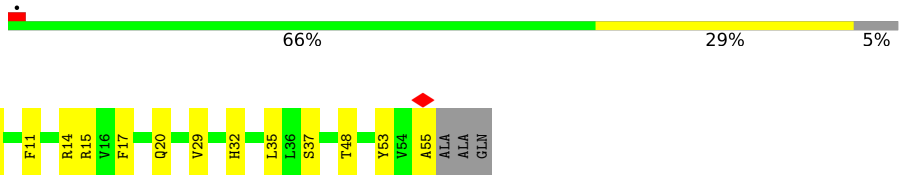
• Molecule 4: Light-harvesting protein B-870 alpha chain

Chain I:



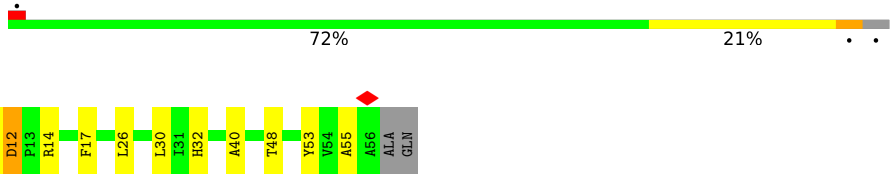
• Molecule 4: Light-harvesting protein B-870 alpha chain

Chain K:



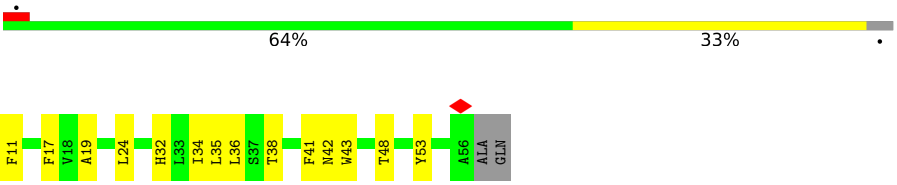
• Molecule 4: Light-harvesting protein B-870 alpha chain

Chain O:



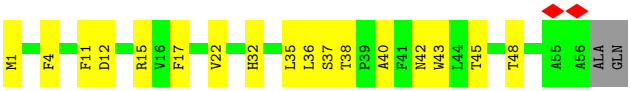
• Molecule 4: Light-harvesting protein B-870 alpha chain

Chain Q:



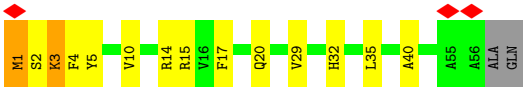
• Molecule 4: Light-harvesting protein B-870 alpha chain

Chain S:



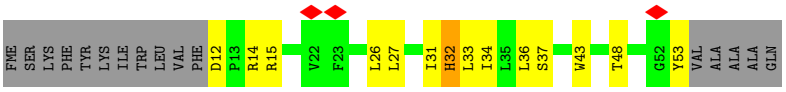
• Molecule 4: Light-harvesting protein B-870 alpha chain

Chain V:



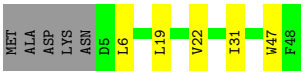
• Molecule 4: Light-harvesting protein B-870 alpha chain

Chain Y:



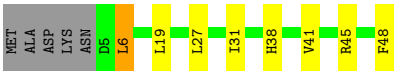
• Molecule 5: Light-harvesting protein B-870 beta chain

Chain B:



• Molecule 5: Light-harvesting protein B-870 beta chain

Chain E:

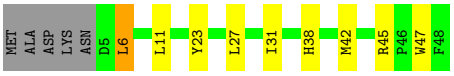


• Molecule 5: Light-harvesting protein B-870 beta chain

Chain G:

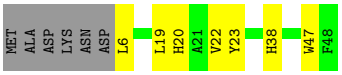
• Molecule 5: Light-harvesting protein B-870 beta chain

Chain J:



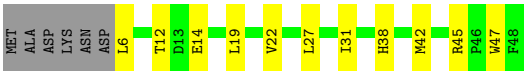
• Molecule 5: Light-harvesting protein B-870 beta chain

Chain N:



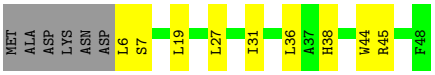
• Molecule 5: Light-harvesting protein B-870 beta chain

Chain P:



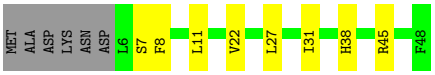
• Molecule 5: Light-harvesting protein B-870 beta chain

Chain R:



• Molecule 5: Light-harvesting protein B-870 beta chain

Chain T:

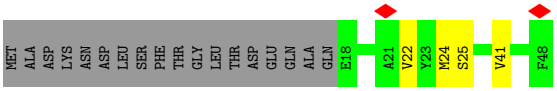


• Molecule 5: Light-harvesting protein B-870 beta chain

Chain W:

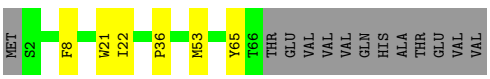
• Molecule 5: Light-harvesting protein B-870 beta chain

Chain Z:



• Molecule 6: Photosynthetic reaction center PufX protein

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224431	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.191	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	L	0.39	0/2328	0.45	0/3180
2	M	0.36	0/2507	0.46	0/3425
3	H	0.33	0/2006	0.48	0/2728
4	A	0.35	0/377	0.42	0/514
4	D	0.36	0/462	0.43	0/631
4	F	0.38	0/452	0.41	0/617
4	I	0.37	0/462	0.41	0/631
4	K	0.36	0/457	0.42	0/624
4	O	0.33	0/458	0.41	0/627
4	Q	0.30	0/462	0.41	0/631
4	S	0.29	0/473	0.43	0/645
4	V	0.28	0/462	0.41	0/631
4	Y	0.24	0/345	0.43	0/472
5	B	0.31	0/356	0.41	0/486
5	E	0.33	0/356	0.43	0/486
5	G	0.33	0/348	0.45	0/475
5	J	0.32	0/356	0.41	0/486
5	N	0.32	0/348	0.41	0/475
5	P	0.31	0/348	0.42	0/475
5	R	0.27	0/344	0.41	0/470
5	T	0.29	0/348	0.40	0/475
5	W	0.26	0/318	0.39	0/435
5	Z	0.23	0/229	0.39	0/313
6	X	0.34	0/519	0.44	0/700
All	All	0.34	0/15121	0.44	0/20632

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	2239	0	2184	30	0
2	M	2417	0	2327	49	0
3	H	1956	0	1923	28	0
4	A	374	0	396	8	0
4	D	457	0	480	13	0
4	F	447	0	470	12	0
4	I	457	0	480	11	0
4	K	452	0	475	17	0
4	O	453	0	469	15	0
4	Q	457	0	480	14	0
4	S	462	0	486	16	0
4	V	457	0	480	14	0
4	Y	335	0	351	12	0
5	B	346	0	337	5	0
5	E	346	0	337	8	0
5	G	338	0	333	11	0
5	J	346	0	337	9	0
5	N	338	0	333	9	0
5	P	338	0	333	10	0
5	R	334	0	329	9	0
5	T	338	0	333	7	0
5	W	309	0	292	5	0
5	Z	224	0	217	3	0
6	X	502	0	488	4	0
7	A	61	0	61	3	0
7	B	66	0	74	6	0
7	D	66	0	74	9	0
7	E	66	0	74	3	0
7	F	132	0	148	10	0
7	G	66	0	74	7	0
7	I	66	0	74	7	0
7	J	66	0	74	7	0
7	K	66	0	74	8	0
7	L	132	0	148	3	0
7	M	132	0	148	7	0
7	N	66	0	74	6	0
7	O	66	0	74	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	66	0	74	8	0
7	Q	66	0	74	2	0
7	R	66	0	74	5	0
7	S	66	0	74	7	0
7	T	66	0	74	5	0
7	V	66	0	74	8	0
7	W	66	0	74	8	0
7	Y	66	0	74	4	0
7	Z	66	0	74	3	0
8	L	65	0	76	3	0
8	M	65	0	76	8	0
9	L	111	0	153	10	0
9	M	68	0	82	5	0
10	H	77	0	92	6	0
10	L	39	0	47	5	0
10	M	154	0	188	14	0
10	Q	35	0	40	5	0
11	L	46	0	69	3	0
12	D	16	0	31	3	0
12	H	30	0	55	3	0
12	L	16	0	31	2	0
12	M	64	0	124	5	0
12	O	16	0	31	1	0
12	Q	21	0	34	3	0
13	A	32	0	37	3	0
13	I	35	0	46	3	0
13	K	35	0	46	2	0
13	L	104	0	133	7	0
13	M	159	0	189	15	0
13	Q	35	0	46	2	0
13	S	59	0	64	8	0
13	X	70	0	92	1	0
13	Y	55	0	56	2	0
14	M	1	0	0	0	0
15	D	126	0	180	17	0
15	E	42	0	60	6	0
15	F	42	0	60	5	0
15	G	42	0	60	3	0
15	I	84	0	120	14	0
15	M	42	0	60	6	0
15	N	42	0	60	6	0
15	O	84	0	120	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	42	0	60	5	0
15	R	42	0	60	6	0
15	S	84	0	120	15	0
15	T	42	0	60	3	0
15	W	42	0	60	8	0
16	F	16	0	27	2	0
17	L	4	0	0	0	0
17	M	3	0	0	0	0
All	All	18554	0	19452	432	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 (432) 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)
4:D:11:PHE:HZ	4:F:17:PHE:HD2	1.21	0.85
4:F:1:FME:HCN	4:F:3:LYS:H	1.41	0.84
4:D:25:PHE:HB2	7:D:102:BCL:H43	1.61	0.81
4:O:40:ALA:O	5:P:45:ARG:NH1	2.18	0.77
10:L:305:PGV:H51	10:L:305:PGV:H232	1.67	0.76
4:Y:15:ARG:HE	13:Y:103:LMT:H6'2	1.50	0.76
13:M:410:LMT:H82	13:S:102:LMT:H62	1.69	0.75
2:M:231:GLU:OE2	3:H:179:ARG:NH1	2.20	0.74
15:I:104:SPO:H37	5:N:22:VAL:HG21	1.67	0.74
15:O:104:SPO:H293	15:R:101:SPO:H37	1.70	0.74
15:D:105:SPO:H6	7:I:102:BCL:HMB2	1.70	0.74
15:D:101:SPO:H6	7:D:102:BCL:HMB2	1.72	0.71
4:V:10:VAL:HG12	4:Y:14:ARG:HB3	1.72	0.71
2:M:240:ARG:NH1	3:H:38:GLU:OE1	2.22	0.71
4:S:35:LEU:HD11	7:T:102:BCL:HHD	1.73	0.71
2:M:233:GLU:OE1	2:M:265:HIS:CE1	2.46	0.69
1:L:231:HIS:CE1	2:M:233:GLU:OE2	2.46	0.69
12:M:418:LDA:H82	12:M:419:LDA:H31	1.73	0.69
1:L:133:VAL:HG23	1:L:134:VAL:HG23	1.76	0.68
15:S:104:SPO:H37	5:T:22:VAL:HG11	1.74	0.68
5:Z:41:VAL:HG11	7:Z:101:BCL:HBC1	1.76	0.68
4:D:32:HIS:CE1	7:E:102:BCL:HMD1	2.28	0.68
5:G:31:ILE:HD12	7:G:101:BCL:H11	1.74	0.68
2:M:55:ALA:HB2	10:M:415:PGV:H012	1.74	0.68
15:G:102:SPO:H37	15:I:103:SPO:H293	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:31:LEU:O	3:H:35:ASN:ND2	2.27	0.67
15:I:103:SPO:H6	7:K:102:BCL:HMB2	1.76	0.67
7:W:102:BCL:HHB	7:W:102:BCL:H8	1.77	0.67
15:I:104:SPO:H401	5:J:6:LEU:HD11	1.76	0.67
3:H:68:ASP:OD2	3:H:70:ARG:NH1	2.28	0.66
13:S:101:LMT:H5'	13:S:102:LMT:H12	1.77	0.66
1:L:77:ASN:HD22	13:A:102:LMT:H6D	1.60	0.66
4:D:19:ALA:HB2	12:D:104:LDA:H51	1.79	0.65
4:S:32:HIS:CE1	7:T:102:BCL:HMD1	2.31	0.65
4:O:7:ILE:HB	15:O:104:SPO:H343	1.79	0.65
11:L:306:PEE:H29	6:X:36:PRO:HB3	1.78	0.65
7:P:102:BCL:HBB2	7:P:102:BCL:H122	1.80	0.64
4:I:7:ILE:HB	15:I:104:SPO:H343	1.79	0.64
4:Q:32:HIS:CE1	7:R:102:BCL:HMD1	2.33	0.64
4:O:12:ASP:OD1	4:O:12:ASP:N	2.29	0.64
4:O:32:HIS:CE1	7:P:102:BCL:HMD1	2.33	0.64
4:I:40:ALA:O	5:J:45:ARG:NH1	2.30	0.64
2:M:279:GLY:HA2	7:M:404:BCL:HED2	1.80	0.64
2:M:118:SER:HB3	15:M:408:SPO:H311	1.80	0.63
4:O:1:FME:SD	4:O:1:FME:N	2.71	0.63
4:Y:12:ASP:HB3	4:Y:15:ARG:HB2	1.80	0.62
13:M:409:LMT:O6'	12:H:301:LDA:O1	2.17	0.62
4:Q:35:LEU:HD11	7:R:102:BCL:HHD	1.82	0.62
13:L:311:LMT:H42	10:H:303:PGV:H011	1.82	0.62
4:S:45:THR:HA	4:S:48:THR:HG22	1.82	0.61
4:K:32:HIS:CE1	7:N:102:BCL:HMD1	2.35	0.61
1:L:267:TRP:HB2	9:M:401:U10:H4M3	1.83	0.61
15:O:104:SPO:H402	5:R:19:LEU:HA	1.81	0.61
8:M:405:BPH:HBB3	8:M:405:BPH:HHC	1.83	0.61
4:Q:7:ILE:HB	15:S:104:SPO:H343	1.81	0.61
3:H:198:LEU:HD22	3:H:207:VAL:HG22	1.83	0.61
7:O:102:BCL:H111	15:P:101:SPO:H341	1.83	0.61
4:I:32:HIS:CE1	7:J:101:BCL:HMD1	2.36	0.61
7:M:403:BCL:H193	12:M:419:LDA:H82	1.82	0.60
4:I:20:GLN:NE2	5:J:23:TYR:OH	2.31	0.60
4:I:40:ALA:HB2	4:K:55:ALA:HB2	1.84	0.60
7:K:102:BCL:HED3	15:N:101:SPO:H25	1.83	0.60
4:V:32:HIS:CE1	7:W:102:BCL:HMD1	2.37	0.60
4:S:40:ALA:O	5:T:45:ARG:NH1	2.35	0.59
15:O:103:SPO:H6	7:Q:105:BCL:HMB2	1.85	0.59
10:H:304:PGV:H012	4:K:15:ARG:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:32:HIS:CE1	7:G:101:BCL:HMD1	2.37	0.59
4:D:40:ALA:O	5:E:45:ARG:NH1	2.36	0.59
7:V:101:BCL:H41	15:W:101:SPO:H352	1.84	0.59
15:S:104:SPO:HM11	4:V:29:VAL:HG13	1.85	0.59
13:M:409:LMT:O3'	13:S:101:LMT:H6D	2.02	0.59
10:H:304:PGV:H031	4:K:15:ARG:HG2	1.83	0.59
4:Y:43:TRP:CZ2	7:Y:102:BCL:HHC	2.38	0.59
13:M:409:LMT:H6D	12:H:301:LDA:H31	1.84	0.59
4:Q:10:VAL:HG23	4:Q:11:PHE:HD1	1.68	0.59
15:S:105:SPO:H31	7:Y:102:BCL:HBB2	1.85	0.58
4:A:32:HIS:CE1	7:B:101:BCL:HMD1	2.38	0.58
2:M:63:GLY:HA3	8:M:405:BPH:H5C1	1.86	0.58
5:E:27:LEU:O	5:E:31:ILE:HG12	2.02	0.58
2:M:300:HIS:ND1	10:M:402:PGV:O14	2.27	0.58
3:H:70:ARG:NH2	3:H:123:GLU:OE1	2.31	0.58
4:K:37:SER:HA	13:K:101:LMT:H5B	1.86	0.58
4:I:6:LYS:HD3	15:I:104:SPO:H403	1.85	0.57
15:S:104:SPO:H6	7:V:101:BCL:HMB2	1.86	0.57
5:P:42:MET:HE3	7:P:102:BCL:H203	1.85	0.57
13:L:311:LMT:H2O2	10:H:303:PGV:H06	1.51	0.57
5:B:31:ILE:HG12	7:B:101:BCL:H2	1.87	0.57
7:N:102:BCL:H42	15:P:101:SPO:H293	1.86	0.57
10:M:415:PGV:H251	10:M:415:PGV:H91	1.87	0.57
2:M:75:TRP:HE1	15:M:408:SPO:HM12	1.68	0.57
15:D:101:SPO:H132	7:D:102:BCL:H42	1.87	0.57
15:D:105:SPO:H182	7:I:102:BCL:H8	1.87	0.57
7:M:403:BCL:H142	8:M:405:BPH:HED2	1.86	0.56
4:D:11:PHE:CZ	4:F:17:PHE:HD2	2.13	0.56
10:L:305:PGV:H222	10:M:402:PGV:H41	1.88	0.56
15:D:105:SPO:H32	5:G:22:VAL:HG12	1.88	0.56
4:V:35:LEU:HD11	7:W:102:BCL:HHD	1.88	0.56
10:M:415:PGV:H061	4:V:14:ARG:HD2	1.88	0.56
3:H:138:ARG:NH1	3:H:225:ASP:OD1	2.37	0.56
4:S:37:SER:HB3	13:S:102:LMT:H2'	1.86	0.56
5:R:6:LEU:HD21	15:S:104:SPO:H401	1.87	0.56
4:F:40:ALA:O	5:G:45:ARG:NH1	2.39	0.56
8:L:302:BPH:HHC	8:L:302:BPH:HBB3	1.88	0.55
15:O:103:SPO:H32	5:P:22:VAL:HG12	1.88	0.55
2:M:75:TRP:HE1	15:M:408:SPO:H22A	1.70	0.55
4:F:6:LYS:HD3	15:I:103:SPO:H393	1.88	0.55
15:O:104:SPO:H391	5:P:6:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:228:PHE:HB2	2:M:243:ALA:HB2	1.89	0.55
8:M:405:BPH:HBC3	8:M:405:BPH:HHD	1.87	0.55
2:M:72:VAL:HG21	13:M:412:LMT:H81	1.88	0.55
15:I:104:SPO:H6	7:O:102:BCL:HMB2	1.89	0.55
1:L:8[B]:ARG:NH2	3:H:47:GLY:HA2	2.23	0.54
2:M:166:LEU:HD11	13:Q:101:LMT:H82	1.89	0.54
4:O:48:THR:HG23	4:O:53:TYR:HB2	1.90	0.54
1:L:174:HIS:CE1	1:L:178:ILE:HD11	2.42	0.54
2:M:108:LEU:HD23	13:M:412:LMT:H6'1	1.88	0.54
4:K:35:LEU:HD11	7:N:102:BCL:HHD	1.89	0.54
15:S:105:SPO:H392	5:W:19:LEU:HA	1.89	0.54
7:M:403:BCL:H13	8:M:405:BPH:HMA1	1.90	0.54
1:L:110:ARG:NH1	11:L:306:PEE:O1P	2.41	0.54
3:H:193:LEU:HB3	3:H:198:LEU:HD21	1.89	0.54
7:P:102:BCL:H202	15:R:101:SPO:H9	1.90	0.54
4:D:11:PHE:HZ	4:F:17:PHE:CD2	2.13	0.53
15:I:104:SPO:H32	4:K:17:PHE:CZ	2.43	0.53
7:D:102:BCL:H52	15:E:101:SPO:H351	1.90	0.53
1:L:92:VAL:HG11	9:L:304:U10:H53	1.90	0.53
5:T:7:SER:OG	5:T:11:LEU:N	2.37	0.53
5:W:47:TRP:CE2	7:W:102:BCL:H2C	2.44	0.53
2:M:68:PHE:HB3	13:M:412:LMT:H82	1.92	0.53
15:I:104:SPO:H32	4:K:17:PHE:CE1	2.44	0.53
3:H:166:ILE:HD12	3:H:181:LEU:HB3	1.90	0.52
15:O:103:SPO:H352	5:P:22:VAL:HB	1.90	0.52
7:P:102:BCL:H42	15:R:101:SPO:H293	1.91	0.52
10:Q:103:PGV:H201	12:Q:104:LDA:H52	1.91	0.52
8:L:302:BPH:HHC	8:L:302:BPH:CBB	2.39	0.52
2:M:15:GLY:H	3:H:176:GLN:HE22	1.57	0.52
2:M:116:ILE:HG21	13:M:412:LMT:H11	1.90	0.52
1:L:9:LYS:HA	3:H:90:LEU:HD11	1.91	0.52
1:L:171:ASN:HB3	1:L:174:HIS:HB2	1.90	0.52
4:Q:48:THR:HG23	4:Q:53:TYR:HB2	1.92	0.52
7:L:310:BCL:HMD1	2:M:205:ILE:HD13	1.91	0.52
7:J:101:BCL:H43	15:N:101:SPO:H292	1.91	0.52
4:F:44:LEU:O	4:F:48:THR:HG23	2.11	0.51
15:O:104:SPO:H41	4:S:32:HIS:CG	2.46	0.51
5:P:27:LEU:O	5:P:31:ILE:HG12	2.10	0.51
4:Y:48:THR:HG23	4:Y:53:TYR:HB2	1.90	0.51
15:O:103:SPO:H351	5:P:19:LEU:HD22	1.92	0.51
4:V:3:LYS:HD3	5:Z:22:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:182:PHE:HB3	8:M:405:BPH:HBB2	1.92	0.51
5:T:8:PHE:HB3	4:V:14:ARG:NH2	2.26	0.51
4:S:11:PHE:HE2	4:V:17:PHE:HD2	1.59	0.51
2:M:288:THR:HB	12:H:301:LDA:H72	1.93	0.50
10:Q:103:PGV:H32	7:S:103:BCL:H72	1.92	0.50
4:Y:33:LEU:HD23	4:Y:36:LEU:HD12	1.92	0.50
4:K:11:PHE:HZ	4:O:17:PHE:HB2	1.76	0.50
2:M:29:GLU:HG3	4:V:15:ARG:HH21	1.76	0.50
1:L:117:HIS:HE1	2:M:5:GLN:O	1.94	0.50
4:K:20:GLN:OE1	5:N:23:TYR:OH	2.24	0.50
5:N:20:HIS:HE1	7:O:102:BCL:H191	1.75	0.50
7:V:101:BCL:H43	15:W:101:SPO:H32	1.92	0.50
5:B:6:LEU:HD23	15:D:103:SPO:H403	1.94	0.50
9:L:304:U10:H4M1	4:A:20:GLN:HG2	1.92	0.50
7:E:102:BCL:H42	15:F:104:SPO:H293	1.94	0.50
4:F:20:GLN:HE21	15:F:104:SPO:H392	1.77	0.50
1:L:40:ILE:HG21	12:D:104:LDA:H111	1.93	0.50
12:L:307:LDA:H21	2:M:3:GLU:HG2	1.93	0.49
4:I:35:LEU:HD11	7:J:101:BCL:HHD	1.93	0.49
7:F:101:BCL:HBB3	16:F:102:MYR:H81	1.93	0.49
7:P:102:BCL:H172	15:R:101:SPO:H11	1.94	0.49
4:Q:19:ALA:HB2	12:Q:104:LDA:H12	1.94	0.49
2:M:36:LEU:HD13	13:M:417:LMT:H5'	1.95	0.49
1:L:29:PRO:HD3	13:L:311:LMT:H2'	1.93	0.49
4:F:35:LEU:HD11	7:G:101:BCL:HHD	1.95	0.49
4:K:29:VAL:HG11	13:K:101:LMT:H111	1.95	0.49
13:I:101:LMT:O6B	13:I:101:LMT:O3'	2.31	0.49
7:J:101:BCL:H92	7:J:101:BCL:HAA1	1.93	0.49
1:L:281:ASN:ND2	2:M:88:ASP:OD1	2.37	0.49
7:B:101:BCL:HBA1	7:B:101:BCL:H71	1.94	0.49
1:L:30:PHE:CD1	9:M:407:U10:H312	2.47	0.49
2:M:66:TRP:CD1	2:M:121:MET:HB2	2.48	0.49
13:M:417:LMT:O3'	13:M:417:LMT:O2B	2.22	0.49
13:M:410:LMT:H62	13:S:102:LMT:H42	1.95	0.48
2:M:94:LEU:HB3	2:M:176:TYR:HB2	1.95	0.48
13:Q:101:LMT:H6'	13:Q:101:LMT:H2O1	1.60	0.48
2:M:225:VAL:HG23	2:M:230:GLY:HA3	1.96	0.48
5:E:48:PHE:HB3	15:F:104:SPO:H82	1.94	0.48
4:K:11:PHE:CZ	4:O:17:PHE:HB2	2.49	0.48
4:I:10:VAL:HG13	4:K:14:ARG:HG2	1.95	0.48
7:W:102:BCL:HBB3	7:Y:102:BCL:NB	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:27:LEU:HD23	7:Z:101:BCL:HED2	1.94	0.48
15:D:105:SPO:H392	5:G:19:LEU:HA	1.96	0.48
4:O:48:THR:HG21	4:O:55:ALA:HB2	1.95	0.48
11:L:306:PEE:H34	13:X:101:LMT:H112	1.96	0.48
1:L:267:TRP:HB3	9:M:401:U10:H3M3	1.96	0.48
3:H:171:VAL:HG12	3:H:178:VAL:HG22	1.96	0.48
1:L:48:LEU:HD13	4:D:30:LEU:HD22	1.96	0.47
15:D:103:SPO:H26	15:E:101:SPO:H37	1.97	0.47
4:S:12:ASP:HB3	4:S:15[A]:ARG:HH11	1.79	0.47
4:S:36:LEU:O	4:S:42:ASN:ND2	2.42	0.47
10:M:413:PGV:H212	3:H:26:TYR:HE2	1.79	0.47
10:H:304:PGV:H62	10:H:304:PGV:H31	1.73	0.47
7:O:102:BCL:H192	7:O:102:BCL:H161	1.73	0.47
2:M:156:TRP:CD1	7:M:403:BCL:HBB1	2.49	0.47
5:T:27:LEU:O	5:T:31:ILE:HG12	2.14	0.47
10:M:413:PGV:H202	10:M:413:PGV:H231	1.65	0.47
4:D:15:ARG:HD2	12:D:104:LDA:H21	1.95	0.47
5:W:12:THR:HG23	5:W:15:GLN:H	1.79	0.47
4:I:29:VAL:HG11	13:I:101:LMT:H92	1.96	0.47
7:A:101:BCL:H121	15:D:101:SPO:H292	1.97	0.47
3:H:122:ASP:OD1	3:H:228:THR:HG21	2.15	0.46
7:K:102:BCL:O1D	15:N:101:SPO:H22	2.14	0.46
7:V:101:BCL:H52	7:V:101:BCL:H8	1.61	0.46
4:Q:36:LEU:O	4:Q:42:ASN:ND2	2.48	0.46
4:S:43:TRP:CD2	7:S:103:BCL:H2C	2.50	0.46
15:S:105:SPO:HM13	4:Y:33:LEU:HG	1.98	0.46
7:F:103:BCL:HMD1	5:G:38:HIS:CE1	2.50	0.46
15:I:104:SPO:H37	5:N:22:VAL:CG2	2.41	0.46
4:Y:34:ILE:O	4:Y:37:SER:OG	2.22	0.46
9:L:304:U10:H1M2	4:D:21:GLY:HA3	1.98	0.46
7:J:101:BCL:HMB1	7:J:101:BCL:HBB2	1.98	0.46
15:I:104:SPO:H391	5:J:6:LEU:HD11	1.98	0.46
15:S:105:SPO:H41	4:Y:32:HIS:CG	2.51	0.46
2:M:103:LEU:HB2	13:S:102:LMT:H11	1.96	0.46
12:M:420:LDA:H82	10:Q:103:PGV:H212	1.96	0.46
3:H:97:GLU:O	4:D:15:ARG:NH2	2.33	0.46
5:B:47:TRP:CD2	7:B:101:BCL:H2C	2.51	0.46
13:M:412:LMT:H52	4:Y:26:LEU:HD22	1.98	0.46
3:H:228:THR:HG22	3:H:230:LEU:H	1.81	0.46
2:M:231:GLU:OE1	2:M:231:GLU:N	2.40	0.46
7:D:102:BCL:H151	7:D:102:BCL:H111	1.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:102:BCL:H2A	15:E:101:SPO:H25	1.96	0.46
5:P:47:TRP:CE2	7:P:102:BCL:H2C	2.51	0.46
2:M:201:HIS:CE1	2:M:205:ILE:HD11	2.51	0.45
10:M:415:PGV:H041	4:V:15:ARG:HH12	1.81	0.45
15:D:105:SPO:H403	5:E:6:LEU:HD21	1.98	0.45
5:G:47:TRP:CE2	7:G:101:BCL:H2C	2.51	0.45
5:Z:24:MET:SD	5:Z:25:SER:N	2.90	0.45
1:L:5:SER:OG	3:H:80:GLU:OE2	2.31	0.45
5:G:8:PHE:HZ	5:J:11:LEU:HD11	1.82	0.45
4:K:48:THR:HG23	4:K:53:TYR:HB2	1.98	0.45
4:O:30:LEU:HD12	12:O:101:LDA:H123	1.97	0.45
5:J:27:LEU:O	5:J:31:ILE:HG12	2.17	0.45
7:T:102:BCL:H92	7:T:102:BCL:HAA1	1.98	0.45
4:D:35:LEU:HD11	7:E:102:BCL:HHD	1.98	0.45
15:O:104:SPO:H20	15:O:104:SPO:H181	1.80	0.45
5:R:31:ILE:HD12	7:R:102:BCL:H2	1.98	0.45
5:R:44:TRP:HB2	15:R:101:SPO:H10	1.99	0.45
15:R:101:SPO:H341	15:R:101:SPO:H361	1.68	0.45
7:F:101:BCL:HAC1	7:I:102:BCL:H101	1.98	0.45
16:F:102:MYR:H82	16:F:102:MYR:H122	1.99	0.45
15:I:104:SPO:H41	4:O:32:HIS:CG	2.52	0.45
15:O:104:SPO:H341	15:O:104:SPO:H362	1.72	0.45
7:Z:101:BCL:H192	7:Z:101:BCL:H162	1.82	0.45
9:L:303:U10:H312	9:L:303:U10:H372	1.98	0.45
2:M:4:TYR:CZ	2:M:6:ASN:HA	2.52	0.45
7:M:403:BCL:HHC	7:M:404:BCL:H42	1.98	0.45
13:M:411:LMT:H11	13:M:411:LMT:H42	1.76	0.44
5:N:47:TRP:CE2	7:N:102:BCL:H2C	2.52	0.44
7:Q:105:BCL:HMD1	5:R:38:HIS:CE1	2.52	0.44
10:L:305:PGV:H21	10:L:305:PGV:H52	1.81	0.44
13:L:311:LMT:H51	13:L:311:LMT:H22	1.58	0.44
2:M:29:GLU:HG3	4:V:15:ARG:NH2	2.32	0.44
4:A:28:ALA:O	4:A:32:HIS:ND1	2.32	0.44
15:G:102:SPO:H25	7:I:102:BCL:HED3	1.97	0.44
15:O:104:SPO:H26	15:O:104:SPO:H241	1.81	0.44
10:L:305:PGV:H11	13:I:101:LMT:H123	1.99	0.44
15:I:103:SPO:H20	15:I:103:SPO:H181	1.82	0.44
15:S:105:SPO:H293	15:W:101:SPO:H392	1.99	0.44
7:W:102:BCL:H112	7:W:102:BCL:H72	1.80	0.44
1:L:116:PHE:CE2	12:L:307:LDA:H12	2.52	0.44
7:A:101:BCL:H62	7:A:101:BCL:H41	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:31:ILE:HD12	7:T:102:BCL:H2	2.00	0.44
9:L:304:U10:H261	4:A:26:LEU:HD22	1.99	0.44
2:M:89:LEU:HB3	9:M:401:U10:H1M3	1.99	0.44
12:M:420:LDA:H52	12:M:420:LDA:H21	1.78	0.44
15:D:101:SPO:H133	15:E:101:SPO:H301	1.98	0.44
10:Q:103:PGV:H32	7:S:103:BCL:H93	1.99	0.44
15:O:103:SPO:H26	15:O:103:SPO:H241	1.86	0.44
15:P:101:SPO:H20	15:P:101:SPO:H181	1.89	0.44
15:W:101:SPO:H15	15:W:101:SPO:H131	1.89	0.44
4:A:39:PRO:HA	4:A:42:ASN:HB2	2.00	0.44
4:S:17:PHE:CE2	15:S:104:SPO:H351	2.53	0.44
7:J:101:BCL:H162	7:J:101:BCL:H141	1.76	0.44
7:R:102:BCL:HMB1	7:R:102:BCL:HBB2	2.00	0.44
7:V:101:BCL:H2A	15:W:101:SPO:H25	2.00	0.44
2:M:296:TRP:O	2:M:300:HIS:HD2	2.01	0.44
4:Q:36:LEU:HG	12:Q:102:LDA:H41	2.00	0.44
15:F:104:SPO:H20	15:F:104:SPO:H181	1.84	0.43
15:O:104:SPO:H6	7:S:103:BCL:HMB2	1.99	0.43
15:P:101:SPO:H10	15:P:101:SPO:H81	1.89	0.43
4:S:1:FME:HA	4:S:4:PHE:CE2	2.53	0.43
1:L:146:ALA:O	6:X:65:TYR:OH	2.28	0.43
3:H:228:THR:HG22	3:H:230:LEU:N	2.33	0.43
15:D:103:SPO:H392	5:E:19:LEU:HA	2.01	0.43
7:F:101:BCL:H2A	7:F:101:BCL:HED3	1.99	0.43
4:K:4:PHE:O	4:K:7:ILE:HG22	2.18	0.43
15:M:408:SPO:H10	15:M:408:SPO:H81	1.91	0.43
4:V:1:FME:HA	4:V:4:PHE:HE1	1.82	0.43
2:M:160:GLY:HA3	15:M:408:SPO:H292	2.01	0.43
4:A:6:LYS:HD3	15:D:103:SPO:H393	2.00	0.43
7:G:101:BCL:H93	7:G:101:BCL:H61	1.81	0.43
7:O:102:BCL:HED3	15:P:101:SPO:H27	2.01	0.43
7:S:103:BCL:HMD1	5:T:38:HIS:CE1	2.54	0.43
7:A:101:BCL:H93	7:A:101:BCL:H61	1.77	0.43
7:K:102:BCL:H41	7:K:102:BCL:H62	1.66	0.43
15:S:105:SPO:H20	15:S:105:SPO:H181	1.79	0.43
10:L:305:PGV:H51	10:L:305:PGV:H261	2.00	0.43
2:M:33:ALA:HB2	2:M:49:PRO:HD3	2.01	0.43
2:M:274:MET:O	2:M:278:THR:OG1	2.32	0.43
13:L:308:LMT:H5B	13:L:308:LMT:H6E	2.00	0.43
15:M:408:SPO:H15	15:M:408:SPO:H131	1.93	0.43
10:M:415:PGV:H72	4:S:22:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:6:LEU:HD11	15:O:103:SPO:H391	2.01	0.43
7:F:103:BCL:HHD	5:G:41:VAL:HG21	2.01	0.43
7:K:102:BCL:HED3	15:N:101:SPO:H27	2.01	0.43
15:N:101:SPO:H15	15:N:101:SPO:H131	1.77	0.43
4:O:1:FME:HA	4:O:4:PHE:CE1	2.53	0.43
13:L:311:LMT:O2'	7:F:101:BCL:HED2	2.18	0.43
7:D:102:BCL:H202	7:D:102:BCL:H162	1.73	0.43
5:G:27:LEU:O	5:G:31:ILE:HG12	2.18	0.43
4:K:3:LYS:NZ	4:K:6:LYS:HD2	2.34	0.43
15:W:101:SPO:H20	15:W:101:SPO:H181	1.89	0.43
15:W:101:SPO:H291	15:W:101:SPO:H312	1.85	0.43
9:L:304:U10:H403	13:A:102:LMT:H82	2.01	0.43
7:F:101:BCL:HBB2	7:F:101:BCL:HMB1	2.00	0.43
2:M:284:LEU:HD23	2:M:284:LEU:HA	1.91	0.42
15:S:104:SPO:H10	15:S:104:SPO:H81	1.93	0.42
2:M:122:ALA:HA	2:M:156:TRP:HH2	1.84	0.42
2:M:203:LEU:HD23	10:M:402:PGV:H241	2.01	0.42
5:W:48:PHE:HD2	7:W:102:BCL:H171	1.84	0.42
2:M:100:GLU:O	13:S:102:LMT:H6'1	2.19	0.42
2:M:105:LEU:HB3	13:Y:101:LMT:O2'	2.19	0.42
3:H:137:MET:HG3	3:H:169:MET:HB2	2.01	0.42
4:Q:34:ILE:O	4:Q:38:THR:HG23	2.19	0.42
7:L:310:BCL:HMB1	7:L:310:BCL:HBB2	2.01	0.42
3:H:194:PRO:O	3:H:198:LEU:HG	2.20	0.42
7:D:102:BCL:HHD	5:E:41:VAL:HG21	2.01	0.42
7:F:101:BCL:C4B	4:I:22:VAL:HG22	2.49	0.42
5:N:47:TRP:CD2	7:N:102:BCL:H2C	2.54	0.42
1:L:250:LEU:HD12	1:L:250:LEU:HA	1.83	0.42
2:M:283:ILE:HG12	7:M:404:BCL:HED3	2.02	0.42
7:K:102:BCL:H161	7:K:102:BCL:H141	1.75	0.42
3:H:192:LEU:HB2	3:H:235:ILE:HD13	2.02	0.42
5:B:22:VAL:HG13	15:D:101:SPO:H362	2.01	0.42
7:D:102:BCL:HMD1	5:E:38:HIS:CE1	2.54	0.42
15:F:104:SPO:H15	15:F:104:SPO:H131	1.96	0.42
13:M:410:LMT:H6'2	4:S:38:THR:HB	2.02	0.42
15:G:102:SPO:H22	7:I:102:BCL:O1D	2.20	0.42
4:Q:5:TYR:CZ	4:Q:6:LYS:HE3	2.54	0.42
5:R:6:LEU:HB3	5:R:7:SER:H	1.71	0.42
15:D:105:SPO:H241	15:D:105:SPO:H26	1.78	0.42
4:O:11:PHE:HE2	4:Q:17:PHE:HD2	1.67	0.42
15:O:104:SPO:H15	15:O:104:SPO:H131	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:186:TRP:CZ3	9:L:303:U10:H153	2.55	0.42
4:A:44:LEU:HD11	13:A:102:LMT:O2'	2.20	0.42
7:B:101:BCL:HMB1	7:B:101:BCL:HBB2	2.01	0.42
1:L:7:GLU:HA	2:M:249:LEU:HD11	2.02	0.42
10:H:303:PGV:H21	10:H:303:PGV:H52	1.86	0.42
15:E:101:SPO:H42	15:E:101:SPO:H83	2.02	0.42
5:J:47:TRP:CE2	7:J:101:BCL:H2C	2.55	0.42
4:Q:24:LEU:HD23	4:Q:24:LEU:HA	1.90	0.42
5:R:27:LEU:O	5:R:31:ILE:HG12	2.20	0.42
7:S:103:BCL:H122	15:T:101:SPO:H341	2.02	0.42
9:L:304:U10:C43	9:L:304:U10:H401	2.49	0.41
4:D:7:ILE:HD11	15:D:105:SPO:H311	2.01	0.41
5:G:47:TRP:CD2	7:G:101:BCL:H2C	2.54	0.41
15:O:104:SPO:H10	15:O:104:SPO:H81	1.94	0.41
6:X:8:PHE:HB2	6:X:21:TRP:CE2	2.55	0.41
1:L:200:ASN:HB3	10:M:413:PGV:H041	2.02	0.41
1:L:264:TRP:HH2	9:L:303:U10:H351	1.85	0.41
8:M:405:BPH:HBA2	8:M:405:BPH:H3A	1.73	0.41
7:O:102:BCL:HMD1	5:P:38:HIS:CE1	2.55	0.41
5:B:31:ILE:HD13	7:B:101:BCL:H51	2.02	0.41
7:R:102:BCL:H52	15:T:101:SPO:H243	2.02	0.41
15:T:101:SPO:H20	15:T:101:SPO:H181	1.82	0.41
4:V:40:ALA:O	5:W:45:ARG:NH1	2.53	0.41
9:L:304:U10:H521	9:L:304:U10:H501	1.71	0.41
2:M:14:ALA:HA	3:H:176:GLN:HE21	1.86	0.41
3:H:217:THR:OG1	3:H:238:TYR:OH	2.29	0.41
4:K:11:PHE:CZ	4:O:14:ARG:HA	2.54	0.41
10:M:413:PGV:H252	10:M:414:PGV:H201	2.01	0.41
15:S:104:SPO:H132	7:V:101:BCL:H61	2.02	0.41
9:M:407:U10:H301	9:M:407:U10:H321	1.74	0.41
15:E:101:SPO:H10	15:E:101:SPO:H81	1.64	0.41
7:F:101:BCL:H191	4:I:33:LEU:HD12	2.03	0.41
7:G:101:BCL:H61	7:G:101:BCL:H2	1.66	0.41
7:K:102:BCL:HHD	7:K:102:BCL:HAC1	1.86	0.41
7:P:102:BCL:H93	7:P:102:BCL:H62	1.75	0.41
7:V:101:BCL:H162	7:V:101:BCL:H141	1.84	0.41
1:L:131:VAL:HA	1:L:135:ILE:HB	2.03	0.41
1:L:250:LEU:O	1:L:254:THR:OG1	2.28	0.41
4:O:26:LEU:HD13	4:O:26:LEU:HA	1.93	0.41
5:R:36:LEU:HD13	5:R:36:LEU:HA	1.91	0.41
15:S:104:SPO:H20	15:S:104:SPO:H181	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:101:BCL:HBB3	7:V:101:BCL:HMB1	2.01	0.41
7:I:102:BCL:H162	7:I:102:BCL:H192	1.76	0.41
4:V:20:GLN:HE21	4:V:20:GLN:HB3	1.66	0.41
1:L:129:TYR:O	1:L:133:VAL:HG22	2.20	0.41
2:M:233:GLU:O	2:M:237:ILE:HG13	2.21	0.41
12:M:420:LDA:H92	12:M:420:LDA:H61	1.87	0.41
4:F:34:ILE:O	4:F:38:THR:HG23	2.20	0.41
7:I:102:BCL:HMD1	5:J:38:HIS:CE1	2.56	0.41
5:J:6:LEU:HD21	5:N:19:LEU:HD12	2.02	0.41
7:N:102:BCL:H162	7:N:102:BCL:H202	1.70	0.41
15:W:101:SPO:H10	15:W:101:SPO:H81	1.81	0.41
1:L:39:THR:HG21	1:L:101:TRP:HE3	1.85	0.41
2:M:277:LEU:HD21	10:M:414:PGV:H261	2.03	0.41
8:M:405:BPH:H6C2	8:M:405:BPH:H4C1	1.82	0.41
13:M:412:LMT:H6E	4:Y:33:LEU:HB3	2.02	0.41
5:E:6:LEU:H	5:G:15:GLN:NE2	2.19	0.41
7:Y:102:BCL:HBB3	7:Y:102:BCL:HMB1	2.02	0.41
3:H:132:ASN:HB2	3:H:135:GLN:HE21	1.86	0.40
3:H:222:LYS:HG2	3:H:231:GLU:OE2	2.20	0.40
3:H:223:SER:HB2	3:H:226:VAL:HB	2.02	0.40
4:A:17:PHE:CE2	6:X:22:ILE:HG12	2.55	0.40
15:D:101:SPO:H26	15:D:101:SPO:H241	1.86	0.40
5:P:12:THR:C	5:P:14:GLU:H	2.25	0.40
4:Q:36:LEU:HD13	4:Q:43:TRP:CH2	2.56	0.40
7:T:102:BCL:H162	7:T:102:BCL:H192	1.73	0.40
13:L:308:LMT:H121	13:L:308:LMT:H92	1.88	0.40
4:F:11:PHE:HB3	4:F:16:VAL:HG21	2.02	0.40
4:Q:41:PHE:CE2	5:R:45:ARG:HG2	2.56	0.40
10:Q:103:PGV:H242	4:S:22:VAL:HG23	2.03	0.40
4:S:37:SER:HA	13:S:101:LMT:H1B	2.03	0.40
7:S:103:BCL:H161	7:S:103:BCL:H202	1.80	0.40
10:M:413:PGV:H131	10:M:413:PGV:H102	1.77	0.40
3:H:61:PRO:HA	3:H:75:PRO:HD2	2.03	0.40
7:K:102:BCL:HMD1	5:N:38:HIS:CE1	2.56	0.40
7:F:101:BCL:H93	7:F:101:BCL:H111	1.95	0.40
8:L:302:BPH:H141	7:L:310:BCL:HBB3	2.03	0.40
15:N:101:SPO:H10	15:N:101:SPO:H81	1.90	0.40
7:W:102:BCL:HBB2	7:W:102:BCL:HMB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	280/282 (99%)	274 (98%)	6 (2%)	0	100	100
2	M	302/307 (98%)	293 (97%)	9 (3%)	0	100	100
3	H	246/253 (97%)	240 (98%)	6 (2%)	0	100	100
4	A	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
4	D	54/58 (93%)	52 (96%)	2 (4%)	0	100	100
4	F	52/58 (90%)	52 (100%)	0	0	100	100
4	I	54/58 (93%)	52 (96%)	2 (4%)	0	100	100
4	K	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	O	54/58 (93%)	52 (96%)	2 (4%)	0	100	100
4	Q	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
4	S	55/58 (95%)	51 (93%)	4 (7%)	0	100	100
4	V	54/58 (93%)	51 (94%)	2 (4%)	1 (2%)	8	15
4	Y	40/58 (69%)	40 (100%)	0	0	100	100
5	B	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	E	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	G	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	J	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	N	41/49 (84%)	41 (100%)	0	0	100	100
5	P	41/49 (84%)	39 (95%)	2 (5%)	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	39/49 (80%)	38 (97%)	1 (3%)	0	100	100
5	Z	29/49 (59%)	29 (100%)	0	0	100	100
6	X	63/78 (81%)	60 (95%)	3 (5%)	0	100	100
All	All	1802/1990 (91%)	1753 (97%)	48 (3%)	1 (0%)	54	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	V	2	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	227/227 (100%)	225 (99%)	2 (1%)	78 91
2	M	236/239 (99%)	234 (99%)	2 (1%)	81 92
3	H	213/217 (98%)	211 (99%)	2 (1%)	78 91
4	A	39/47 (83%)	35 (90%)	4 (10%)	7 13
4	D	46/47 (98%)	45 (98%)	1 (2%)	52 76
4	F	46/47 (98%)	45 (98%)	1 (2%)	52 76
4	I	46/47 (98%)	46 (100%)	0	100 100
4	K	46/47 (98%)	46 (100%)	0	100 100
4	O	45/47 (96%)	44 (98%)	1 (2%)	52 76
4	Q	46/47 (98%)	46 (100%)	0	100 100
4	S	47/47 (100%)	47 (100%)	0	100 100
4	V	46/47 (98%)	44 (96%)	2 (4%)	29 54
4	Y	35/47 (74%)	33 (94%)	2 (6%)	20 41
5	B	35/39 (90%)	34 (97%)	1 (3%)	42 68
5	E	35/39 (90%)	34 (97%)	1 (3%)	42 68
5	G	34/39 (87%)	33 (97%)	1 (3%)	42 68
5	J	35/39 (90%)	33 (94%)	2 (6%)	20 41
5	N	34/39 (87%)	34 (100%)	0	100 100
5	P	34/39 (87%)	34 (100%)	0	100 100
5	R	33/39 (85%)	33 (100%)	0	100 100
5	T	34/39 (87%)	34 (100%)	0	100 100
5	W	28/39 (72%)	28 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	Z	20/39 (51%)	20 (100%)	0	100 100
6	X	50/62 (81%)	49 (98%)	1 (2%)	55 78
All	All	1490/1605 (93%)	1467 (98%)	23 (2%)	66 83

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	248	CYS
1	L	273	TRP
2	M	52	LEU
2	M	215	PHE
3	H	151	ARG
3	H	233	ASP
4	A	3	LYS
4	A	35	LEU
4	A	43	TRP
4	A	44	LEU
5	B	19	LEU
4	D	3	LYS
5	E	6	LEU
4	F	54	VAL
5	G	19	LEU
5	J	6	LEU
5	J	42	MET
4	O	12	ASP
4	V	3	LYS
4	V	5	TYR
4	Y	31	ILE
4	Y	32	HIS
6	X	53	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	77	ASN
1	L	117	HIS
2	M	12	GLN
2	M	44	ASN
2	M	144	HIS
3	H	44	ASN

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Mol	Chain	Res	Type
3	H	176	GLN
5	E	17	GLN
4	I	20	GLN
5	J	17	GLN
4	K	20	GLN
5	N	15	GLN
4	O	51	HIS
4	V	20	GLN
5	W	17	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

9 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	I	1	4	8,9,10	0.52	0	7,9,11	0.95	1 (14%)
4	FME	A	1	4	8,9,10	0.52	0	7,9,11	0.92	1 (14%)
4	FME	S	1	4	5,6,10	0.82	0	3,6,11	0.75	0
4	FME	D	1	4	8,9,10	0.51	0	7,9,11	1.02	1 (14%)
4	FME	Q	1	4	8,9,10	0.53	0	7,9,11	0.96	1 (14%)
4	FME	F	1	4	8,9,10	0.49	0	7,9,11	1.18	1 (14%)
4	FME	V	1	4	8,9,10	0.55	0	7,9,11	0.93	1 (14%)
4	FME	K	1	4	8,9,10	0.53	0	7,9,11	0.97	1 (14%)
4	FME	O	1	4	8,9,10	0.51	0	7,9,11	1.06	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	I	1	4	-	1/7/9/11	-
4	FME	A	1	4	-	1/7/9/11	-
4	FME	S	1	4	-	1/2/5/11	-
4	FME	D	1	4	-	0/7/9/11	-
4	FME	Q	1	4	-	0/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	V	1	4	-	1/7/9/11	-
4	FME	K	1	4	-	1/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	1	FME	O-C-CA	-2.59	118.00	124.78
4	F	1	FME	O-C-CA	-2.53	118.16	124.78
4	D	1	FME	O-C-CA	-2.52	118.18	124.78
4	I	1	FME	O-C-CA	-2.45	118.35	124.78
4	V	1	FME	O-C-CA	-2.43	118.42	124.78
4	K	1	FME	O-C-CA	-2.41	118.47	124.78
4	Q	1	FME	O-C-CA	-2.41	118.47	124.78
4	A	1	FME	O-C-CA	-2.35	118.63	124.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	F	1	FME	O1-CN-N-CA
4	O	1	FME	O1-CN-N-CA
4	S	1	FME	O1-CN-N-CA
4	I	1	FME	N-CA-CB-CG
4	V	1	FME	N-CA-CB-CG
4	K	1	FME	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1	FME	1	0
4	F	1	FME	1	0
4	V	1	FME	1	0
4	O	1	FME	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 89 ligands modelled in this entry, 1 is monoatomic - leaving 88 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	D	105	-	40,41,41	0.67	0	47,50,50	1.75	13 (27%)
13	LMT	X	102	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
10	PGV	M	414	-	34,34,50	1.09	2 (5%)	37,40,56	1.15	3 (8%)
12	LDA	O	101	-	12,15,15	2.06	1 (8%)	14,17,17	0.53	0
7	BCL	T	102	-	58,74,74	1.65	10 (17%)	69,115,115	1.67	12 (17%)
7	BCL	Q	105	-	58,74,74	1.63	9 (15%)	69,115,115	1.80	16 (23%)
9	U10	L	303	-	48,48,63	0.70	2 (4%)	58,61,79	0.60	0
7	BCL	K	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.83	17 (24%)
10	PGV	Q	103	-	34,34,50	1.11	2 (5%)	37,40,56	1.14	3 (8%)
13	LMT	K	101	-	36,36,36	0.40	0	47,47,47	0.84	1 (2%)
12	LDA	M	419	-	12,15,15	2.09	1 (8%)	14,17,17	0.46	0
7	BCL	D	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.87	17 (24%)
7	BCL	J	101	-	58,74,74	1.61	10 (17%)	69,115,115	1.67	13 (18%)
9	U10	M	401	-	20,20,63	0.99	2 (10%)	24,27,79	0.82	0
13	LMT	Y	101	-	29,29,36	0.42	0	40,40,47	0.75	1 (2%)
11	PEE	L	306	-	45,45,50	0.77	2 (4%)	48,50,55	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	LDA	H	302	-	10,13,15	2.28	1 (10%)	12,15,17	0.47	0
15	SPO	E	101	-	40,41,41	0.66	0	47,50,50	2.08	14 (29%)
13	LMT	L	309	-	35,35,36	0.39	0	46,46,47	0.72	1 (2%)
10	PGV	M	413	-	44,44,50	0.97	2 (4%)	47,50,56	1.10	2 (4%)
10	PGV	H	304	-	33,33,50	1.10	2 (6%)	36,39,56	1.14	2 (5%)
9	U10	L	304	-	63,63,63	0.64	2 (3%)	76,79,79	0.58	0
15	SPO	M	408	-	40,41,41	0.64	0	47,50,50	1.75	12 (25%)
15	SPO	N	101	-	40,41,41	0.67	0	47,50,50	1.95	16 (34%)
7	BCL	B	101	-	58,74,74	1.66	9 (15%)	69,115,115	1.64	14 (20%)
13	LMT	I	101	-	36,36,36	0.32	0	47,47,47	1.03	4 (8%)
15	SPO	G	102	-	40,41,41	0.67	0	47,50,50	1.99	14 (29%)
13	LMT	Q	101	-	36,36,36	0.45	0	47,47,47	0.82	1 (2%)
7	BCL	L	301	-	58,74,74	1.61	8 (13%)	69,115,115	1.71	14 (20%)
13	LMT	L	311	-	36,36,36	0.37	0	47,47,47	0.93	1 (2%)
13	LMT	M	411	-	36,36,36	0.35	0	47,47,47	0.74	1 (2%)
12	LDA	D	104	-	12,15,15	2.06	1 (8%)	14,17,17	0.61	0
13	LMT	A	102	-	33,33,36	0.47	0	44,44,47	0.97	2 (4%)
16	MYR	F	102	7	15,15,15	0.56	0	15,15,15	0.54	0
13	LMT	M	410	-	36,36,36	0.36	0	47,47,47	0.86	2 (4%)
13	LMT	M	412	-	33,33,36	0.38	0	44,44,47	0.81	1 (2%)
7	BCL	O	102	-	58,74,74	1.60	9 (15%)	69,115,115	1.84	14 (20%)
13	LMT	Y	103	-	28,28,36	0.45	0	39,39,47	0.75	1 (2%)
15	SPO	P	101	-	40,41,41	0.65	0	47,50,50	1.81	14 (29%)
7	BCL	G	101	-	58,74,74	1.64	10 (17%)	69,115,115	1.63	12 (17%)
8	BPH	M	405	-	51,70,70	0.60	2 (3%)	52,101,101	0.75	2 (3%)
13	LMT	M	417	-	34,34,36	0.38	0	45,45,47	0.68	1 (2%)
9	U10	M	407	-	48,48,63	0.73	2 (4%)	58,61,79	0.60	1 (1%)
13	LMT	M	409	-	25,25,36	0.48	0	36,36,47	0.99	1 (2%)
10	PGV	L	305	-	38,38,50	1.05	2 (5%)	41,44,56	1.11	2 (4%)
7	BCL	V	101	-	58,74,74	1.64	10 (17%)	69,115,115	1.72	14 (20%)
12	LDA	L	307	-	12,15,15	2.09	1 (8%)	14,17,17	0.49	0
7	BCL	Y	102	-	58,74,74	1.72	11 (18%)	69,115,115	1.65	15 (21%)
12	LDA	M	418	-	12,15,15	2.08	1 (8%)	14,17,17	0.53	0
7	BCL	W	102	-	58,74,74	1.68	10 (17%)	69,115,115	1.65	14 (20%)
13	LMT	S	102	-	34,34,36	0.37	0	45,45,47	0.72	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BCL	R	102	-	58,74,74	1.65	11 (18%)	69,115,115	1.68	14 (20%)
7	BCL	F	103	-	58,74,74	1.61	9 (15%)	69,115,115	1.75	12 (17%)
7	BCL	M	404	-	58,74,74	1.65	11 (18%)	69,115,115	1.74	13 (18%)
12	LDA	Q	104	-	8,11,15	2.54	1 (12%)	10,13,17	0.44	0
15	SPO	D	101	-	40,41,41	0.64	0	47,50,50	1.58	11 (23%)
15	SPO	W	101	-	40,41,41	0.65	0	47,50,50	1.77	12 (25%)
15	SPO	S	105	-	40,41,41	0.62	0	47,50,50	1.83	12 (25%)
10	PGV	M	415	-	37,37,50	1.06	2 (5%)	40,43,56	1.12	3 (7%)
7	BCL	I	102	-	58,74,74	1.62	9 (15%)	69,115,115	1.85	16 (23%)
7	BCL	E	102	-	58,74,74	1.64	10 (17%)	69,115,115	1.76	12 (17%)
13	LMT	L	308	-	36,36,36	0.35	0	47,47,47	0.72	0
15	SPO	F	104	-	40,41,41	0.65	0	47,50,50	1.98	14 (29%)
7	BCL	F	101	16	58,74,74	1.70	11 (18%)	69,115,115	1.68	12 (17%)
7	BCL	A	101	-	53,69,74	1.77	11 (20%)	63,109,115	1.87	14 (22%)
7	BCL	P	102	-	58,74,74	1.62	10 (17%)	69,115,115	1.71	16 (23%)
13	LMT	X	101	-	36,36,36	0.43	0	47,47,47	0.90	2 (4%)
7	BCL	Z	101	-	58,74,74	1.74	11 (18%)	69,115,115	1.60	12 (17%)
8	BPH	L	302	-	51,70,70	0.65	2 (3%)	52,101,101	0.71	1 (1%)
10	PGV	M	402	-	35,35,50	1.07	2 (5%)	38,41,56	1.14	3 (7%)
7	BCL	N	102	-	58,74,74	1.62	9 (15%)	69,115,115	1.72	12 (17%)
12	LDA	M	416	-	12,15,15	2.09	1 (8%)	14,17,17	0.47	0
10	PGV	H	303	-	42,42,50	0.98	2 (4%)	44,48,56	1.15	4 (9%)
15	SPO	D	103	-	40,41,41	0.67	0	47,50,50	1.80	13 (27%)
15	SPO	T	101	-	40,41,41	0.63	0	47,50,50	1.75	12 (25%)
12	LDA	Q	102	-	5,8,15	3.23	1 (20%)	7,10,17	0.33	0
7	BCL	S	103	-	58,74,74	1.62	8 (13%)	69,115,115	1.80	13 (18%)
15	SPO	O	104	-	40,41,41	0.67	0	47,50,50	1.87	15 (31%)
15	SPO	I	103	-	40,41,41	0.65	0	47,50,50	1.68	12 (25%)
13	LMT	S	101	-	27,27,36	0.44	0	37,38,47	0.86	2 (5%)
12	LDA	H	301	-	12,15,15	2.11	1 (8%)	14,17,17	0.49	0
15	SPO	O	103	-	40,41,41	0.63	0	47,50,50	1.62	10 (21%)
7	BCL	L	310	-	58,74,74	1.61	9 (15%)	69,115,115	1.75	14 (20%)
15	SPO	I	104	-	40,41,41	0.67	0	47,50,50	1.80	16 (34%)
7	BCL	M	403	-	58,74,74	1.65	11 (18%)	69,115,115	1.68	13 (18%)
12	LDA	M	420	-	12,15,15	2.10	1 (8%)	14,17,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	SPO	S	104	-	40,41,41	0.66	0	47,50,50	1.82	14 (29%)
15	SPO	R	101	-	40,41,41	0.68	0	47,50,50	3.72	16 (34%)

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	D	105	-	-	4/47/47/47	-
13	LMT	X	102	-	-	4/21/61/61	0/2/2/2
10	PGV	M	414	-	-	7/39/39/55	-
12	LDA	O	101	-	-	2/13/13/13	-
7	BCL	T	102	-	-	11/37/137/137	-
7	BCL	Q	105	-	-	15/37/137/137	-
9	U10	L	303	-	-	12/45/69/87	0/1/1/1
7	BCL	K	102	-	-	10/37/137/137	-
10	PGV	Q	103	-	-	11/39/39/55	-
13	LMT	K	101	-	-	4/21/61/61	0/2/2/2
12	LDA	M	419	-	-	2/13/13/13	-
7	BCL	D	102	-	-	14/37/137/137	-
7	BCL	J	101	-	-	14/37/137/137	-
9	U10	M	401	-	-	4/12/36/87	0/1/1/1
13	LMT	Y	101	-	-	3/14/54/61	0/2/2/2
11	PEE	L	306	-	-	12/49/49/54	-
12	LDA	H	302	-	-	2/11/11/13	-
15	SPO	E	101	-	-	14/47/47/47	-
13	LMT	L	309	-	-	8/20/60/61	0/2/2/2
10	PGV	M	413	-	-	15/49/49/55	-
10	PGV	H	304	-	-	18/38/38/55	-
9	U10	L	304	-	-	17/63/87/87	0/1/1/1
15	SPO	M	408	-	-	4/47/47/47	-
15	SPO	N	101	-	-	9/47/47/47	-
7	BCL	B	101	-	-	11/37/137/137	-
13	LMT	I	101	-	-	6/21/61/61	0/2/2/2
15	SPO	G	102	-	-	13/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LMT	Q	101	-	-	8/21/61/61	0/2/2/2
7	BCL	L	301	-	-	8/37/137/137	-
13	LMT	L	311	-	-	6/21/61/61	0/2/2/2
13	LMT	M	411	-	-	2/21/61/61	0/2/2/2
12	LDA	D	104	-	-	9/13/13/13	-
13	LMT	A	102	-	-	6/18/58/61	0/2/2/2
16	MYR	F	102	7	-	5/13/13/13	-
13	LMT	M	410	-	-	5/21/61/61	0/2/2/2
13	LMT	M	412	-	-	1/18/58/61	0/2/2/2
7	BCL	O	102	-	-	11/37/137/137	-
13	LMT	Y	103	-	-	6/13/53/61	0/2/2/2
15	SPO	P	101	-	-	5/47/47/47	-
7	BCL	G	101	-	-	15/37/137/137	-
8	BPH	M	405	-	-	5/37/105/105	0/5/6/6
13	LMT	M	417	-	-	7/19/59/61	0/2/2/2
9	U10	M	407	-	-	5/45/69/87	0/1/1/1
13	LMT	M	409	-	-	1/10/50/61	0/2/2/2
10	PGV	L	305	-	-	15/43/43/55	-
7	BCL	V	101	-	-	12/37/137/137	-
12	LDA	L	307	-	-	2/13/13/13	-
7	BCL	Y	102	-	-	10/37/137/137	-
12	LDA	M	418	-	-	2/13/13/13	-
7	BCL	W	102	-	-	14/37/137/137	-
13	LMT	S	102	-	-	4/19/59/61	0/2/2/2
7	BCL	R	102	-	-	14/37/137/137	-
7	BCL	F	103	-	-	10/37/137/137	-
7	BCL	M	404	-	-	7/37/137/137	-
12	LDA	Q	104	-	-	2/9/9/13	-
15	SPO	D	101	-	-	6/47/47/47	-
15	SPO	W	101	-	-	3/47/47/47	-
15	SPO	S	105	-	-	5/47/47/47	-
10	PGV	M	415	-	-	9/42/42/55	-
7	BCL	I	102	-	-	9/37/137/137	-
7	BCL	E	102	-	-	13/37/137/137	-
13	LMT	L	308	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SPO	F	104	-	-	10/47/47/47	-
7	BCL	F	101	16	-	16/37/137/137	-
7	BCL	A	101	-	-	12/31/131/137	-
7	BCL	P	102	-	-	10/37/137/137	-
13	LMT	X	101	-	-	6/21/61/61	0/2/2/2
7	BCL	Z	101	-	-	12/37/137/137	-
8	BPH	L	302	-	-	6/37/105/105	0/5/6/6
10	PGV	M	402	-	-	16/40/40/55	-
7	BCL	N	102	-	-	15/37/137/137	-
12	LDA	M	416	-	-	1/13/13/13	-
10	PGV	H	303	-	-	10/47/47/55	-
15	SPO	D	103	-	-	6/47/47/47	-
15	SPO	T	101	-	-	4/47/47/47	-
12	LDA	Q	102	-	-	0/6/6/13	-
7	BCL	S	103	-	-	8/37/137/137	-
15	SPO	O	104	-	-	4/47/47/47	-
15	SPO	I	103	-	-	4/47/47/47	-
13	LMT	S	101	-	-	6/12/52/61	0/2/2/2
12	LDA	H	301	-	-	7/13/13/13	-
15	SPO	O	103	-	-	1/47/47/47	-
7	BCL	L	310	-	-	8/37/137/137	-
15	SPO	I	104	-	-	4/47/47/47	-
7	BCL	M	403	-	-	17/37/137/137	-
12	LDA	M	420	-	-	3/13/13/13	-
15	SPO	S	104	-	-	4/47/47/47	-
15	SPO	R	101	-	-	9/47/47/47	-

All (287) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	301	LDA	O1-N1	-7.29	1.25	1.42
12	M	420	LDA	O1-N1	-7.24	1.25	1.42
12	M	419	LDA	O1-N1	-7.22	1.25	1.42
12	Q	102	LDA	O1-N1	-7.21	1.25	1.42
12	M	416	LDA	O1-N1	-7.20	1.25	1.42
12	L	307	LDA	O1-N1	-7.20	1.25	1.42
12	M	418	LDA	O1-N1	-7.19	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	302	LDA	O1-N1	-7.17	1.25	1.42
12	Q	104	LDA	O1-N1	-7.17	1.25	1.42
12	O	101	LDA	O1-N1	-7.12	1.25	1.42
12	D	104	LDA	O1-N1	-7.12	1.25	1.42
7	A	101	BCL	O2D-CGD	5.11	1.45	1.33
7	Z	101	BCL	O2D-CGD	5.11	1.45	1.33
7	M	404	BCL	O2D-CGD	5.11	1.45	1.33
7	B	101	BCL	O2D-CGD	5.10	1.45	1.33
7	Y	102	BCL	O2D-CGD	5.10	1.45	1.33
7	F	101	BCL	O2D-CGD	5.08	1.45	1.33
7	W	102	BCL	O2D-CGD	5.07	1.45	1.33
7	L	301	BCL	O2D-CGD	5.04	1.45	1.33
7	R	102	BCL	O2D-CGD	5.02	1.45	1.33
7	J	101	BCL	O2D-CGD	5.00	1.45	1.33
7	N	102	BCL	O2D-CGD	4.99	1.45	1.33
7	F	103	BCL	O2D-CGD	4.98	1.45	1.33
7	T	102	BCL	O2D-CGD	4.98	1.45	1.33
7	D	102	BCL	O2D-CGD	4.97	1.45	1.33
7	P	102	BCL	O2D-CGD	4.97	1.45	1.33
7	S	103	BCL	O2D-CGD	4.95	1.45	1.33
7	Q	105	BCL	O2D-CGD	4.95	1.45	1.33
7	O	102	BCL	O2D-CGD	4.93	1.45	1.33
7	G	101	BCL	O2D-CGD	4.93	1.45	1.33
7	V	101	BCL	O2D-CGD	4.92	1.45	1.33
7	K	102	BCL	O2D-CGD	4.91	1.45	1.33
7	E	102	BCL	O2D-CGD	4.90	1.45	1.33
7	I	102	BCL	O2D-CGD	4.89	1.45	1.33
7	Y	102	BCL	C3B-C2B	4.84	1.48	1.39
7	Z	101	BCL	C3B-C2B	4.84	1.48	1.39
7	T	102	BCL	C3B-C2B	4.84	1.48	1.39
7	M	403	BCL	O2D-CGD	4.83	1.45	1.33
7	W	102	BCL	C3B-C2B	4.82	1.48	1.39
7	M	404	BCL	C3B-C2B	4.81	1.48	1.39
7	L	310	BCL	O2D-CGD	4.79	1.44	1.33
7	E	102	BCL	C3B-C2B	4.76	1.48	1.39
7	A	101	BCL	C3B-C2B	4.76	1.48	1.39
7	F	101	BCL	C3B-C2B	4.75	1.47	1.39
7	N	102	BCL	C3B-C2B	4.74	1.47	1.39
7	Z	101	BCL	C3D-C2D	4.72	1.47	1.39
7	R	102	BCL	C3B-C2B	4.72	1.47	1.39
7	K	102	BCL	C3B-C2B	4.71	1.47	1.39
7	Q	105	BCL	C3B-C2B	4.69	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	102	BCL	C3B-C2B	4.69	1.47	1.39
7	G	101	BCL	C3B-C2B	4.68	1.47	1.39
7	L	310	BCL	C3B-C2B	4.67	1.47	1.39
7	M	403	BCL	C3B-C2B	4.66	1.47	1.39
7	B	101	BCL	C3B-C2B	4.66	1.47	1.39
7	L	301	BCL	C3B-C2B	4.63	1.47	1.39
7	V	101	BCL	C3B-C2B	4.63	1.47	1.39
7	P	102	BCL	C3B-C2B	4.61	1.47	1.39
7	Y	102	BCL	OBD-CAD	4.60	1.28	1.22
7	F	101	BCL	OBD-CAD	4.58	1.28	1.22
7	S	103	BCL	C3B-C2B	4.58	1.47	1.39
7	F	103	BCL	C3B-C2B	4.54	1.47	1.39
7	Z	101	BCL	OBD-CAD	4.52	1.28	1.22
7	J	101	BCL	C3B-C2B	4.50	1.47	1.39
7	D	102	BCL	C3B-C2B	4.49	1.47	1.39
7	Y	102	BCL	C3D-C2D	4.49	1.47	1.39
7	W	102	BCL	OBD-CAD	4.46	1.28	1.22
7	O	102	BCL	C3B-C2B	4.42	1.47	1.39
7	A	101	BCL	OBD-CAD	4.42	1.28	1.22
7	R	102	BCL	OBD-CAD	4.40	1.28	1.22
7	V	101	BCL	OBD-CAD	4.39	1.28	1.22
7	M	403	BCL	OBD-CAD	4.38	1.28	1.22
7	W	102	BCL	C3D-C2D	4.38	1.47	1.39
7	F	101	BCL	C3D-C2D	4.37	1.47	1.39
7	M	403	BCL	C3D-C2D	4.35	1.47	1.39
7	A	101	BCL	C3D-C2D	4.32	1.47	1.39
7	T	102	BCL	C3D-C2D	4.31	1.47	1.39
7	S	103	BCL	OBD-CAD	4.30	1.28	1.22
7	B	101	BCL	OBD-CAD	4.30	1.28	1.22
7	M	404	BCL	OBD-CAD	4.30	1.28	1.22
7	L	310	BCL	C3D-C2D	4.30	1.47	1.39
7	Z	101	BCL	O2A-CGA	4.29	1.45	1.33
10	L	305	PGV	O03-C19	4.29	1.45	1.33
7	R	102	BCL	C3D-C2D	4.29	1.47	1.39
7	G	101	BCL	O2A-CGA	4.28	1.45	1.33
7	P	102	BCL	OBD-CAD	4.26	1.28	1.22
7	L	310	BCL	O2A-CGA	4.26	1.45	1.33
7	N	102	BCL	OBD-CAD	4.25	1.28	1.22
7	T	102	BCL	OBD-CAD	4.25	1.28	1.22
7	G	101	BCL	OBD-CAD	4.25	1.28	1.22
10	Q	103	PGV	O03-C19	4.25	1.45	1.33
7	V	101	BCL	O2A-CGA	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	102	BCL	C3D-C2D	4.24	1.47	1.39
7	Y	102	BCL	O2A-CGA	4.23	1.45	1.33
7	Q	105	BCL	OBD-CAD	4.23	1.28	1.22
10	M	413	PGV	O03-C19	4.22	1.45	1.33
7	W	102	BCL	O2A-CGA	4.22	1.45	1.33
7	F	101	BCL	O2A-CGA	4.22	1.45	1.33
7	K	102	BCL	OBD-CAD	4.20	1.28	1.22
7	B	101	BCL	C3D-C2D	4.20	1.47	1.39
7	P	102	BCL	C3D-C2D	4.20	1.46	1.39
10	H	304	PGV	O03-C19	4.19	1.45	1.33
7	M	403	BCL	O2A-CGA	4.19	1.45	1.33
7	G	101	BCL	C3D-C2D	4.19	1.46	1.39
7	Q	105	BCL	O2A-CGA	4.18	1.45	1.33
10	M	414	PGV	O03-C19	4.18	1.45	1.33
7	E	102	BCL	C3D-C2D	4.18	1.46	1.39
7	D	102	BCL	C3D-C2D	4.17	1.46	1.39
7	D	102	BCL	O2A-CGA	4.17	1.45	1.33
7	F	103	BCL	OBD-CAD	4.17	1.28	1.22
10	M	415	PGV	O03-C19	4.16	1.45	1.33
7	O	102	BCL	OBD-CAD	4.16	1.28	1.22
7	E	102	BCL	OBD-CAD	4.15	1.28	1.22
7	J	101	BCL	OBD-CAD	4.14	1.28	1.22
7	D	102	BCL	OBD-CAD	4.14	1.28	1.22
10	H	303	PGV	O03-C19	4.13	1.45	1.33
7	E	102	BCL	O2A-CGA	4.12	1.45	1.33
7	L	310	BCL	OBD-CAD	4.12	1.28	1.22
7	S	103	BCL	O2A-CGA	4.12	1.45	1.33
7	L	301	BCL	OBD-CAD	4.11	1.28	1.22
10	M	402	PGV	O03-C19	4.11	1.45	1.33
7	V	101	BCL	C3D-C2D	4.11	1.46	1.39
7	F	103	BCL	O2A-CGA	4.10	1.45	1.33
7	J	101	BCL	O2A-CGA	4.10	1.45	1.33
10	M	413	PGV	O01-C1	4.09	1.45	1.34
7	I	102	BCL	OBD-CAD	4.09	1.28	1.22
7	A	101	BCL	O2A-CGA	4.09	1.45	1.33
7	O	102	BCL	C3D-C2D	4.08	1.46	1.39
7	B	101	BCL	O2A-CGA	4.08	1.45	1.33
7	R	102	BCL	O2A-CGA	4.08	1.45	1.33
7	T	102	BCL	O2A-CGA	4.07	1.45	1.33
7	I	102	BCL	C3D-C2D	4.07	1.46	1.39
7	L	301	BCL	O2A-CGA	4.07	1.45	1.33
7	J	101	BCL	C3D-C2D	4.07	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	102	BCL	C3D-C2D	4.06	1.46	1.39
10	L	305	PGV	O01-C1	4.06	1.45	1.34
7	M	404	BCL	C3D-C2D	4.05	1.46	1.39
7	F	103	BCL	C3D-C2D	4.05	1.46	1.39
7	O	102	BCL	O2A-CGA	4.05	1.45	1.33
7	Q	105	BCL	C3D-C2D	4.04	1.46	1.39
7	K	102	BCL	O2A-CGA	4.04	1.45	1.33
7	P	102	BCL	O2A-CGA	4.03	1.45	1.33
10	M	415	PGV	O01-C1	4.03	1.45	1.34
10	Q	103	PGV	O01-C1	4.03	1.45	1.34
7	N	102	BCL	O2A-CGA	4.03	1.45	1.33
7	I	102	BCL	O2A-CGA	4.02	1.45	1.33
10	M	402	PGV	O01-C1	4.01	1.45	1.34
7	M	404	BCL	O2A-CGA	4.00	1.45	1.33
10	M	414	PGV	O01-C1	3.97	1.45	1.34
10	H	304	PGV	O01-C1	3.96	1.45	1.34
10	H	303	PGV	O01-C1	3.96	1.45	1.34
7	L	301	BCL	C3D-C2D	3.91	1.46	1.39
7	S	103	BCL	C3D-C2D	3.87	1.46	1.39
7	Z	101	BCL	C2D-C1D	3.86	1.51	1.42
7	Y	102	BCL	C2D-C1D	3.81	1.51	1.42
7	A	101	BCL	C2D-C1D	3.66	1.50	1.42
7	F	101	BCL	C2D-C1D	3.66	1.50	1.42
7	V	101	BCL	C2D-C1D	3.50	1.50	1.42
7	S	103	BCL	C2D-C1D	3.45	1.50	1.42
11	L	306	PEE	C39-C38	3.39	1.51	1.31
11	L	306	PEE	C18-C19	3.35	1.51	1.31
7	M	404	BCL	C2D-C1D	3.32	1.50	1.42
7	Q	105	BCL	C2D-C1D	3.31	1.50	1.42
7	W	102	BCL	C2D-C1D	3.30	1.50	1.42
7	L	301	BCL	C2D-C1D	3.19	1.49	1.42
7	K	102	BCL	C2D-C1D	3.17	1.49	1.42
7	R	102	BCL	C2D-C1D	3.12	1.49	1.42
7	I	102	BCL	C2D-C1D	3.11	1.49	1.42
7	O	102	BCL	C2D-C1D	3.11	1.49	1.42
7	F	103	BCL	C2D-C1D	3.07	1.49	1.42
7	T	102	BCL	C2D-C1D	3.04	1.49	1.42
7	Z	101	BCL	MG-NC	-3.04	1.99	2.06
7	D	102	BCL	C2D-C1D	3.04	1.49	1.42
7	B	101	BCL	C2D-C1D	3.04	1.49	1.42
7	A	101	BCL	MG-NC	-3.02	1.99	2.06
7	G	101	BCL	C2D-C1D	3.01	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	102	BCL	MG-NC	-2.98	1.99	2.06
7	L	310	BCL	C2D-C1D	2.96	1.49	1.42
7	M	403	BCL	C2D-C1D	2.95	1.49	1.42
7	P	102	BCL	C2D-C1D	2.95	1.49	1.42
7	N	102	BCL	C2D-C1D	2.87	1.49	1.42
7	Z	101	BCL	MG-NA	-2.85	1.99	2.06
7	J	101	BCL	C2D-C1D	2.84	1.49	1.42
9	L	303	U10	C4-C5	-2.80	1.40	1.48
7	F	101	BCL	MG-NC	-2.77	1.99	2.06
7	A	101	BCL	MG-NA	-2.74	1.99	2.06
9	M	407	U10	C4-C5	-2.73	1.41	1.48
7	E	102	BCL	C2D-C1D	2.70	1.48	1.42
7	W	102	BCL	MG-NC	-2.69	1.99	2.06
9	L	304	U10	C3-C2	-2.68	1.41	1.48
8	M	405	BPH	C3A-C2A	-2.66	1.52	1.54
7	W	102	BCL	MG-NA	-2.61	2.00	2.06
7	Y	102	BCL	MG-NA	-2.59	2.00	2.06
7	F	101	BCL	MG-NA	-2.59	2.00	2.06
9	M	401	U10	C4-C5	-2.57	1.41	1.48
7	T	102	BCL	MG-NA	-2.54	2.00	2.06
8	L	302	BPH	C3A-C2A	-2.52	1.52	1.54
7	Z	101	BCL	CHD-C4C	2.49	1.48	1.41
9	M	407	U10	C3-C2	-2.48	1.41	1.48
7	R	102	BCL	MG-NA	-2.48	2.00	2.06
7	Y	102	BCL	C1B-CHB	2.48	1.47	1.41
7	D	102	BCL	MG-NA	-2.48	2.00	2.06
8	L	302	BPH	CBD-CGD	-2.47	1.49	1.52
7	B	101	BCL	MG-NA	-2.45	2.00	2.06
7	O	102	BCL	MG-NA	-2.45	2.00	2.06
7	B	101	BCL	MG-NC	-2.43	2.00	2.06
9	L	304	U10	C4-C5	-2.42	1.41	1.48
7	L	310	BCL	MG-NA	-2.42	2.00	2.06
7	A	101	BCL	C1B-CHB	2.42	1.47	1.41
7	Z	101	BCL	C1B-CHB	2.42	1.47	1.41
7	I	102	BCL	MG-NA	-2.41	2.00	2.06
7	M	403	BCL	MG-NA	-2.41	2.00	2.06
7	E	102	BCL	MG-NA	-2.41	2.00	2.06
7	T	102	BCL	MG-NC	-2.40	2.00	2.06
7	K	102	BCL	MG-NA	-2.39	2.00	2.06
7	Z	101	BCL	C4B-CHC	2.39	1.47	1.41
7	D	102	BCL	C3C-C4C	-2.38	1.48	1.51
7	K	102	BCL	C3C-C4C	-2.38	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	102	BCL	C3C-C4C	-2.37	1.48	1.51
7	V	101	BCL	MG-NC	-2.37	2.00	2.06
7	M	403	BCL	C4B-NB	-2.33	1.33	1.35
7	V	101	BCL	MG-NA	-2.33	2.00	2.06
7	M	403	BCL	MG-NC	-2.32	2.00	2.06
7	Q	105	BCL	MG-NA	-2.32	2.00	2.06
7	F	101	BCL	CHD-C4C	2.31	1.47	1.41
7	E	102	BCL	MG-NC	-2.31	2.00	2.06
7	E	102	BCL	C3C-C4C	-2.31	1.48	1.51
7	S	103	BCL	MG-NC	-2.30	2.00	2.06
9	L	303	U10	C3-C2	-2.28	1.42	1.48
7	P	102	BCL	MG-NA	-2.27	2.00	2.06
7	M	404	BCL	MG-NA	-2.27	2.00	2.06
7	R	102	BCL	MG-NC	-2.27	2.00	2.06
7	A	101	BCL	CHD-C4C	2.27	1.47	1.41
7	F	101	BCL	C1B-CHB	2.27	1.47	1.41
7	S	103	BCL	MG-NA	-2.26	2.00	2.06
7	F	103	BCL	MG-NA	-2.25	2.00	2.06
7	L	301	BCL	C3C-C4C	-2.23	1.48	1.51
7	L	301	BCL	MG-NC	-2.23	2.01	2.06
7	Y	102	BCL	CHD-C4C	2.23	1.47	1.41
7	W	102	BCL	C1B-CHB	2.22	1.47	1.41
7	J	101	BCL	MG-NA	-2.21	2.01	2.06
7	N	102	BCL	MG-NA	-2.20	2.01	2.06
7	Y	102	BCL	C4B-CHC	2.20	1.47	1.41
9	M	401	U10	C3-C2	-2.19	1.42	1.48
8	M	405	BPH	CBD-CGD	-2.18	1.49	1.52
7	L	310	BCL	C1B-CHB	2.18	1.47	1.41
7	G	101	BCL	MG-NA	-2.17	2.01	2.06
7	M	404	BCL	MG-NC	-2.17	2.01	2.06
7	P	102	BCL	C3C-C4C	-2.16	1.48	1.51
7	P	102	BCL	MG-NC	-2.16	2.01	2.06
7	L	310	BCL	MG-NC	-2.16	2.01	2.06
7	M	404	BCL	C3C-C4C	-2.15	1.48	1.51
7	F	103	BCL	C3C-C4C	-2.14	1.48	1.51
7	G	101	BCL	C3C-C4C	-2.14	1.48	1.51
7	Q	105	BCL	MG-NC	-2.14	2.01	2.06
7	J	101	BCL	MG-NC	-2.14	2.01	2.06
7	F	103	BCL	MG-NC	-2.12	2.01	2.06
7	M	403	BCL	C1B-CHB	2.12	1.46	1.41
7	G	101	BCL	MG-NC	-2.12	2.01	2.06
7	T	102	BCL	C1B-CHB	2.12	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	102	BCL	C4B-CHC	2.12	1.46	1.41
7	G	101	BCL	C1B-CHB	2.11	1.46	1.41
7	T	102	BCL	C4B-CHC	2.11	1.46	1.41
7	R	102	BCL	C1B-CHB	2.11	1.46	1.41
7	N	102	BCL	MG-NC	-2.10	2.01	2.06
7	B	101	BCL	C3C-C4C	-2.10	1.49	1.51
7	J	101	BCL	C3C-C4C	-2.10	1.49	1.51
7	O	102	BCL	MG-NC	-2.08	2.01	2.06
7	O	102	BCL	C3C-C4C	-2.08	1.49	1.51
7	I	102	BCL	MG-NC	-2.08	2.01	2.06
7	F	101	BCL	C4B-CHC	2.08	1.46	1.41
7	V	101	BCL	C1B-CHB	2.06	1.46	1.41
7	K	102	BCL	C1B-CHB	2.06	1.46	1.41
7	A	101	BCL	C4B-CHC	2.05	1.46	1.41
7	K	102	BCL	MG-NC	-2.05	2.01	2.06
7	N	102	BCL	C4B-CHC	2.04	1.46	1.41
7	M	404	BCL	C4B-CHC	2.04	1.46	1.41
7	M	403	BCL	C3C-C4C	-2.04	1.49	1.51
7	Q	105	BCL	C3C-C4C	-2.03	1.49	1.51
7	R	102	BCL	C3C-C4C	-2.03	1.49	1.51
7	E	102	BCL	C1B-CHB	2.03	1.46	1.41
7	M	404	BCL	C1B-CHB	2.02	1.46	1.41
7	D	102	BCL	C1B-CHB	2.02	1.46	1.41
7	P	102	BCL	C1B-CHB	2.02	1.46	1.41
7	J	101	BCL	C1B-CHB	2.02	1.46	1.41
7	V	101	BCL	CHD-C4C	2.01	1.47	1.41
7	D	102	BCL	MG-NC	-2.01	2.01	2.06
7	W	102	BCL	CHD-C4C	2.00	1.47	1.41

All (635) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	R	101	SPO	C2-C1-C4	-15.71	86.74	110.86
15	R	101	SPO	C3-C1-C4	-14.76	88.19	110.86
15	E	101	SPO	C10-C9-C7	-7.44	116.69	127.31
7	A	101	BCL	C4B-CHC-C1C	-5.98	118.28	130.12
15	F	104	SPO	C5-C6-C7	-5.96	116.89	125.89
7	L	310	BCL	O2D-CGD-CBD	5.96	121.86	111.27
7	M	403	BCL	O2D-CGD-CBD	5.86	121.67	111.27
7	Y	102	BCL	O2D-CGD-CBD	5.54	121.12	111.27
15	O	104	SPO	C21-C22-C23	-5.25	119.81	127.31
15	R	101	SPO	C3-C1-C2	5.25	120.24	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	102	BCL	CHD-C4C-NC	5.10	130.74	125.08
15	G	102	SPO	C15-C14-C12	-5.09	120.04	127.31
7	Q	105	BCL	CMB-C2B-C3B	5.06	134.14	124.68
7	D	102	BCL	CHD-C4C-NC	5.04	130.67	125.08
7	Q	105	BCL	O2D-CGD-CBD	4.99	120.14	111.27
7	O	102	BCL	CHD-C4C-NC	4.98	130.60	125.08
7	V	101	BCL	O2D-CGD-CBD	4.97	120.09	111.27
7	I	102	BCL	CHD-C4C-NC	4.96	130.58	125.08
7	K	102	BCL	CMB-C2B-C3B	4.95	133.93	124.68
7	K	102	BCL	C3C-C4C-CHD	-4.92	112.88	123.39
7	F	103	BCL	CMB-C2B-C3B	4.92	133.88	124.68
7	F	103	BCL	CHD-C4C-NC	4.92	130.54	125.08
7	S	103	BCL	O2D-CGD-CBD	4.91	119.99	111.27
15	M	408	SPO	C20-C19-C17	-4.90	120.32	127.31
7	M	404	BCL	CHD-C4C-NC	4.89	130.51	125.08
7	A	101	BCL	C4A-NA-C1A	4.87	108.90	106.71
7	D	102	BCL	C3C-C4C-CHD	-4.85	113.04	123.39
7	E	102	BCL	CHD-C4C-NC	4.84	130.46	125.08
7	I	102	BCL	CMB-C2B-C3B	4.84	133.73	124.68
7	I	102	BCL	C3C-C4C-CHD	-4.83	113.08	123.39
7	O	102	BCL	CMB-C2B-C3B	4.82	133.70	124.68
7	K	102	BCL	O2D-CGD-CBD	4.82	119.83	111.27
7	Q	105	BCL	CHD-C4C-NC	4.80	130.40	125.08
7	O	102	BCL	O2D-CGD-CBD	4.79	119.78	111.27
7	O	102	BCL	C3C-C4C-CHD	-4.79	113.16	123.39
7	I	102	BCL	O2D-CGD-CBD	4.77	119.75	111.27
7	S	103	BCL	CHD-C4C-NC	4.77	130.37	125.08
7	F	103	BCL	O2D-CGD-CBD	4.74	119.68	111.27
7	R	102	BCL	CHD-C4C-NC	4.73	130.33	125.08
7	Z	101	BCL	O2D-CGD-CBD	4.73	119.67	111.27
7	F	101	BCL	O2D-CGD-CBD	4.73	119.67	111.27
7	M	404	BCL	CMB-C2B-C3B	4.70	133.48	124.68
7	F	103	BCL	C3C-C4C-CHD	-4.69	113.38	123.39
15	S	105	SPO	C20-C19-C17	-4.69	120.62	127.31
7	B	101	BCL	CHD-C4C-NC	4.68	130.28	125.08
7	L	301	BCL	CHD-C4C-NC	4.68	130.27	125.08
7	N	102	BCL	O2D-CGD-CBD	4.67	119.57	111.27
7	T	102	BCL	O2D-CGD-CBD	4.66	119.55	111.27
15	M	408	SPO	C21-C22-C23	-4.65	120.67	127.31
7	N	102	BCL	CMB-C2B-C3B	4.63	133.33	124.68
7	P	102	BCL	CHD-C4C-NC	4.62	130.21	125.08
15	R	101	SPO	C5-C6-C7	-4.61	118.92	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	103	BCL	CMB-C2B-C3B	4.61	133.30	124.68
7	A	101	BCL	O2D-CGD-CBD	4.61	119.45	111.27
7	D	102	BCL	CMB-C2B-C3B	4.60	133.28	124.68
7	J	101	BCL	CHD-C4C-NC	4.58	130.16	125.08
7	N	102	BCL	CHD-C4C-NC	4.57	130.16	125.08
7	E	102	BCL	C3C-C4C-CHD	-4.57	113.62	123.39
7	L	301	BCL	CMB-C2B-C3B	4.56	133.22	124.68
7	E	102	BCL	CMB-C2B-C3B	4.56	133.22	124.68
15	S	104	SPO	C21-C22-C23	-4.56	120.80	127.31
7	Q	105	BCL	C3C-C4C-CHD	-4.55	113.67	123.39
7	G	101	BCL	CHD-C4C-NC	4.55	130.13	125.08
15	G	102	SPO	C5-C6-C7	-4.54	119.03	125.89
7	G	101	BCL	CMB-C2B-C3B	4.54	133.17	124.68
7	L	301	BCL	C3C-C4C-CHD	-4.53	113.70	123.39
7	P	102	BCL	C3C-C4C-CHD	-4.53	113.71	123.39
7	N	102	BCL	C3C-C4C-CHD	-4.51	113.76	123.39
10	M	413	PGV	O01-C1-C2	4.49	121.17	111.50
7	G	101	BCL	C3C-C4C-CHD	-4.47	113.84	123.39
7	J	101	BCL	C3C-C4C-CHD	-4.47	113.84	123.39
7	M	403	BCL	CMB-C2B-C3B	4.47	133.03	124.68
7	R	102	BCL	O2D-CGD-CBD	4.46	119.20	111.27
7	E	102	BCL	O2D-CGD-CBD	4.46	119.20	111.27
7	M	404	BCL	C3C-C4C-CHD	-4.45	113.89	123.39
7	R	102	BCL	C3C-C4C-CHD	-4.44	113.90	123.39
7	T	102	BCL	CHD-C4C-NC	4.44	130.01	125.08
7	V	101	BCL	CMB-C2B-C3B	4.44	132.98	124.68
7	M	404	BCL	O2D-CGD-CBD	4.42	119.12	111.27
7	T	102	BCL	CMB-C2B-C3B	4.42	132.94	124.68
7	J	101	BCL	CMB-C2B-C3B	4.41	132.93	124.68
7	A	101	BCL	C1B-CHB-C4A	-4.40	121.40	130.12
15	D	105	SPO	C21-C22-C23	-4.39	121.04	127.31
10	H	303	PGV	O01-C1-C2	4.36	120.89	111.50
7	Z	101	BCL	C1B-CHB-C4A	-4.34	121.53	130.12
7	T	102	BCL	C3C-C4C-CHD	-4.33	114.14	123.39
7	Y	102	BCL	C4B-CHC-C1C	-4.31	121.59	130.12
7	D	102	BCL	C1-C2-C3	-4.30	118.60	126.04
7	L	310	BCL	CHD-C4C-NC	4.30	129.85	125.08
7	L	310	BCL	CMB-C2B-C3B	4.29	132.70	124.68
7	B	101	BCL	CMB-C2B-C3B	4.28	132.69	124.68
7	D	102	BCL	O2D-CGD-CBD	4.28	118.88	111.27
7	B	101	BCL	O2D-CGD-CBD	4.28	118.87	111.27
7	B	101	BCL	C3C-C4C-CHD	-4.26	114.29	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	103	BCL	C3C-C4C-CHD	-4.23	114.35	123.39
7	P	102	BCL	CMB-C2B-C3B	4.22	132.57	124.68
15	S	104	SPO	C20-C19-C17	-4.21	121.30	127.31
7	G	101	BCL	O2D-CGD-CBD	4.18	118.70	111.27
7	L	310	BCL	C3C-C4C-CHD	-4.18	114.46	123.39
10	L	305	PGV	O01-C1-C2	4.17	120.50	111.50
7	W	102	BCL	O2D-CGD-CBD	4.17	118.68	111.27
15	D	103	SPO	C21-C22-C23	-4.17	121.36	127.31
10	M	402	PGV	O01-C1-C2	4.15	120.44	111.50
7	J	101	BCL	O2D-CGD-CBD	4.14	118.63	111.27
7	R	102	BCL	CMB-C2B-C3B	4.14	132.42	124.68
15	R	101	SPO	C21-C22-C23	-4.13	121.41	127.31
7	P	102	BCL	O2D-CGD-CBD	4.10	118.56	111.27
15	P	101	SPO	C5-C6-C7	-4.10	119.69	125.89
15	O	104	SPO	C20-C19-C17	-4.02	121.58	127.31
15	W	101	SPO	C10-C9-C7	-4.01	121.58	127.31
15	D	103	SPO	C20-C19-C17	-4.01	121.59	127.31
7	L	301	BCL	O2D-CGD-CBD	4.00	118.37	111.27
15	T	101	SPO	C21-C22-C23	-3.98	121.62	127.31
15	N	101	SPO	C8-C7-C6	3.98	124.35	118.08
15	I	104	SPO	C21-C22-C23	-3.98	121.63	127.31
15	N	101	SPO	C15-C14-C12	-3.98	121.63	127.31
15	I	103	SPO	C20-C19-C17	-3.97	121.64	127.31
7	M	403	BCL	CHD-C4C-NC	3.97	129.49	125.08
7	W	102	BCL	C4B-CHC-C1C	-3.96	122.28	130.12
15	E	101	SPO	C20-C19-C17	-3.95	121.67	127.31
7	F	101	BCL	CMB-C2B-C3B	3.93	132.04	124.68
10	H	304	PGV	O01-C1-C2	3.93	119.97	111.50
15	I	104	SPO	C20-C19-C17	-3.91	121.72	127.31
13	Q	101	LMT	O1B-C4'-C3'	3.90	117.67	107.28
10	Q	103	PGV	O01-C1-C2	3.88	119.87	111.50
15	O	103	SPO	C21-C22-C23	-3.88	121.77	127.31
15	W	101	SPO	C21-C22-C23	-3.88	121.78	127.31
15	G	102	SPO	C20-C19-C17	-3.86	121.80	127.31
7	M	403	BCL	C3C-C4C-CHD	-3.84	115.18	123.39
15	S	105	SPO	C21-C22-C23	-3.83	121.85	127.31
15	D	105	SPO	C20-C19-C17	-3.81	121.87	127.31
10	M	414	PGV	O01-C1-C2	3.81	119.71	111.50
10	M	415	PGV	O01-C1-C2	3.81	119.70	111.50
7	V	101	BCL	CHD-C4C-NC	3.80	129.29	125.08
15	N	101	SPO	C5-C6-C7	3.79	131.62	125.89
15	F	104	SPO	C10-C9-C7	-3.79	121.90	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Y	102	BCL	C4A-NA-C1A	3.77	108.40	106.71
7	F	101	BCL	C1B-CHB-C4A	-3.76	122.66	130.12
7	F	101	BCL	C4B-CHC-C1C	-3.75	122.70	130.12
7	D	102	BCL	O2A-CGA-CBA	3.74	123.63	111.91
15	O	103	SPO	C20-C19-C17	-3.73	121.98	127.31
15	N	101	SPO	C21-C22-C23	-3.71	122.02	127.31
7	S	103	BCL	C1-C2-C3	-3.68	119.67	126.04
7	W	102	BCL	C1B-CHB-C4A	-3.68	122.82	130.12
15	F	104	SPO	C21-C22-C23	-3.68	122.05	127.31
15	D	101	SPO	C21-C22-C23	-3.66	122.09	127.31
15	G	102	SPO	C21-C22-C23	-3.66	122.09	127.31
15	T	101	SPO	C20-C19-C17	-3.64	122.11	127.31
7	A	101	BCL	C1-C2-C3	-3.64	119.75	126.04
7	Y	102	BCL	C4C-CHD-C1D	-3.64	120.51	125.88
7	W	102	BCL	CMB-C2B-C3B	3.63	131.46	124.68
15	N	101	SPO	C20-C19-C17	-3.63	122.14	127.31
7	L	301	BCL	C4C-CHD-C1D	-3.60	120.57	125.88
7	V	101	BCL	C1-C2-C3	-3.59	119.83	126.04
15	D	105	SPO	C31-C32-C33	-3.58	119.05	127.66
7	E	102	BCL	C4-C3-C5	3.54	121.23	115.27
15	E	101	SPO	C14-C15-C16	-3.54	112.18	123.22
7	L	301	BCL	O2A-CGA-CBA	3.54	123.00	111.91
7	Y	102	BCL	CMB-C2B-C3B	3.53	131.29	124.68
7	O	102	BCL	C1-C2-C3	-3.53	119.93	126.04
7	P	102	BCL	C4C-CHD-C1D	-3.53	120.67	125.88
15	F	104	SPO	C20-C19-C17	-3.50	122.31	127.31
7	F	101	BCL	C4A-NA-C1A	3.50	108.28	106.71
7	Z	101	BCL	CHD-C4C-NC	3.50	128.96	125.08
15	G	102	SPO	C34-C33-C35	3.49	121.14	115.27
7	L	310	BCL	C1-C2-C3	-3.49	120.01	126.04
15	O	104	SPO	C31-C32-C33	-3.47	119.30	127.66
7	V	101	BCL	C3C-C4C-CHD	-3.47	115.98	123.39
7	K	102	BCL	C4-C3-C5	3.46	121.08	115.27
7	I	102	BCL	C4C-CHD-C1D	-3.46	120.78	125.88
7	E	102	BCL	C4C-CHD-C1D	-3.45	120.80	125.88
7	K	102	BCL	C4C-CHD-C1D	-3.44	120.80	125.88
7	F	101	BCL	CHD-C4C-NC	3.44	128.90	125.08
15	T	101	SPO	C29-C28-C30	3.44	121.05	115.27
7	L	310	BCL	C4C-CHD-C1D	-3.43	120.82	125.88
7	S	103	BCL	C4-C3-C5	3.42	121.03	115.27
15	W	101	SPO	C5-C6-C7	-3.42	120.73	125.89
15	S	105	SPO	C31-C32-C33	-3.41	119.44	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Z	101	BCL	C1C-NC-C4C	3.41	108.24	106.71
7	D	102	BCL	C4C-CHD-C1D	-3.41	120.86	125.88
7	O	102	BCL	C4C-CHD-C1D	-3.40	120.86	125.88
7	W	102	BCL	CHD-C4C-NC	3.40	128.85	125.08
15	T	101	SPO	C5-C6-C7	-3.39	120.77	125.89
7	Q	105	BCL	C1-C2-C3	-3.39	120.18	126.04
7	M	403	BCL	C4C-CHD-C1D	-3.37	120.91	125.88
7	D	102	BCL	C1C-NC-C4C	-3.36	105.19	106.71
7	J	101	BCL	C4C-CHD-C1D	-3.34	120.95	125.88
15	P	101	SPO	C29-C28-C30	3.34	120.89	115.27
15	D	103	SPO	C31-C32-C33	-3.34	119.62	127.66
7	L	310	BCL	O2D-CGD-O1D	-3.33	117.33	123.84
7	G	101	BCL	C4C-CHD-C1D	-3.32	120.99	125.88
7	S	103	BCL	CHC-C1C-NC	3.29	129.07	124.51
7	W	102	BCL	C4C-CHD-C1D	-3.29	121.02	125.88
15	F	104	SPO	C29-C28-C30	3.29	120.80	115.27
15	S	104	SPO	C31-C32-C33	-3.29	119.74	127.66
7	R	102	BCL	C4C-CHD-C1D	-3.27	121.05	125.88
15	E	101	SPO	C21-C22-C23	-3.27	122.64	127.31
15	P	101	SPO	C21-C22-C23	-3.26	122.66	127.31
7	F	101	BCL	C4C-CHD-C1D	-3.26	121.07	125.88
15	E	101	SPO	C29-C28-C30	3.25	120.73	115.27
7	N	102	BCL	C4C-CHD-C1D	-3.24	121.11	125.88
15	P	101	SPO	C34-C33-C35	3.23	120.71	115.27
13	M	412	LMT	C1B-O1B-C4'	-3.23	109.97	117.96
15	F	104	SPO	C34-C33-C35	3.22	120.69	115.27
7	N	102	BCL	C4-C3-C5	3.22	120.69	115.27
7	F	103	BCL	C4C-CHD-C1D	-3.20	121.16	125.88
7	D	102	BCL	CHC-C1C-NC	3.19	128.93	124.51
7	T	102	BCL	C4-C3-C5	3.19	120.64	115.27
7	V	101	BCL	C4C-CHD-C1D	-3.18	121.18	125.88
13	M	409	LMT	C1B-O1B-C4'	-3.18	110.09	117.96
7	Z	101	BCL	CMB-C2B-C3B	3.18	130.63	124.68
15	G	102	SPO	C29-C28-C30	3.17	120.60	115.27
7	B	101	BCL	C4C-CHD-C1D	-3.17	121.21	125.88
15	I	104	SPO	C29-C28-C30	3.15	120.57	115.27
15	S	105	SPO	C29-C28-C30	3.15	120.57	115.27
7	D	102	BCL	C4A-NA-C1A	3.15	108.12	106.71
15	R	101	SPO	C29-C28-C30	3.15	120.57	115.27
7	N	102	BCL	C1-C2-C3	-3.15	120.60	126.04
15	P	101	SPO	C10-C9-C7	-3.14	122.83	127.31
7	A	101	BCL	C4C-CHD-C1D	-3.14	121.25	125.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	404	BCL	C4C-CHD-C1D	-3.13	121.26	125.88
7	O	102	BCL	CHC-C1C-NC	3.13	128.84	124.51
7	I	102	BCL	O2A-CGA-CBA	3.13	121.72	111.91
7	P	102	BCL	O2A-CGA-CBA	3.13	121.72	111.91
15	I	103	SPO	C31-C32-C33	-3.12	120.14	127.66
15	D	105	SPO	C9-C10-C11	-3.12	113.48	123.22
15	N	101	SPO	C34-C33-C35	3.11	120.51	115.27
7	P	102	BCL	C1-C2-C3	-3.11	120.66	126.04
7	T	102	BCL	C4C-CHD-C1D	-3.11	121.29	125.88
7	Y	102	BCL	C1-C2-C3	-3.11	120.67	126.04
7	R	102	BCL	C1-C2-C3	-3.10	120.67	126.04
15	E	101	SPO	C13-C12-C11	3.10	122.97	118.08
15	I	103	SPO	C21-C22-C23	-3.10	122.88	127.31
15	R	101	SPO	C15-C14-C12	-3.10	122.89	127.31
7	F	103	BCL	CHC-C1C-NC	3.10	128.80	124.51
7	S	103	BCL	C4C-CHD-C1D	-3.10	121.31	125.88
7	P	102	BCL	C4-C3-C5	3.09	120.48	115.27
15	S	105	SPO	C5-C6-C7	-3.09	121.22	125.89
15	R	101	SPO	C20-C19-C17	-3.09	122.90	127.31
15	D	103	SPO	C29-C28-C30	3.08	120.45	115.27
15	R	101	SPO	C34-C33-C35	3.07	120.44	115.27
7	Q	105	BCL	C4C-CHD-C1D	-3.07	121.36	125.88
7	L	301	BCL	C4-C3-C5	3.06	120.42	115.27
15	E	101	SPO	C34-C33-C35	3.05	120.41	115.27
7	I	102	BCL	C4-C3-C5	3.05	120.40	115.27
13	X	101	LMT	C1B-O1B-C4'	-3.05	110.42	117.96
7	J	101	BCL	O2A-CGA-CBA	3.05	121.47	111.91
7	O	102	BCL	C4-C3-C5	3.04	120.39	115.27
15	W	101	SPO	C29-C28-C30	3.04	120.38	115.27
15	M	408	SPO	C31-C32-C33	-3.04	120.35	127.66
7	A	101	BCL	CMB-C2B-C3B	3.03	130.35	124.68
15	S	105	SPO	C10-C9-C7	-3.03	122.98	127.31
7	M	403	BCL	O2D-CGD-O1D	-3.01	117.95	123.84
7	Z	101	BCL	C1-C2-C3	-3.01	120.84	126.04
7	B	101	BCL	CHB-C4A-NA	3.01	128.67	124.51
15	O	104	SPO	C15-C14-C12	-2.99	123.04	127.31
7	W	102	BCL	C4-C3-C5	2.98	120.28	115.27
7	M	403	BCL	O2A-CGA-CBA	2.98	121.25	111.91
15	D	101	SPO	C31-C32-C33	-2.97	120.50	127.66
15	F	104	SPO	C13-C12-C11	2.97	122.75	118.08
7	Q	105	BCL	CHC-C1C-NC	2.97	128.61	124.51
7	E	102	BCL	C1-C2-C3	-2.96	120.92	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	102	BCL	O2A-CGA-CBA	2.96	121.19	111.91
15	F	104	SPO	C14-C15-C16	-2.95	114.00	123.22
7	O	102	BCL	C1C-NC-C4C	-2.95	105.38	106.71
15	D	103	SPO	C15-C14-C12	-2.94	123.11	127.31
7	M	404	BCL	C1-C2-C3	-2.94	120.96	126.04
7	R	102	BCL	C4-C3-C5	2.94	120.22	115.27
7	W	102	BCL	C3C-C4C-CHD	-2.93	117.12	123.39
15	D	103	SPO	C9-C10-C11	-2.93	114.06	123.22
7	F	103	BCL	C4-C3-C5	2.93	120.20	115.27
7	I	102	BCL	C4A-NA-C1A	2.93	108.02	106.71
7	W	102	BCL	C4A-NA-C1A	2.93	108.02	106.71
15	S	104	SPO	C34-C33-C35	2.93	120.19	115.27
15	I	103	SPO	C29-C28-C30	2.92	120.19	115.27
7	Q	105	BCL	O2A-CGA-CBA	2.92	121.08	111.91
15	W	101	SPO	C21-C20-C19	-2.92	117.49	123.47
7	M	403	BCL	C4-C3-C5	2.92	120.18	115.27
15	P	101	SPO	C20-C19-C17	-2.91	123.15	127.31
13	A	102	LMT	O1B-C1B-C2B	2.90	115.61	108.10
7	T	102	BCL	O2A-CGA-CBA	2.90	121.00	111.91
15	N	101	SPO	C29-C28-C30	2.89	120.13	115.27
7	A	101	BCL	C4-C3-C5	2.88	120.12	115.27
15	P	101	SPO	C14-C15-C16	-2.88	114.22	123.22
7	Q	105	BCL	C4-C3-C5	2.88	120.12	115.27
7	I	102	BCL	CHC-C1C-NC	2.88	128.49	124.51
7	R	102	BCL	O2A-CGA-CBA	2.88	120.94	111.91
7	E	102	BCL	CHC-C1C-NC	2.87	128.48	124.51
7	G	101	BCL	O2A-CGA-CBA	2.87	120.92	111.91
7	K	102	BCL	CHC-C1C-NC	2.87	128.48	124.51
15	I	104	SPO	C31-C32-C33	-2.87	120.75	127.66
10	M	414	PGV	C02-O01-C1	-2.86	110.74	117.79
15	T	101	SPO	C31-C32-C33	-2.86	120.77	127.66
7	B	101	BCL	C4-C3-C5	2.86	120.08	115.27
7	W	102	BCL	C1-C2-C3	-2.85	121.11	126.04
15	I	103	SPO	C9-C10-C11	-2.85	114.32	123.22
7	I	102	BCL	C1-C2-C3	-2.85	121.11	126.04
15	W	101	SPO	C34-C33-C35	2.85	120.06	115.27
7	N	102	BCL	O2D-CGD-O1D	-2.84	118.28	123.84
7	S	103	BCL	O2A-CGA-CBA	2.84	120.83	111.91
15	I	104	SPO	C9-C10-C11	-2.84	114.36	123.22
7	W	102	BCL	O2A-CGA-CBA	2.84	120.81	111.91
15	E	101	SPO	C8-C7-C9	-2.83	118.96	122.92
7	Y	102	BCL	C4-C3-C5	2.82	120.02	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Z	101	BCL	C4C-CHD-C1D	-2.82	121.72	125.88
10	H	303	PGV	O03-C19-C20	2.82	120.75	111.91
7	F	101	BCL	C3C-C4C-CHD	-2.81	117.38	123.39
15	D	105	SPO	C29-C28-C30	2.81	120.00	115.27
7	I	102	BCL	O2D-CGD-O1D	-2.80	118.36	123.84
15	P	101	SPO	C27-C26-C25	-2.80	114.48	123.22
7	K	102	BCL	O2D-CGD-O1D	-2.80	118.36	123.84
7	Y	102	BCL	C1B-CHB-C4A	-2.80	124.58	130.12
15	P	101	SPO	C21-C20-C19	-2.79	117.75	123.47
15	E	101	SPO	C31-C32-C33	-2.79	120.93	127.66
15	D	101	SPO	C20-C19-C17	-2.79	123.33	127.31
15	S	104	SPO	C9-C10-C11	-2.79	114.52	123.22
7	S	103	BCL	CHB-C4A-NA	2.78	128.36	124.51
15	D	101	SPO	C14-C15-C16	-2.78	114.53	123.22
7	G	101	BCL	CHB-C4A-NA	2.78	128.36	124.51
10	H	304	PGV	O03-C19-C20	2.78	120.63	111.91
7	V	101	BCL	CHB-C4A-NA	2.77	128.35	124.51
15	I	104	SPO	C34-C33-C35	2.77	119.93	115.27
15	M	408	SPO	C34-C33-C35	2.77	119.93	115.27
7	O	102	BCL	O2A-CGA-CBA	2.77	120.60	111.91
10	M	413	PGV	O03-C19-C20	2.77	120.59	111.91
7	G	101	BCL	C4-C3-C5	2.76	119.92	115.27
7	L	310	BCL	C4-C3-C5	2.76	119.91	115.27
15	O	104	SPO	C9-C10-C11	-2.76	114.61	123.22
7	Z	101	BCL	C4-C3-C5	2.76	119.91	115.27
15	S	104	SPO	C29-C28-C30	2.75	119.90	115.27
15	O	103	SPO	C9-C10-C11	-2.75	114.63	123.22
7	L	310	BCL	C1C-NC-C4C	-2.75	105.47	106.71
15	R	101	SPO	C10-C9-C7	-2.74	123.40	127.31
7	M	404	BCL	C4-C3-C5	2.74	119.88	115.27
7	P	102	BCL	CHB-C4A-NA	2.74	128.29	124.51
7	F	101	BCL	O2A-CGA-CBA	2.73	120.49	111.91
7	Q	105	BCL	O2D-CGD-O1D	-2.73	118.49	123.84
15	W	101	SPO	C31-C32-C33	-2.73	121.09	127.66
7	F	103	BCL	C1-C2-C3	-2.73	121.33	126.04
7	F	101	BCL	C4-C3-C5	2.73	119.86	115.27
7	N	102	BCL	O2A-CGA-CBA	2.72	120.44	111.91
10	Q	103	PGV	O03-C19-C20	2.71	120.42	111.91
7	M	403	BCL	C1-C2-C3	-2.71	121.36	126.04
7	B	101	BCL	CHC-C1C-NC	2.70	128.25	124.51
13	L	309	LMT	C1B-O1B-C4'	-2.70	111.28	117.96
15	W	101	SPO	C15-C14-C12	-2.70	123.46	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	102	BCL	CAC-C3C-C4C	-2.70	106.60	112.58
7	E	102	BCL	CHB-C4A-NA	2.70	128.24	124.51
7	K	102	BCL	O2A-CGA-CBA	2.69	120.35	111.91
7	V	101	BCL	CHC-C1C-NC	2.69	128.23	124.51
7	V	101	BCL	C4-C3-C5	2.69	119.79	115.27
15	T	101	SPO	C34-C33-C35	2.69	119.79	115.27
7	M	404	BCL	CED-O2D-CGD	2.68	122.01	115.94
15	F	104	SPO	C27-C26-C25	-2.68	114.85	123.22
13	X	102	LMT	C1B-O1B-C4'	-2.68	111.33	117.96
15	D	101	SPO	C9-C10-C11	-2.67	114.87	123.22
7	J	101	BCL	CHC-C1C-NC	2.67	128.21	124.51
7	F	103	BCL	CHB-C4A-NA	2.67	128.21	124.51
7	N	102	BCL	CHB-C4A-NA	2.67	128.20	124.51
7	F	103	BCL	O2A-CGA-CBA	2.66	120.27	111.91
15	O	103	SPO	C29-C28-C30	2.66	119.75	115.27
7	Z	101	BCL	O2A-CGA-CBA	2.66	120.25	111.91
15	I	103	SPO	C34-C33-C35	2.66	119.74	115.27
13	I	101	LMT	O1B-C4'-C5'	-2.66	102.17	109.45
7	Y	102	BCL	CHD-C4C-NC	2.65	128.02	125.08
15	S	105	SPO	C15-C14-C12	-2.65	123.53	127.31
13	M	410	LMT	C1-O1'-C1'	-2.64	109.46	113.84
10	M	415	PGV	O03-C19-C20	2.64	120.18	111.91
7	I	102	BCL	C1C-NC-C4C	-2.63	105.52	106.71
7	Z	101	BCL	C3C-C4C-CHD	-2.63	117.78	123.39
7	J	101	BCL	C4-C3-C5	2.63	119.69	115.27
7	L	310	BCL	O2A-CGA-CBA	2.63	120.15	111.91
7	V	101	BCL	O2D-CGD-O1D	-2.62	118.71	123.84
15	I	104	SPO	C14-C15-C16	-2.62	115.04	123.22
15	D	103	SPO	C34-C33-C35	2.62	119.67	115.27
7	E	102	BCL	C2A-C1A-CHA	-2.61	119.29	123.86
7	J	101	BCL	CHB-C4A-NA	2.60	128.11	124.51
15	G	102	SPO	C40-C38-C39	2.60	120.35	114.60
7	L	301	BCL	CED-O2D-CGD	2.60	121.82	115.94
7	T	102	BCL	CHB-C4A-NA	2.60	128.11	124.51
7	G	101	BCL	C2A-C1A-CHA	-2.60	119.31	123.86
7	K	102	BCL	CHB-C4A-NA	2.60	128.10	124.51
7	T	102	BCL	C1-C2-C3	-2.60	121.55	126.04
10	M	402	PGV	O03-C19-C20	2.59	120.05	111.91
15	S	104	SPO	C40-C38-C39	2.59	120.33	114.60
15	W	101	SPO	C20-C19-C17	-2.59	123.61	127.31
7	Z	101	BCL	O2D-CGD-O1D	-2.59	118.78	123.84
7	K	102	BCL	CAC-C3C-C4C	-2.59	106.84	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	101	SPO	C31-C32-C33	-2.59	121.43	127.66
7	L	301	BCL	CHC-C1C-NC	2.59	128.09	124.51
7	J	101	BCL	C2A-C1A-CHA	-2.59	119.34	123.86
7	O	102	BCL	O2D-CGD-O1D	-2.59	118.78	123.84
7	L	301	BCL	C1-C2-C3	-2.59	121.57	126.04
10	Q	103	PGV	C02-O01-C1	-2.58	111.43	117.79
15	M	408	SPO	C40-C38-C39	2.58	120.31	114.60
7	L	301	BCL	O2A-CGA-O1A	-2.58	117.08	123.59
7	L	310	BCL	CHC-C1C-NC	2.58	128.08	124.51
13	M	410	LMT	O1'-C1'-C2'	2.58	112.33	108.30
7	V	101	BCL	O2A-CGA-CBA	2.58	119.99	111.91
7	E	102	BCL	O2D-CGD-O1D	-2.58	118.80	123.84
15	O	104	SPO	C21-C20-C19	-2.58	118.20	123.47
7	M	404	BCL	O2A-CGA-CBA	2.57	119.99	111.91
10	M	415	PGV	C02-O01-C1	-2.57	111.45	117.79
15	G	102	SPO	C31-C32-C33	-2.57	121.46	127.66
10	H	303	PGV	C02-O01-C1	-2.57	111.46	117.79
7	R	102	BCL	CHB-C4A-NA	2.57	128.07	124.51
15	D	105	SPO	C8-C7-C6	2.57	122.12	118.08
15	N	101	SPO	C21-C20-C19	-2.57	118.21	123.47
7	F	101	BCL	C1-C2-C3	-2.57	121.60	126.04
15	O	104	SPO	C34-C33-C35	2.57	119.59	115.27
10	M	414	PGV	O03-C19-C20	2.56	119.95	111.91
8	L	302	BPH	CMA-C3A-C4A	-2.56	108.77	114.38
7	I	102	BCL	CHB-C4A-NA	2.56	128.05	124.51
15	D	103	SPO	C8-C7-C6	2.56	122.11	118.08
15	N	101	SPO	C13-C12-C14	-2.56	119.34	122.92
7	K	102	BCL	C1-C2-C3	-2.55	121.62	126.04
7	M	404	BCL	CHB-C4A-NA	2.55	128.04	124.51
7	B	101	BCL	O2D-CGD-O1D	-2.55	118.86	123.84
7	A	101	BCL	C3C-C2C-C1C	-2.55	97.76	101.87
7	F	103	BCL	O2D-CGD-O1D	-2.54	118.87	123.84
7	M	404	BCL	CAA-C2A-C3A	-2.54	105.82	112.78
7	V	101	BCL	C4B-CHC-C1C	-2.54	125.09	130.12
7	R	102	BCL	C4B-CHC-C1C	-2.54	125.09	130.12
7	K	102	BCL	C4A-NA-C1A	2.54	107.85	106.71
7	D	102	BCL	O2A-CGA-O1A	-2.53	117.20	123.59
7	J	101	BCL	O2D-CGD-O1D	-2.53	118.89	123.84
15	N	101	SPO	C9-C10-C11	-2.53	115.32	123.22
15	D	101	SPO	C29-C28-C30	2.52	119.52	115.27
7	B	101	BCL	C2A-C1A-CHA	-2.52	119.46	123.86
7	F	103	BCL	CAC-C3C-C4C	-2.52	107.00	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	102	BCL	C1C-NC-C4C	-2.52	105.58	106.71
7	S	103	BCL	O2D-CGD-O1D	-2.51	118.92	123.84
7	Y	102	BCL	O2D-CGD-O1D	-2.51	118.92	123.84
15	D	105	SPO	C34-C33-C35	2.51	119.49	115.27
7	D	102	BCL	CHB-C4A-NA	2.51	127.98	124.51
7	B	101	BCL	C1-C2-C3	-2.51	121.71	126.04
7	O	102	BCL	C4A-NA-C1A	2.50	107.83	106.71
15	N	101	SPO	C27-C26-C25	-2.50	115.40	123.22
15	O	103	SPO	C34-C33-C35	2.50	119.47	115.27
15	O	104	SPO	C29-C28-C30	2.50	119.47	115.27
15	O	103	SPO	C14-C15-C16	-2.50	115.42	123.22
15	M	408	SPO	C10-C9-C7	-2.50	123.75	127.31
15	S	104	SPO	C5-C6-C7	-2.50	122.12	125.89
7	A	101	BCL	O2A-CGA-CBA	2.49	119.74	111.91
7	G	101	BCL	CHC-C1C-NC	2.49	127.95	124.51
15	T	101	SPO	C9-C10-C11	-2.48	115.46	123.22
15	T	101	SPO	C14-C15-C16	-2.48	115.47	123.22
7	N	102	BCL	C2A-C1A-CHA	-2.48	119.52	123.86
15	I	103	SPO	C14-C15-C16	-2.48	115.47	123.22
10	L	305	PGV	O03-C19-C20	2.48	119.69	111.91
7	T	102	BCL	O2D-CGD-O1D	-2.47	119.01	123.84
15	M	408	SPO	C9-C10-C11	-2.47	115.51	123.22
15	D	105	SPO	C14-C15-C16	-2.47	115.51	123.22
7	O	102	BCL	CHB-C4A-NA	2.47	127.92	124.51
13	S	101	LMT	O1B-C4'-C3'	2.47	113.84	107.28
15	G	102	SPO	C27-C26-C25	-2.46	115.53	123.22
7	M	404	BCL	CHC-C1C-NC	2.46	127.91	124.51
7	P	102	BCL	C2A-C1A-CHA	-2.45	119.58	123.86
15	G	102	SPO	C21-C20-C19	-2.45	118.46	123.47
15	T	101	SPO	C40-C38-C39	2.43	119.98	114.60
15	E	101	SPO	C27-C26-C25	-2.43	115.63	123.22
15	F	104	SPO	C9-C10-C11	-2.43	115.63	123.22
7	Q	105	BCL	CHB-C4A-NA	2.42	127.86	124.51
15	R	101	SPO	C21-C20-C19	-2.42	118.51	123.47
15	I	104	SPO	C40-C38-C39	2.42	119.94	114.60
7	Z	101	BCL	C4B-CHC-C1C	-2.42	125.33	130.12
10	M	402	PGV	C02-O01-C1	-2.41	111.85	117.79
15	G	102	SPO	C9-C10-C11	-2.41	115.69	123.22
13	L	311	LMT	O1B-C4'-C3'	2.41	113.69	107.28
15	R	101	SPO	C40-C38-C39	2.41	119.92	114.60
15	S	104	SPO	C13-C12-C11	2.40	121.87	118.08
15	D	101	SPO	C40-C38-C39	2.40	119.91	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	417	LMT	C1B-O1B-C4'	-2.40	112.02	117.96
15	P	101	SPO	C40-C38-C39	2.39	119.89	114.60
15	I	104	SPO	C10-C9-C7	-2.39	123.89	127.31
7	R	102	BCL	O2D-CGD-O1D	-2.38	119.18	123.84
15	T	101	SPO	C21-C20-C19	-2.38	118.61	123.47
15	I	104	SPO	C13-C12-C11	2.38	121.82	118.08
15	S	105	SPO	C40-C38-C39	2.37	119.84	114.60
15	I	104	SPO	C21-C20-C19	-2.37	118.62	123.47
15	E	101	SPO	C40-C38-C39	2.37	119.84	114.60
7	G	101	BCL	O2D-CGD-O1D	-2.37	119.20	123.84
15	O	103	SPO	C8-C7-C6	2.37	121.81	118.08
7	M	404	BCL	O2D-CGD-O1D	-2.37	119.21	123.84
15	D	101	SPO	C5-C6-C7	-2.37	122.32	125.89
15	I	103	SPO	C20-C21-C22	-2.36	118.63	123.47
7	L	310	BCL	C2A-C1A-CHA	-2.36	119.73	123.86
7	N	102	BCL	CHC-C1C-NC	2.36	127.78	124.51
15	P	101	SPO	C13-C12-C11	2.36	121.80	118.08
15	S	104	SPO	C10-C9-C7	-2.36	123.94	127.31
15	N	101	SPO	C8-C7-C9	-2.36	119.62	122.92
15	D	101	SPO	C34-C33-C35	2.35	119.23	115.27
15	F	104	SPO	C21-C20-C19	-2.35	118.66	123.47
15	N	101	SPO	C40-C38-C39	2.35	119.80	114.60
15	O	104	SPO	C40-C38-C39	2.35	119.79	114.60
8	M	405	BPH	CMA-C3A-C4A	-2.35	109.23	114.38
15	N	101	SPO	C31-C32-C33	-2.34	122.02	127.66
7	Y	102	BCL	O2A-CGA-CBA	2.34	119.26	111.91
15	D	103	SPO	C14-C15-C16	-2.34	115.91	123.22
15	W	101	SPO	C40-C38-C39	2.34	119.76	114.60
15	W	101	SPO	C14-C15-C16	-2.34	115.93	123.22
15	O	104	SPO	C13-C12-C11	2.33	121.76	118.08
15	O	104	SPO	C14-C15-C16	-2.33	115.93	123.22
15	G	102	SPO	C13-C12-C14	-2.33	119.65	122.92
15	D	105	SPO	C21-C20-C19	-2.33	118.71	123.47
7	D	102	BCL	CAC-C3C-C4C	-2.33	107.42	112.58
15	D	103	SPO	C13-C12-C11	2.32	121.73	118.08
7	P	102	BCL	CHC-C1C-NC	2.31	127.71	124.51
15	I	104	SPO	C8-C7-C6	2.31	121.72	118.08
13	M	411	LMT	C1-O1'-C1'	-2.31	110.01	113.84
15	N	101	SPO	C1-C4-C5	-2.31	106.94	113.06
13	Y	103	LMT	O1B-C4'-C3'	2.31	113.42	107.28
15	S	105	SPO	C20-C21-C22	-2.30	118.76	123.47
7	T	102	BCL	C2A-C1A-CHA	-2.30	119.84	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	102	SPO	C8-C7-C6	2.29	121.69	118.08
15	M	408	SPO	C15-C14-C12	-2.28	124.05	127.31
7	M	403	BCL	C2A-C1A-CHA	-2.28	119.88	123.86
15	N	101	SPO	C14-C15-C16	-2.28	116.11	123.22
15	M	408	SPO	C5-C6-C7	-2.28	122.45	125.89
15	R	101	SPO	C13-C12-C14	-2.27	119.74	122.92
7	A	101	BCL	CHD-C4C-NC	2.27	127.60	125.08
7	I	102	BCL	O2A-CGA-O1A	-2.26	117.88	123.59
15	P	101	SPO	C15-C14-C12	-2.26	124.08	127.31
15	S	104	SPO	C14-C15-C16	-2.26	116.17	123.22
7	D	102	BCL	C4B-CHC-C1C	-2.25	125.65	130.12
15	I	104	SPO	C15-C14-C12	-2.25	124.10	127.31
7	P	102	BCL	O2D-CGD-O1D	-2.25	119.45	123.84
15	T	101	SPO	C27-C26-C25	-2.24	116.22	123.22
7	R	102	BCL	C2A-C1A-CHA	-2.24	119.94	123.86
7	S	103	BCL	CAD-C3D-C4D	2.24	109.72	108.47
7	F	101	BCL	O2D-CGD-O1D	-2.24	119.47	123.84
7	I	102	BCL	CAD-C3D-C4D	2.23	109.72	108.47
15	M	408	SPO	C8-C7-C6	2.22	121.58	118.08
7	L	301	BCL	CHB-C4A-NA	2.22	127.59	124.51
15	S	105	SPO	C34-C33-C35	2.22	119.01	115.27
15	S	105	SPO	C9-C10-C11	-2.22	116.29	123.22
7	D	102	BCL	O2D-CGD-O1D	-2.22	119.50	123.84
7	Y	102	BCL	CAC-C3C-C4C	-2.22	107.66	112.58
7	L	310	BCL	CHB-C4A-NA	2.22	127.58	124.51
15	F	104	SPO	C31-C32-C33	-2.22	122.33	127.66
7	P	102	BCL	C4B-CHC-C1C	-2.21	125.73	130.12
15	R	101	SPO	C31-C32-C33	-2.21	122.33	127.66
7	Y	102	BCL	O1D-CGD-CBD	-2.21	119.96	124.48
15	D	103	SPO	C21-C20-C19	-2.21	118.94	123.47
15	W	101	SPO	C27-C26-C25	-2.21	116.32	123.22
15	I	103	SPO	C13-C12-C11	2.21	121.55	118.08
15	O	104	SPO	C10-C9-C7	-2.20	124.17	127.31
15	I	103	SPO	C40-C38-C39	2.20	119.47	114.60
7	T	102	BCL	CHC-C1C-NC	2.20	127.55	124.51
15	D	105	SPO	C26-C25-C23	-2.20	120.25	126.42
7	J	101	BCL	C1-C2-C3	-2.19	122.25	126.04
15	D	103	SPO	C40-C38-C39	2.19	119.44	114.60
7	Q	105	BCL	C1C-NC-C4C	-2.19	105.72	106.71
15	I	104	SPO	C20-C21-C22	-2.19	118.99	123.47
15	S	105	SPO	C14-C15-C16	-2.18	116.40	123.22
7	R	102	BCL	CHC-C1C-NC	2.18	127.53	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	104	SPO	C40-C38-C39	2.18	119.41	114.60
15	E	101	SPO	C21-C20-C19	-2.18	119.02	123.47
7	R	102	BCL	CAC-C3C-C4C	-2.17	107.76	112.58
15	D	103	SPO	C20-C21-C22	-2.16	119.04	123.47
7	M	403	BCL	C4B-CHC-C1C	-2.16	125.83	130.12
7	Q	105	BCL	C2A-C1A-CHA	-2.16	120.08	123.86
7	A	101	BCL	CBA-CAA-C2A	-2.16	107.49	113.86
15	O	104	SPO	C8-C7-C6	2.16	121.47	118.08
7	Q	105	BCL	CAC-C3C-C4C	-2.15	107.80	112.58
7	W	102	BCL	CBC-CAC-C3C	-2.15	108.67	113.47
13	S	102	LMT	C1B-O1B-C4'	-2.14	112.66	117.96
7	L	310	BCL	C1-O2A-CGA	2.14	122.06	116.44
7	L	301	BCL	CAD-C3D-C4D	2.14	109.66	108.47
8	M	405	BPH	CBA-CAA-C2A	-2.14	107.56	113.81
15	I	104	SPO	C27-C26-C25	-2.14	116.54	123.22
7	B	101	BCL	CED-O2D-CGD	2.14	120.77	115.94
15	G	102	SPO	C20-C21-C22	-2.14	119.10	123.47
15	I	103	SPO	C8-C7-C6	2.13	121.43	118.08
7	V	101	BCL	C4A-NA-C1A	2.13	107.66	106.71
13	A	102	LMT	O2B-C2B-C1B	2.13	115.21	110.05
15	O	103	SPO	C40-C38-C39	2.13	119.30	114.60
15	F	104	SPO	C24-C23-C25	2.12	121.42	118.08
7	Q	105	BCL	CMB-C2B-C1B	-2.12	125.20	128.46
7	Y	102	BCL	C3C-C4C-CHD	-2.12	118.87	123.39
7	P	102	BCL	O2A-CGA-O1A	-2.12	118.25	123.59
15	I	104	SPO	C18-C17-C16	2.11	121.41	118.08
15	D	105	SPO	C15-C14-C12	-2.11	124.30	127.31
13	I	101	LMT	O1B-C4'-C3'	2.11	112.90	107.28
7	V	101	BCL	C1C-NC-C4C	-2.11	105.76	106.71
15	P	101	SPO	C24-C23-C25	2.11	121.40	118.08
15	O	104	SPO	C26-C25-C23	-2.10	120.50	126.42
7	G	101	BCL	CAD-C3D-C4D	2.10	109.64	108.47
13	K	101	LMT	C1B-O1B-C4'	-2.10	112.76	117.96
13	X	101	LMT	O5B-C1B-C2B	2.10	114.79	110.35
13	Y	101	LMT	C1B-O1B-C4'	-2.10	112.78	117.96
13	S	101	LMT	O5'-C5'-C6'	2.09	111.64	106.44
10	H	303	PGV	O03-C19-O04	-2.09	118.31	123.59
7	K	102	BCL	C2A-C1A-CHA	-2.09	120.21	123.86
7	S	103	BCL	CAC-C3C-C4C	-2.09	107.95	112.58
7	A	101	BCL	CED-O2D-CGD	2.08	120.63	115.94
15	E	101	SPO	C10-C11-C12	2.08	132.25	126.42
15	R	101	SPO	C14-C15-C16	-2.07	116.75	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	102	BCL	CAD-C3D-C4D	2.07	109.62	108.47
15	D	105	SPO	C13-C12-C11	2.06	121.33	118.08
7	L	301	BCL	C2A-C1A-CHA	-2.06	120.26	123.86
15	O	103	SPO	C20-C21-C22	-2.06	119.26	123.47
15	M	408	SPO	C14-C15-C16	-2.06	116.80	123.22
7	Y	102	BCL	C2A-C1A-CHA	-2.06	120.26	123.86
7	K	102	BCL	CAD-C3D-C4D	2.05	109.61	108.47
7	B	101	BCL	CAD-C3D-C4D	2.05	109.61	108.47
7	J	101	BCL	O2A-CGA-O1A	-2.05	118.42	123.59
15	R	101	SPO	C13-C12-C11	2.05	121.31	118.08
7	W	102	BCL	CED-O2D-CGD	2.05	120.57	115.94
7	K	102	BCL	CMB-C2B-C1B	-2.04	125.32	128.46
7	Q	105	BCL	CAD-C3D-C4D	2.04	109.61	108.47
7	B	101	BCL	O2A-CGA-CBA	2.04	118.31	111.91
7	W	102	BCL	O2D-CGD-O1D	-2.04	119.85	123.84
9	M	407	U10	O4-C4-C5	-2.04	109.66	116.56
15	O	103	SPO	C15-C14-C12	-2.04	124.41	127.31
15	T	101	SPO	C13-C12-C11	2.04	121.28	118.08
7	P	102	BCL	CAD-C3D-C4D	2.03	109.60	108.47
15	E	101	SPO	C9-C10-C11	2.03	129.55	123.22
7	A	101	BCL	O1D-CGD-CBD	-2.03	120.34	124.48
15	S	104	SPO	C21-C20-C19	-2.02	119.33	123.47
15	I	103	SPO	C18-C17-C16	2.02	121.27	118.08
15	D	101	SPO	C13-C12-C11	2.02	121.26	118.08
7	M	403	BCL	C1B-CHB-C4A	-2.02	126.11	130.12
15	S	104	SPO	C15-C14-C12	-2.02	124.43	127.31
15	M	408	SPO	C29-C28-C30	2.02	118.67	115.27
15	O	104	SPO	C5-C6-C7	-2.02	122.84	125.89
13	I	101	LMT	C3B-C4B-C5B	2.02	113.84	110.24
13	I	101	LMT	O5'-C1'-C2'	-2.01	106.09	110.35
15	S	104	SPO	C36-C37-C38	-2.01	120.87	127.75
7	D	102	BCL	C4-C3-C5	2.01	118.65	115.27
7	M	403	BCL	O1D-CGD-CBD	-2.01	120.38	124.48
15	D	105	SPO	C34-C33-C32	-2.01	118.53	123.68
7	P	102	BCL	CED-O2D-CGD	2.00	120.47	115.94
7	O	102	BCL	CAC-C3C-C4C	-2.00	108.14	112.58
15	D	101	SPO	C21-C20-C19	-2.00	119.38	123.47

There are no chirality outliers.

All (688) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	403	BCL	C1A-C2A-CAA-CBA
7	M	403	BCL	C3A-C2A-CAA-CBA
7	A	101	BCL	C2C-C3C-CAC-CBC
7	A	101	BCL	C4C-C3C-CAC-CBC
7	D	102	BCL	C1A-C2A-CAA-CBA
7	E	102	BCL	C1A-C2A-CAA-CBA
7	E	102	BCL	C3A-C2A-CAA-CBA
7	F	101	BCL	C1A-C2A-CAA-CBA
7	F	103	BCL	C11-C10-C8-C9
7	K	102	BCL	C2-C3-C5-C6
7	K	102	BCL	C4-C3-C5-C6
7	N	102	BCL	C1A-C2A-CAA-CBA
7	N	102	BCL	C3A-C2A-CAA-CBA
7	O	102	BCL	C2-C3-C5-C6
7	O	102	BCL	C4-C3-C5-C6
7	P	102	BCL	C1A-C2A-CAA-CBA
7	P	102	BCL	C3A-C2A-CAA-CBA
7	R	102	BCL	C1A-C2A-CAA-CBA
7	R	102	BCL	C3A-C2A-CAA-CBA
7	S	103	BCL	C4C-C3C-CAC-CBC
7	V	101	BCL	C4C-C3C-CAC-CBC
7	W	102	BCL	C1A-C2A-CAA-CBA
7	W	102	BCL	C4C-C3C-CAC-CBC
7	Y	102	BCL	CHA-CBD-CGD-O1D
7	Z	101	BCL	C3A-C2A-CAA-CBA
9	L	304	U10	C40-C39-C41-C42
9	L	304	U10	C50-C49-C51-C52
9	M	407	U10	C30-C29-C31-C32
10	M	402	PGV	C03-O11-P-O12
10	M	402	PGV	C03-O11-P-O13
10	M	402	PGV	C03-O11-P-O14
10	M	402	PGV	C04-O12-P-O11
10	M	402	PGV	C04-O12-P-O13
10	M	402	PGV	O12-C04-C05-O05
10	M	413	PGV	C03-O11-P-O12
10	M	413	PGV	C04-O12-P-O11
10	M	413	PGV	C2-C1-O01-C02
10	M	415	PGV	C03-O11-P-O12
10	M	415	PGV	C03-O11-P-O13
10	M	415	PGV	C03-O11-P-O14
10	H	304	PGV	C03-O11-P-O13
10	H	304	PGV	C03-O11-P-O14
10	H	304	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
10	Q	103	PGV	C03-O11-P-O12
11	L	306	PEE	C2-C1-O3P-P
12	L	307	LDA	N1-C1-C2-C3
12	H	301	LDA	C2-C1-N1-CM2
12	H	301	LDA	N1-C1-C2-C3
12	H	302	LDA	N1-C1-C2-C3
12	D	104	LDA	C2-C1-N1-CM2
13	A	102	LMT	C2B-C1B-O1B-C4'
13	Q	101	LMT	C2'-C1'-O1'-C1
13	Q	101	LMT	O5'-C1'-O1'-C1
13	X	101	LMT	O5'-C1'-O1'-C1
15	D	103	SPO	C10-C11-C12-C13
15	D	103	SPO	C10-C11-C12-C14
15	D	103	SPO	C28-C30-C31-C32
15	D	103	SPO	C32-C33-C35-C36
15	D	103	SPO	C34-C33-C35-C36
15	D	103	SPO	C33-C35-C36-C37
15	E	101	SPO	C10-C11-C12-C13
15	E	101	SPO	C10-C11-C12-C14
15	E	101	SPO	C15-C16-C17-C18
15	E	101	SPO	C15-C16-C17-C19
15	E	101	SPO	C27-C28-C30-C31
15	E	101	SPO	C29-C28-C30-C31
15	E	101	SPO	C32-C33-C35-C36
15	E	101	SPO	C34-C33-C35-C36
15	F	104	SPO	O1-C1-C4-C5
15	F	104	SPO	C2-C1-C4-C5
15	F	104	SPO	C3-C1-C4-C5
15	F	104	SPO	C5-C6-C7-C8
15	F	104	SPO	C5-C6-C7-C9
15	F	104	SPO	C27-C28-C30-C31
15	F	104	SPO	C29-C28-C30-C31
15	F	104	SPO	C32-C33-C35-C36
15	F	104	SPO	C34-C33-C35-C36
15	G	102	SPO	C5-C6-C7-C8
15	G	102	SPO	C5-C6-C7-C9
15	G	102	SPO	C34-C33-C35-C36
15	I	103	SPO	C32-C33-C35-C36
15	I	103	SPO	C34-C33-C35-C36
15	I	103	SPO	C33-C35-C36-C37
15	I	104	SPO	C32-C33-C35-C36
15	I	104	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
15	I	104	SPO	C33-C35-C36-C37
15	N	101	SPO	C5-C6-C7-C8
15	N	101	SPO	C5-C6-C7-C9
15	N	101	SPO	C10-C11-C12-C13
15	N	101	SPO	C10-C11-C12-C14
15	O	104	SPO	C28-C30-C31-C32
15	O	104	SPO	C32-C33-C35-C36
15	O	104	SPO	C34-C33-C35-C36
15	O	104	SPO	C33-C35-C36-C37
15	P	101	SPO	C27-C28-C30-C31
15	P	101	SPO	C29-C28-C30-C31
15	P	101	SPO	C34-C33-C35-C36
15	R	101	SPO	C2-C1-O1-CM1
15	R	101	SPO	C27-C28-C30-C31
15	R	101	SPO	C29-C28-C30-C31
15	S	104	SPO	C28-C30-C31-C32
15	S	104	SPO	C32-C33-C35-C36
15	S	104	SPO	C34-C33-C35-C36
15	S	104	SPO	C33-C35-C36-C37
7	F	101	BCL	CBD-CGD-O2D-CED
7	Z	101	BCL	CBD-CGD-O2D-CED
13	S	101	LMT	O5B-C1B-O1B-C4'
13	Q	101	LMT	C3'-C4'-O1B-C1B
13	L	311	LMT	O5B-C1B-O1B-C4'
13	I	101	LMT	O5B-C1B-O1B-C4'
13	Y	103	LMT	O5B-C1B-O1B-C4'
7	A	101	BCL	CBD-CGD-O2D-CED
10	M	413	PGV	O02-C1-O01-C02
10	H	304	PGV	O02-C1-O01-C02
7	Q	105	BCL	C4-C3-C5-C6
15	G	102	SPO	C29-C28-C30-C31
15	T	101	SPO	C29-C28-C30-C31
9	L	304	U10	C38-C39-C41-C42
9	M	407	U10	C28-C29-C31-C32
15	G	102	SPO	C32-C33-C35-C36
9	M	407	U10	C27-C28-C29-C30
7	M	404	BCL	CBD-CGD-O2D-CED
7	Z	101	BCL	O1D-CGD-O2D-CED
9	M	407	U10	C27-C28-C29-C31
7	Q	105	BCL	C3-C5-C6-C7
7	M	403	BCL	CBA-CGA-O2A-C1
7	B	101	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
7	F	101	BCL	O1D-CGD-O2D-CED
13	M	411	LMT	O5'-C5'-C6'-O6'
7	B	101	BCL	O1A-CGA-O2A-C1
13	X	102	LMT	O5'-C5'-C6'-O6'
9	L	303	U10	C15-C14-C16-C17
9	L	304	U10	C35-C34-C36-C37
15	R	101	SPO	C34-C33-C35-C36
9	L	303	U10	C13-C14-C16-C17
9	L	304	U10	C33-C34-C36-C37
9	L	304	U10	C48-C49-C51-C52
15	G	102	SPO	C27-C28-C30-C31
15	P	101	SPO	C32-C33-C35-C36
15	R	101	SPO	C32-C33-C35-C36
7	M	403	BCL	O1A-CGA-O2A-C1
15	D	101	SPO	C28-C30-C31-C32
15	D	105	SPO	C28-C30-C31-C32
15	E	101	SPO	C28-C30-C31-C32
15	I	103	SPO	C28-C30-C31-C32
15	I	104	SPO	C28-C30-C31-C32
15	N	101	SPO	C28-C30-C31-C32
15	N	101	SPO	C33-C35-C36-C37
15	O	103	SPO	C28-C30-C31-C32
15	R	101	SPO	C33-C35-C36-C37
15	T	101	SPO	C33-C35-C36-C37
10	M	402	PGV	O12-C04-C05-C06
7	S	103	BCL	C15-C16-C17-C18
10	H	304	PGV	O12-C04-C05-O05
15	D	101	SPO	C29-C28-C30-C31
15	T	101	SPO	C27-C28-C30-C31
7	L	310	BCL	C6-C7-C8-C9
7	B	101	BCL	C6-C7-C8-C9
7	D	102	BCL	C14-C13-C15-C16
7	G	101	BCL	C6-C7-C8-C9
7	G	101	BCL	C14-C13-C15-C16
7	J	101	BCL	C6-C7-C8-C9
7	N	102	BCL	C6-C7-C8-C9
7	P	102	BCL	C6-C7-C8-C9
7	Q	105	BCL	C11-C12-C13-C14
7	R	102	BCL	C6-C7-C8-C9
7	S	103	BCL	C11-C10-C8-C9
7	T	102	BCL	C6-C7-C8-C9
7	Y	102	BCL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
7	Z	101	BCL	C11-C10-C8-C9
7	R	102	BCL	C10-C11-C12-C13
15	G	102	SPO	C10-C11-C12-C13
15	S	105	SPO	C10-C11-C12-C13
15	G	102	SPO	C10-C11-C12-C14
13	X	102	LMT	C4'-C5'-C6'-O6'
7	J	101	BCL	C15-C16-C17-C18
7	Q	105	BCL	C13-C15-C16-C17
7	D	102	BCL	C3-C5-C6-C7
7	D	102	BCL	C5-C6-C7-C8
7	G	101	BCL	C10-C11-C12-C13
7	V	101	BCL	C8-C10-C11-C12
11	L	306	PEE	C37-C38-C39-C40
7	M	403	BCL	C15-C16-C17-C18
7	F	101	BCL	C10-C11-C12-C13
7	G	101	BCL	C8-C10-C11-C12
7	J	101	BCL	C13-C15-C16-C17
7	O	102	BCL	C10-C11-C12-C13
7	Z	101	BCL	C5-C6-C7-C8
13	K	101	LMT	C3'-C4'-O1B-C1B
7	L	301	BCL	CBD-CGD-O2D-CED
13	L	311	LMT	C5'-C4'-O1B-C1B
7	F	103	BCL	C6-C7-C8-C10
7	Q	105	BCL	C6-C7-C8-C10
7	S	103	BCL	C6-C7-C8-C10
7	W	102	BCL	C11-C10-C8-C7
7	Y	102	BCL	C6-C7-C8-C10
7	N	102	BCL	C2A-CAA-CBA-CGA
7	E	102	BCL	C10-C11-C12-C13
7	K	102	BCL	C8-C10-C11-C12
7	O	102	BCL	C5-C6-C7-C8
13	S	102	LMT	O5'-C1'-O1'-C1
7	A	101	BCL	O1D-CGD-O2D-CED
9	L	303	U10	C24-C26-C27-C28
15	D	101	SPO	C33-C35-C36-C37
15	D	105	SPO	C33-C35-C36-C37
15	S	105	SPO	C33-C35-C36-C37
15	W	101	SPO	C33-C35-C36-C37
7	M	404	BCL	C10-C11-C12-C13
7	B	101	BCL	C15-C16-C17-C18
7	N	102	BCL	C10-C11-C12-C13
13	Y	103	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
7	Y	102	BCL	C8-C10-C11-C12
10	L	305	PGV	C2-C1-O01-C02
7	F	103	BCL	C15-C16-C17-C18
7	V	101	BCL	C15-C16-C17-C18
10	H	304	PGV	C03-O11-P-O12
10	H	304	PGV	C04-O12-P-O11
10	Q	103	PGV	C04-O12-P-O11
7	I	102	BCL	C3-C5-C6-C7
7	B	101	BCL	C8-C10-C11-C12
10	L	305	PGV	O02-C1-O01-C02
7	W	102	BCL	C4-C3-C5-C6
15	W	101	SPO	C29-C28-C30-C31
9	L	303	U10	C32-C33-C34-C36
7	I	102	BCL	C15-C16-C17-C18
7	R	102	BCL	C16-C17-C18-C19
13	M	410	LMT	O1'-C1-C2-C3
7	M	404	BCL	O1D-CGD-O2D-CED
12	D	104	LDA	C5-C6-C7-C8
12	D	104	LDA	C7-C8-C9-C10
10	L	305	PGV	C5-C6-C7-C8
13	M	417	LMT	C5-C6-C7-C8
7	F	101	BCL	C15-C16-C17-C18
13	A	102	LMT	C3-C4-C5-C6
7	W	102	BCL	C3-C5-C6-C7
7	R	102	BCL	C11-C10-C8-C9
13	L	311	LMT	C3'-C4'-O1B-C1B
7	E	102	BCL	C2A-CAA-CBA-CGA
15	E	101	SPO	C5-C6-C7-C8
13	M	410	LMT	C2-C3-C4-C5
15	E	101	SPO	C5-C6-C7-C9
10	L	305	PGV	C24-C25-C26-C27
10	M	402	PGV	C22-C23-C24-C25
10	Q	103	PGV	C22-C23-C24-C25
12	M	419	LDA	C11-C10-C9-C8
13	Y	103	LMT	C3'-C4'-O1B-C1B
7	E	102	BCL	C16-C17-C18-C19
13	M	412	LMT	O5'-C1'-O1'-C1
7	T	102	BCL	C15-C16-C17-C18
10	H	304	PGV	C1-C2-C3-C4
7	D	102	BCL	C3A-C2A-CAA-CBA
7	G	101	BCL	C3A-C2A-CAA-CBA
7	J	101	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
7	T	102	BCL	C3A-C2A-CAA-CBA
7	W	102	BCL	C3A-C2A-CAA-CBA
7	Q	105	BCL	C10-C11-C12-C13
13	K	101	LMT	C2-C1-O1'-C1'
13	S	102	LMT	C2-C1-O1'-C1'
10	M	402	PGV	C23-C24-C25-C26
12	L	307	LDA	C2-C3-C4-C5
13	M	417	LMT	C4-C5-C6-C7
8	L	302	BPH	O2A-C1-C2-C3
7	J	101	BCL	C3-C5-C6-C7
15	S	105	SPO	C34-C33-C35-C36
7	Q	105	BCL	C2-C3-C5-C6
15	S	105	SPO	C32-C33-C35-C36
10	L	305	PGV	C7-C8-C9-C10
12	H	301	LDA	C7-C8-C9-C10
12	H	301	LDA	C1-C2-C3-C4
7	G	101	BCL	CBA-CGA-O2A-C1
10	M	414	PGV	C23-C24-C25-C26
13	Q	101	LMT	C2-C3-C4-C5
7	L	301	BCL	C15-C16-C17-C18
7	L	301	BCL	C11-C10-C8-C7
7	L	310	BCL	C6-C7-C8-C10
7	B	101	BCL	C6-C7-C8-C10
7	D	102	BCL	C11-C12-C13-C15
7	E	102	BCL	C6-C7-C8-C10
7	G	101	BCL	C6-C7-C8-C10
7	J	101	BCL	C6-C7-C8-C10
7	N	102	BCL	C6-C7-C8-C10
7	N	102	BCL	C11-C10-C8-C7
7	R	102	BCL	C11-C10-C8-C7
7	T	102	BCL	C6-C7-C8-C10
7	V	101	BCL	C2-C3-C5-C6
13	Q	101	LMT	C3-C4-C5-C6
10	M	415	PGV	O02-C1-O01-C02
7	W	102	BCL	C2A-CAA-CBA-CGA
7	M	404	BCL	C5-C6-C7-C8
12	H	302	LDA	C5-C6-C7-C8
13	I	101	LMT	C5'-C4'-O1B-C1B
13	Q	101	LMT	O1'-C1-C2-C3
7	V	101	BCL	C16-C17-C18-C19
12	D	104	LDA	C1-C2-C3-C4
10	M	414	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
10	M	415	PGV	C2-C1-O01-C02
13	A	102	LMT	C5'-C4'-O1B-C1B
7	G	101	BCL	O1A-CGA-O2A-C1
16	F	102	MYR	C6-C7-C8-C9
10	M	414	PGV	O02-C1-O01-C02
13	M	417	LMT	O5B-C5B-C6B-O6B
13	Q	101	LMT	O5'-C5'-C6'-O6'
7	R	102	BCL	C16-C17-C18-C20
12	O	101	LDA	C4-C5-C6-C7
13	L	309	LMT	C2-C3-C4-C5
10	H	303	PGV	C11-C10-C9-C8
7	A	101	BCL	C4-C3-C5-C6
7	V	101	BCL	C4-C3-C5-C6
10	H	303	PGV	C1-C2-C3-C4
7	W	102	BCL	C2-C3-C5-C6
15	D	101	SPO	C27-C28-C30-C31
15	W	101	SPO	C27-C28-C30-C31
7	K	102	BCL	C11-C10-C8-C9
7	N	102	BCL	C11-C10-C8-C9
7	Q	105	BCL	C6-C7-C8-C9
7	Y	102	BCL	C6-C7-C8-C9
13	S	102	LMT	O5'-C5'-C6'-O6'
13	S	101	LMT	C4'-C5'-C6'-O6'
7	P	102	BCL	C2A-CAA-CBA-CGA
7	F	101	BCL	CBA-CGA-O2A-C1
13	A	102	LMT	C3'-C4'-O1B-C1B
13	I	101	LMT	C3'-C4'-O1B-C1B
7	L	310	BCL	C1A-C2A-CAA-CBA
7	J	101	BCL	C1A-C2A-CAA-CBA
7	T	102	BCL	C1A-C2A-CAA-CBA
7	Z	101	BCL	C1A-C2A-CAA-CBA
7	E	102	BCL	C16-C17-C18-C20
7	V	101	BCL	C16-C17-C18-C20
7	P	102	BCL	C5-C6-C7-C8
11	L	306	PEE	C1-O3P-P-O4P
13	M	411	LMT	C4'-C5'-C6'-O6'
7	Q	105	BCL	C15-C16-C17-C18
7	S	103	BCL	C2C-C3C-CAC-CBC
7	V	101	BCL	C2C-C3C-CAC-CBC
7	W	102	BCL	C2C-C3C-CAC-CBC
12	D	104	LDA	C3-C4-C5-C6
13	K	101	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
13	I	101	LMT	C2-C3-C4-C5
10	Q	103	PGV	C2-C1-O01-C02
13	Y	101	LMT	O5B-C5B-C6B-O6B
12	M	420	LDA	C4-C5-C6-C7
13	L	309	LMT	O5'-C1'-O1'-C1
13	L	309	LMT	O1'-C1-C2-C3
7	D	102	BCL	C13-C15-C16-C17
7	O	102	BCL	C15-C16-C17-C18
10	M	413	PGV	C19-C20-C21-C22
13	M	409	LMT	O5'-C5'-C6'-O6'
13	Y	101	LMT	O5'-C5'-C6'-O6'
13	Y	103	LMT	O5B-C5B-C6B-O6B
12	D	104	LDA	C4-C5-C6-C7
7	L	301	BCL	O1D-CGD-O2D-CED
13	M	417	LMT	O5'-C5'-C6'-O6'
7	L	310	BCL	C15-C16-C17-C18
7	I	102	BCL	C13-C15-C16-C17
10	M	402	PGV	O01-C02-C03-O11
13	Y	103	LMT	C1-C2-C3-C4
7	F	101	BCL	O1A-CGA-O2A-C1
15	R	101	SPO	C3-C1-O1-CM1
15	G	102	SPO	C3-C1-C4-C5
7	M	403	BCL	C4-C3-C5-C6
7	M	403	BCL	C11-C10-C8-C7
7	A	101	BCL	C11-C10-C8-C7
7	E	102	BCL	C11-C10-C8-C7
7	K	102	BCL	C11-C10-C8-C7
7	P	102	BCL	C6-C7-C8-C10
7	Q	105	BCL	C11-C12-C13-C15
7	R	102	BCL	C6-C7-C8-C10
7	Y	102	BCL	C11-C10-C8-C7
13	M	417	LMT	O1'-C1-C2-C3
7	L	301	BCL	C11-C10-C8-C9
7	M	403	BCL	C11-C10-C8-C9
7	A	101	BCL	C11-C10-C8-C9
7	E	102	BCL	C11-C10-C8-C9
7	O	102	BCL	C6-C7-C8-C9
7	O	102	BCL	C11-C10-C8-C9
7	Q	105	BCL	C11-C10-C8-C9
13	L	311	LMT	C7-C8-C9-C10
12	Q	104	LDA	N1-C1-C2-C3
13	X	102	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	E	102	BCL	C15-C16-C17-C18
10	M	402	PGV	C01-C02-C03-O11
9	L	304	U10	C9-C11-C12-C13
7	T	102	BCL	C4-C3-C5-C6
7	Z	101	BCL	C4-C3-C5-C6
7	M	403	BCL	C2-C3-C5-C6
7	G	101	BCL	C2-C3-C5-C6
7	T	102	BCL	C2-C3-C5-C6
7	Z	101	BCL	C2-C3-C5-C6
7	M	403	BCL	C2A-CAA-CBA-CGA
7	F	101	BCL	C3A-C2A-CAA-CBA
7	K	102	BCL	C3-C5-C6-C7
7	G	101	BCL	C4-C3-C5-C6
10	L	305	PGV	C23-C24-C25-C26
7	D	102	BCL	C2A-CAA-CBA-CGA
7	R	102	BCL	C2A-CAA-CBA-CGA
10	M	413	PGV	O01-C02-C03-O11
10	H	303	PGV	O01-C02-C03-O11
13	I	101	LMT	C1-C2-C3-C4
12	M	418	LDA	C4-C5-C6-C7
13	L	309	LMT	C5'-C4'-O1B-C1B
7	M	403	BCL	C8-C10-C11-C12
15	E	101	SPO	C33-C35-C36-C37
15	T	101	SPO	C28-C30-C31-C32
10	Q	103	PGV	O02-C1-O01-C02
7	K	102	BCL	C2-C1-O2A-CGA
7	Z	101	BCL	C2-C1-O2A-CGA
7	K	102	BCL	C5-C6-C7-C8
7	N	102	BCL	C14-C13-C15-C16
7	W	102	BCL	C6-C7-C8-C9
7	I	102	BCL	C10-C11-C12-C13
15	S	105	SPO	C10-C11-C12-C14
13	L	309	LMT	C3'-C4'-O1B-C1B
7	N	102	BCL	C15-C16-C17-C18
10	H	303	PGV	C01-C02-C03-O11
10	H	304	PGV	C01-C02-C03-O11
7	D	102	BCL	C11-C10-C8-C7
7	O	102	BCL	C6-C7-C8-C10
7	O	102	BCL	C11-C10-C8-C7
7	Q	105	BCL	C11-C10-C8-C7
7	W	102	BCL	C6-C7-C8-C10
12	M	418	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
7	W	102	BCL	C5-C6-C7-C8
7	M	403	BCL	CAD-CBD-CGD-O2D
7	M	404	BCL	CAD-CBD-CGD-O2D
8	M	405	BPH	CAD-CBD-CGD-O2D
9	L	303	U10	C32-C33-C34-C35
7	E	102	BCL	C5-C6-C7-C8
15	P	101	SPO	C28-C30-C31-C32
10	H	304	PGV	O01-C02-C03-O11
10	M	402	PGV	C21-C22-C23-C24
7	Y	102	BCL	CHA-CBD-CGD-O2D
12	H	301	LDA	C2-C1-N1-CM1
12	D	104	LDA	C2-C1-N1-CM1
7	V	101	BCL	C5-C6-C7-C8
10	L	305	PGV	O03-C01-C02-O01
10	M	413	PGV	C20-C21-C22-C23
9	L	304	U10	C12-C11-C9-C10
15	D	105	SPO	C34-C33-C35-C36
7	N	102	BCL	C8-C10-C11-C12
7	F	101	BCL	C6-C7-C8-C9
7	J	101	BCL	C11-C10-C8-C9
13	S	101	LMT	C3'-C4'-O1B-C1B
13	S	101	LMT	C5'-C4'-O1B-C1B
7	J	101	BCL	C2A-CAA-CBA-CGA
7	G	101	BCL	C1A-C2A-CAA-CBA
7	M	404	BCL	C16-C17-C18-C19
10	M	415	PGV	C04-O12-P-O11
9	L	304	U10	C45-C44-C46-C47
9	M	401	U10	C12-C11-C9-C10
7	A	101	BCL	C2-C3-C5-C6
9	L	304	U10	C12-C11-C9-C8
10	M	413	PGV	C03-O11-P-O14
10	M	413	PGV	C04-O12-P-O14
10	H	304	PGV	C04-O12-P-O13
10	Q	103	PGV	C03-O11-P-O14
10	Q	103	PGV	C04-O12-P-O14
11	L	306	PEE	C1-O3P-P-O2P
7	J	101	BCL	CBA-CGA-O2A-C1
10	L	305	PGV	C01-C02-C03-O11
10	M	413	PGV	C01-C02-C03-O11
10	Q	103	PGV	C01-C02-C03-O11
13	K	101	LMT	C6-C7-C8-C9
7	F	101	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
12	H	301	LDA	C2-C1-N1-O1
12	D	104	LDA	C2-C1-N1-O1
7	L	310	BCL	C13-C15-C16-C17
15	N	101	SPO	C1-C4-C5-C6
13	M	410	LMT	C3-C4-C5-C6
10	H	304	PGV	O12-C04-C05-C06
15	M	408	SPO	C34-C33-C35-C36
7	F	101	BCL	C6-C7-C8-C10
7	V	101	BCL	C6-C7-C8-C10
10	L	305	PGV	O01-C02-C03-O11
10	Q	103	PGV	O01-C02-C03-O11
7	B	101	BCL	C16-C17-C18-C19
10	L	305	PGV	C22-C23-C24-C25
7	J	101	BCL	O1A-CGA-O2A-C1
10	M	413	PGV	C4-C5-C6-C7
7	L	310	BCL	C8-C10-C11-C12
7	A	101	BCL	O1A-CGA-O2A-C1
7	P	102	BCL	C4-C3-C5-C6
15	D	105	SPO	C32-C33-C35-C36
7	D	102	BCL	C11-C10-C8-C9
7	W	102	BCL	C11-C10-C8-C9
10	M	415	PGV	C5-C6-C7-C8
13	M	417	LMT	C3-C4-C5-C6
15	E	101	SPO	C9-C10-C11-C12
7	N	102	BCL	C16-C17-C18-C20
13	A	102	LMT	O5B-C5B-C6B-O6B
9	M	401	U10	C12-C11-C9-C8
11	L	306	PEE	C18-C19-C20-C21
7	Q	105	BCL	C5-C6-C7-C8
7	A	101	BCL	CBA-CGA-O2A-C1
7	L	301	BCL	C2-C1-O2A-CGA
7	M	403	BCL	C2-C1-O2A-CGA
15	F	104	SPO	C11-C10-C9-C7
8	L	302	BPH	C16-C17-C18-C20
9	L	304	U10	C43-C44-C46-C47
10	M	413	PGV	O03-C01-C02-O01
13	I	101	LMT	C7-C8-C9-C10
10	L	305	PGV	C03-O11-P-O12
10	L	305	PGV	C04-O12-P-O11
10	M	414	PGV	C03-O11-P-O12
10	M	414	PGV	C04-O12-P-O11
10	H	303	PGV	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
10	H	303	PGV	C04-O12-P-O11
11	L	306	PEE	C4-O4P-P-O3P
15	G	102	SPO	C2-C1-C4-C5
10	H	304	PGV	O03-C01-C02-C03
7	I	102	BCL	C6-C7-C8-C10
10	M	402	PGV	C3-C4-C5-C6
13	X	101	LMT	C7-C8-C9-C10
7	D	102	BCL	C11-C12-C13-C14
7	P	102	BCL	C16-C17-C18-C19
13	Y	103	LMT	O1'-C1-C2-C3
13	L	311	LMT	C2-C3-C4-C5
7	F	101	BCL	C5-C6-C7-C8
8	M	405	BPH	C13-C15-C16-C17
15	G	102	SPO	O1-C1-C4-C5
11	L	306	PEE	C16-C17-C18-C19
7	G	101	BCL	C13-C15-C16-C17
12	D	104	LDA	C2-C3-C4-C5
13	M	417	LMT	C2-C3-C4-C5
12	M	419	LDA	C3-C4-C5-C6
13	X	101	LMT	C6-C7-C8-C9
9	L	303	U10	C30-C29-C31-C32
7	F	101	BCL	C16-C17-C18-C19
7	L	301	BCL	C2A-CAA-CBA-CGA
7	N	102	BCL	C16-C17-C18-C19
10	H	303	PGV	C4-C5-C6-C7
13	S	102	LMT	C4-C5-C6-C7
15	R	101	SPO	C28-C30-C31-C32
7	F	103	BCL	C2-C1-O2A-CGA
7	O	102	BCL	C2-C1-O2A-CGA
7	S	103	BCL	C2-C1-O2A-CGA
10	H	303	PGV	C19-C20-C21-C22
13	X	101	LMT	C2'-C1'-O1'-C1
7	T	102	BCL	C2A-CAA-CBA-CGA
7	K	102	BCL	C13-C15-C16-C17
11	L	306	PEE	C38-C39-C40-C41
7	J	101	BCL	C4-C3-C5-C6
13	S	101	LMT	O5'-C5'-C6'-O6'
10	H	304	PGV	C2-C3-C4-C5
7	M	403	BCL	C11-C12-C13-C14
7	E	102	BCL	C6-C7-C8-C9
7	S	103	BCL	C6-C7-C8-C9
7	T	102	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
7	V	101	BCL	C6-C7-C8-C9
10	L	305	PGV	O03-C01-C02-C03
7	B	101	BCL	C16-C17-C18-C20
15	D	101	SPO	C10-C11-C12-C13
16	F	102	MYR	O2-C1-C2-C3
7	D	102	BCL	C10-C11-C12-C13
7	I	102	BCL	C1A-C2A-CAA-CBA
12	O	101	LDA	C11-C10-C9-C8
7	D	102	BCL	C6-C7-C8-C10
7	J	101	BCL	C11-C10-C8-C7
7	E	102	BCL	C3-C5-C6-C7
16	F	102	MYR	O1-C1-C2-C3
13	L	309	LMT	C5-C6-C7-C8
16	F	102	MYR	C3-C4-C5-C6
11	L	306	PEE	O3P-C1-C2-O2
9	L	304	U10	C6-C7-C8-C9
10	Q	103	PGV	C21-C22-C23-C24
7	P	102	BCL	C2-C3-C5-C6
9	L	303	U10	C28-C29-C31-C32
16	F	102	MYR	C11-C10-C9-C8
15	E	101	SPO	C11-C10-C9-C7
15	N	101	SPO	C25-C26-C27-C28
15	R	101	SPO	C1-C4-C5-C6
7	Z	101	BCL	C16-C17-C18-C19
10	M	415	PGV	O12-C04-C05-C06
7	Q	105	BCL	C2-C1-O2A-CGA
7	F	103	BCL	C6-C7-C8-C9
7	T	102	BCL	C11-C10-C8-C9
8	L	302	BPH	C14-C13-C15-C16
7	W	102	BCL	C16-C17-C18-C19
7	F	103	BCL	C4-C3-C5-C6
7	N	102	BCL	C4-C3-C5-C6
7	R	102	BCL	C4-C3-C5-C6
9	L	304	U10	C25-C24-C26-C27
7	Y	102	BCL	C15-C16-C17-C18
7	G	101	BCL	CAA-CBA-CGA-O2A
13	L	311	LMT	C1-C2-C3-C4
7	K	102	BCL	C16-C17-C18-C19
11	L	306	PEE	C36-C37-C38-C39
10	H	303	PGV	C11-C12-C13-C14
10	M	413	PGV	C7-C8-C9-C10
15	M	408	SPO	C29-C28-C30-C31

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Mol	Chain	Res	Type	Atoms
7	J	101	BCL	C2-C3-C5-C6
7	N	102	BCL	C2-C3-C5-C6
7	R	102	BCL	C2-C3-C5-C6
9	L	304	U10	C13-C14-C16-C17
15	M	408	SPO	C27-C28-C30-C31
15	G	102	SPO	C11-C10-C9-C7
7	R	102	BCL	C8-C10-C11-C12
7	D	102	BCL	C8-C10-C11-C12
7	O	102	BCL	C16-C17-C18-C19
7	P	102	BCL	C16-C17-C18-C20
8	M	405	BPH	C4-C3-C5-C6
15	M	408	SPO	C32-C33-C35-C36
12	Q	104	LDA	C1-C2-C3-C4
7	Y	102	BCL	C14-C13-C15-C16
13	Y	101	LMT	C5'-C4'-O1B-C1B
7	L	301	BCL	CAD-CBD-CGD-O2D
7	A	101	BCL	CAD-CBD-CGD-O2D
8	L	302	BPH	CAD-CBD-CGD-O2D
9	L	303	U10	C35-C34-C36-C37
9	L	304	U10	C15-C14-C16-C17
7	F	103	BCL	C13-C15-C16-C17
9	L	304	U10	C23-C24-C26-C27
9	L	303	U10	C5-C4-O4-C4M
9	M	407	U10	C5-C4-O4-C4M
10	M	413	PGV	O03-C01-C02-C03
13	A	102	LMT	C6-C7-C8-C9
7	B	101	BCL	O2A-C1-C2-C3
8	M	405	BPH	O2A-C1-C2-C3
13	S	101	LMT	O5B-C5B-C6B-O6B
7	Y	102	BCL	C2A-CAA-CBA-CGA
10	L	305	PGV	C3-C4-C5-C6
8	M	405	BPH	C10-C11-C12-C13
7	M	403	BCL	C16-C17-C18-C19
7	L	310	BCL	CHA-CBD-CGD-O1D
7	L	310	BCL	CHA-CBD-CGD-O2D
7	M	404	BCL	CHA-CBD-CGD-O2D
7	F	101	BCL	CHA-CBD-CGD-O1D
7	F	101	BCL	CHA-CBD-CGD-O2D
12	M	420	LDA	C2-C1-N1-CM1
9	L	303	U10	C33-C34-C36-C37
10	H	303	PGV	C3-C4-C5-C6
10	Q	103	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
11	L	306	PEE	O3P-C1-C2-C3
10	M	413	PGV	C6-C7-C8-C9
13	X	101	LMT	C5-C6-C7-C8
10	M	415	PGV	C21-C22-C23-C24
10	M	402	PGV	O03-C01-C02-O01
11	L	306	PEE	O2-C2-C3-O3
12	M	420	LDA	C1-C2-C3-C4
10	H	304	PGV	C3-C4-C5-C6
7	M	403	BCL	C11-C12-C13-C15
7	I	102	BCL	C11-C12-C13-C15
7	I	102	BCL	C11-C12-C13-C14
9	M	401	U10	C3-C4-O4-C4M
13	X	101	LMT	C4-C5-C6-C7
10	H	304	PGV	O03-C19-C20-C21
9	L	304	U10	C2-C3-O3-C3M
15	N	101	SPO	C30-C31-C32-C33
13	L	309	LMT	C6-C7-C8-C9
10	M	402	PGV	C20-C19-O03-C01
12	H	301	LDA	C4-C5-C6-C7
13	L	308	LMT	C11-C10-C9-C8
7	A	101	BCL	C1A-C2A-CAA-CBA
7	G	101	BCL	C2-C1-O2A-CGA
13	L	309	LMT	C4-C5-C6-C7
10	M	414	PGV	C04-O12-P-O13
10	M	414	PGV	C22-C23-C24-C25
7	M	403	BCL	C3-C5-C6-C7
9	M	401	U10	C5-C4-O4-C4M
10	H	304	PGV	C23-C24-C25-C26
7	V	101	BCL	CAD-CBD-CGD-O1D
7	Z	101	BCL	CAD-CBD-CGD-O1D
10	H	304	PGV	O04-C19-C20-C21
10	L	305	PGV	O01-C1-C2-C3
7	B	101	BCL	CAA-CBA-CGA-O2A
9	L	303	U10	C11-C12-C13-C14
9	L	303	U10	C26-C27-C28-C29
13	X	102	LMT	C2-C3-C4-C5
7	F	101	BCL	C4-C3-C5-C6
7	S	103	BCL	C4-C3-C5-C6
8	L	302	BPH	C4-C3-C5-C6
13	M	410	LMT	C4'-C5'-C6'-O6'
7	F	103	BCL	C2-C3-C5-C6
7	F	103	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
7	G	101	BCL	C2C-C3C-CAC-CBC
7	I	102	BCL	C3A-C2A-CAA-CBA
7	T	102	BCL	C11-C10-C8-C7
7	Z	101	BCL	C11-C10-C8-C7
8	L	302	BPH	C11-C12-C13-C15
7	F	103	BCL	O1A-CGA-O2A-C1
7	Q	105	BCL	C8-C10-C11-C12
15	D	101	SPO	C10-C11-C12-C14
12	M	416	LDA	C2-C3-C4-C5
13	M	410	LMT	C2-C1-O1'-C1'
13	Q	101	LMT	C2-C1-O1'-C1'
10	M	402	PGV	O04-C19-O03-C01
15	G	102	SPO	C33-C35-C36-C37
7	B	101	BCL	CAA-CBA-CGA-O1A
7	R	102	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

83 monomers are involved in 304 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	D	105	SPO	7	0
10	M	414	PGV	2	0
12	O	101	LDA	1	0
7	T	102	BCL	5	0
7	Q	105	BCL	2	0
9	L	303	U10	3	0
7	K	102	BCL	8	0
10	Q	103	PGV	5	0
13	K	101	LMT	2	0
12	M	419	LDA	2	0
7	D	102	BCL	9	0
7	J	101	BCL	7	0
9	M	401	U10	3	0
13	Y	101	LMT	1	0
11	L	306	PEE	3	0
15	E	101	SPO	6	0
10	M	413	PGV	5	0
10	H	304	PGV	3	0
9	L	304	U10	7	0
15	M	408	SPO	6	0
15	N	101	SPO	6	0
7	B	101	BCL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	I	101	LMT	3	0
15	G	102	SPO	3	0
13	Q	101	LMT	2	0
13	L	311	LMT	5	0
13	M	411	LMT	1	0
12	D	104	LDA	3	0
13	A	102	LMT	3	0
16	F	102	MYR	2	0
13	M	410	LMT	3	0
13	M	412	LMT	6	0
7	O	102	BCL	6	0
13	Y	103	LMT	1	0
15	P	101	SPO	5	0
7	G	101	BCL	7	0
8	M	405	BPH	8	0
13	M	417	LMT	2	0
9	M	407	U10	2	0
13	M	409	LMT	3	0
10	L	305	PGV	5	0
7	V	101	BCL	8	0
12	L	307	LDA	2	0
7	Y	102	BCL	4	0
12	M	418	LDA	1	0
7	W	102	BCL	8	0
13	S	102	LMT	6	0
7	R	102	BCL	5	0
7	F	103	BCL	2	0
7	M	404	BCL	3	0
12	Q	104	LDA	2	0
15	D	101	SPO	6	0
15	W	101	SPO	8	0
15	S	105	SPO	6	0
10	M	415	PGV	5	0
7	I	102	BCL	7	0
7	E	102	BCL	3	0
13	L	308	LMT	2	0
15	F	104	SPO	5	0
7	F	101	BCL	8	0
7	A	101	BCL	3	0
7	P	102	BCL	8	0
13	X	101	LMT	1	0
7	Z	101	BCL	3	0

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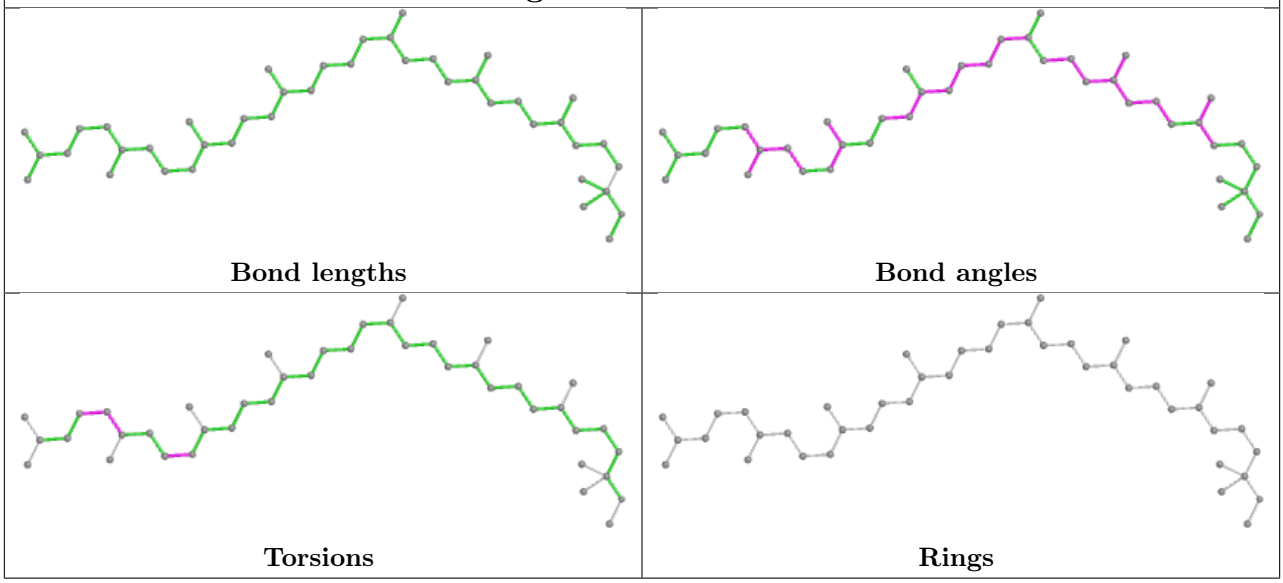
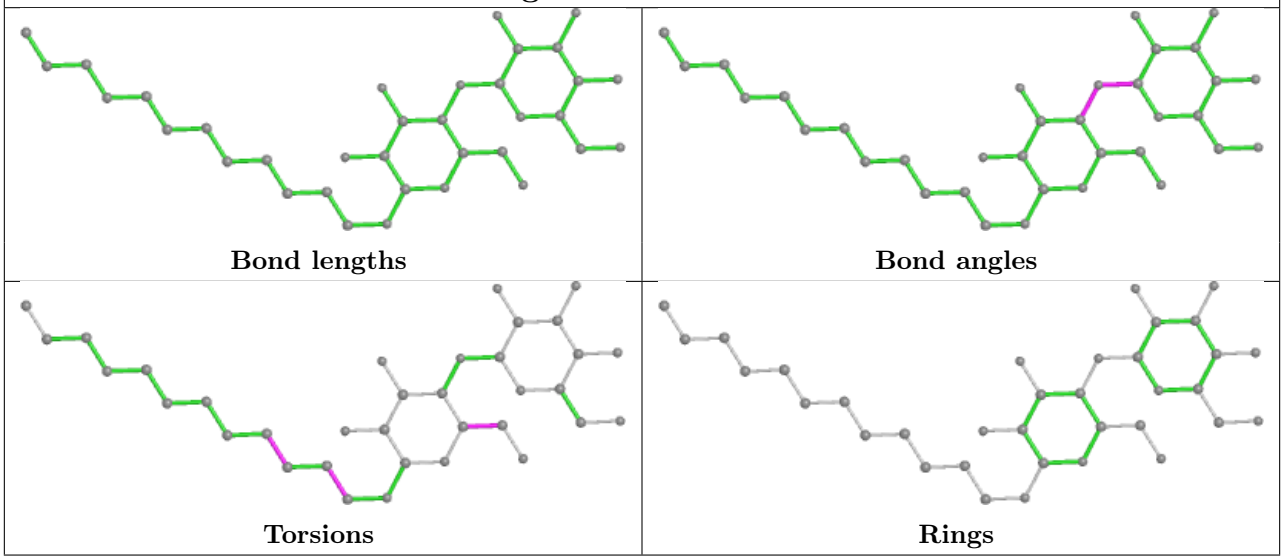
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	302	BPH	3	0
10	M	402	PGV	3	0
7	N	102	BCL	6	0
10	H	303	PGV	3	0
15	D	103	SPO	4	0
15	T	101	SPO	3	0
12	Q	102	LDA	1	0
7	S	103	BCL	7	0
15	O	104	SPO	11	0
15	I	103	SPO	4	0
13	S	101	LMT	3	0
12	H	301	LDA	3	0
15	O	103	SPO	6	0
7	L	310	BCL	3	0
15	I	104	SPO	10	0
7	M	403	BCL	5	0
12	M	420	LDA	3	0
15	S	104	SPO	9	0
15	R	101	SPO	6	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.

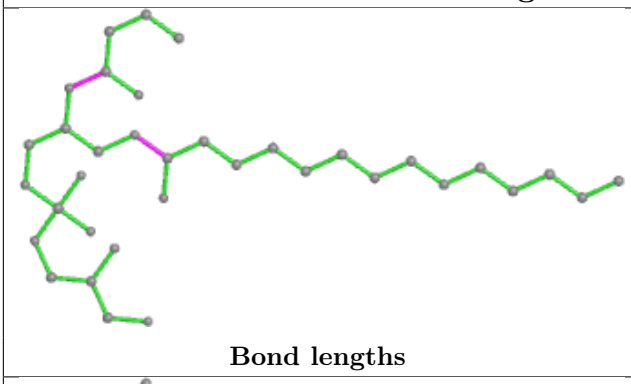
Ligand SPO D 105



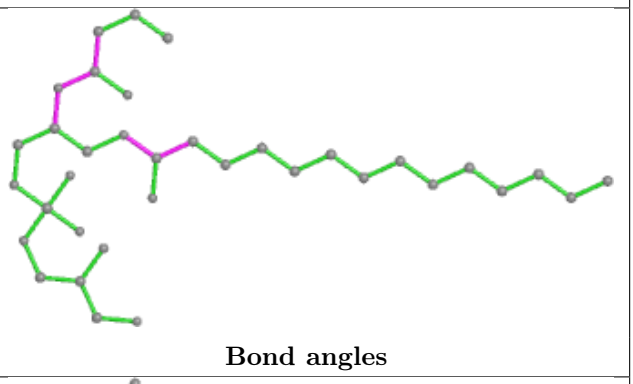
Ligand LMT X 102



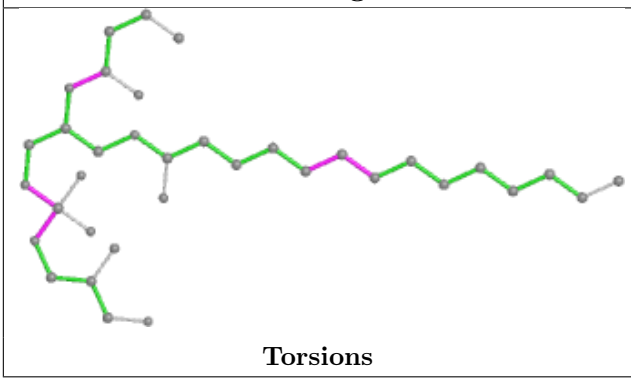
Ligand PGV M 414



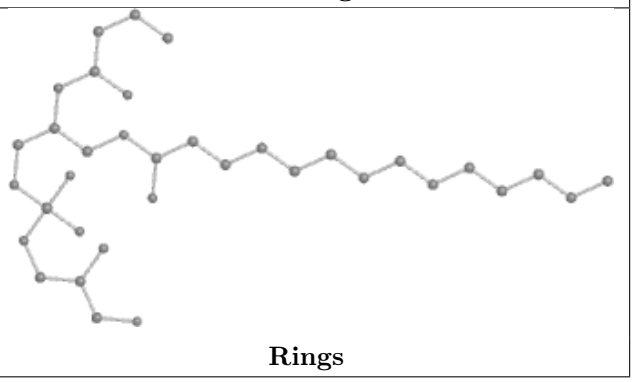
Bond lengths



Bond angles

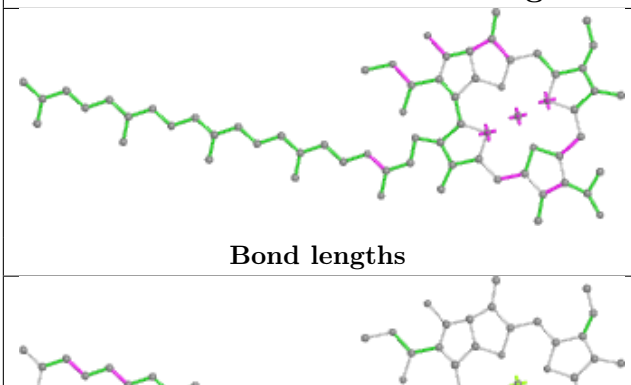


Torsions

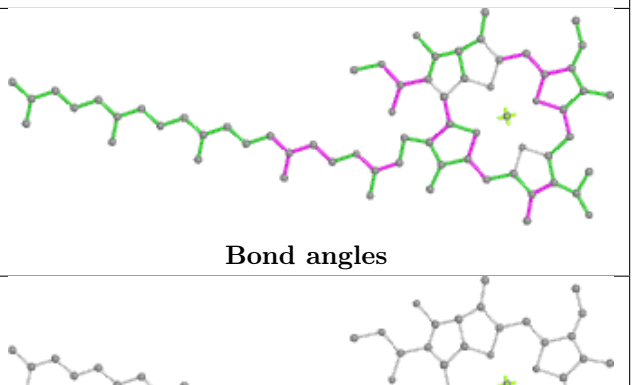


Rings

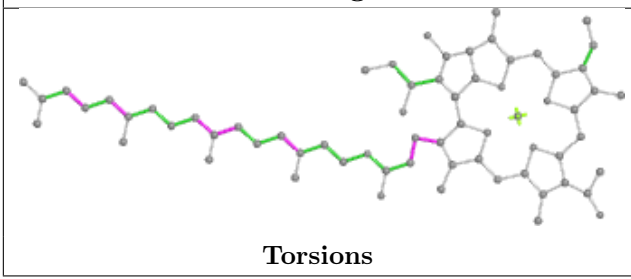
Ligand BCL T 102



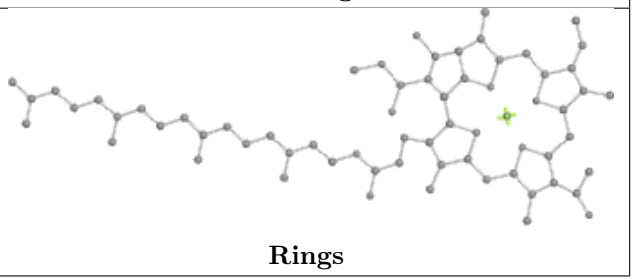
Bond lengths



Bond angles

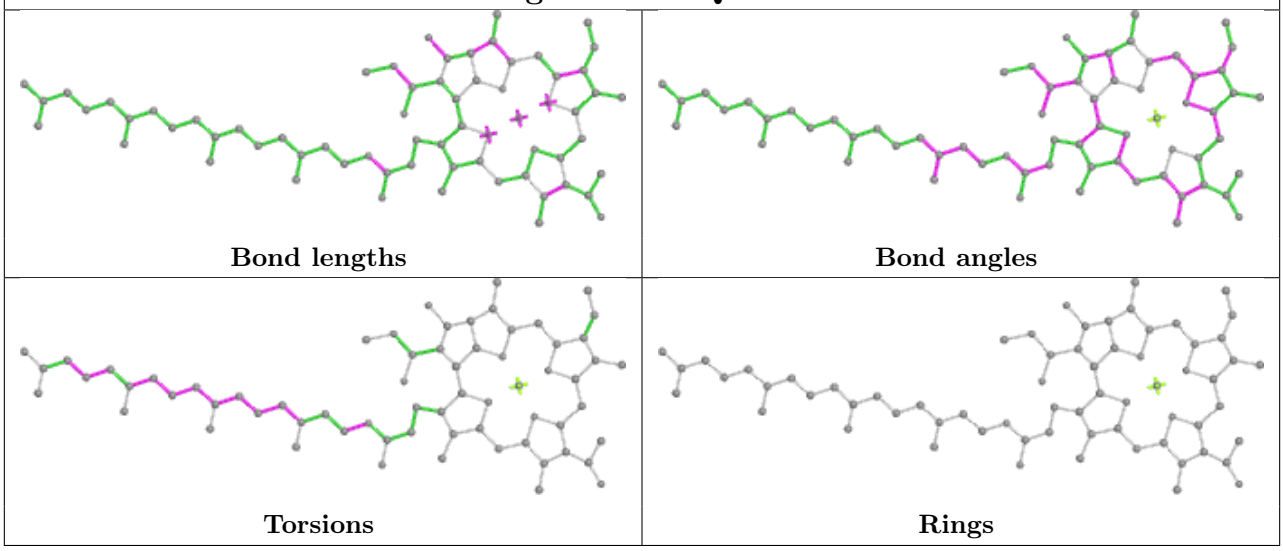


Torsions

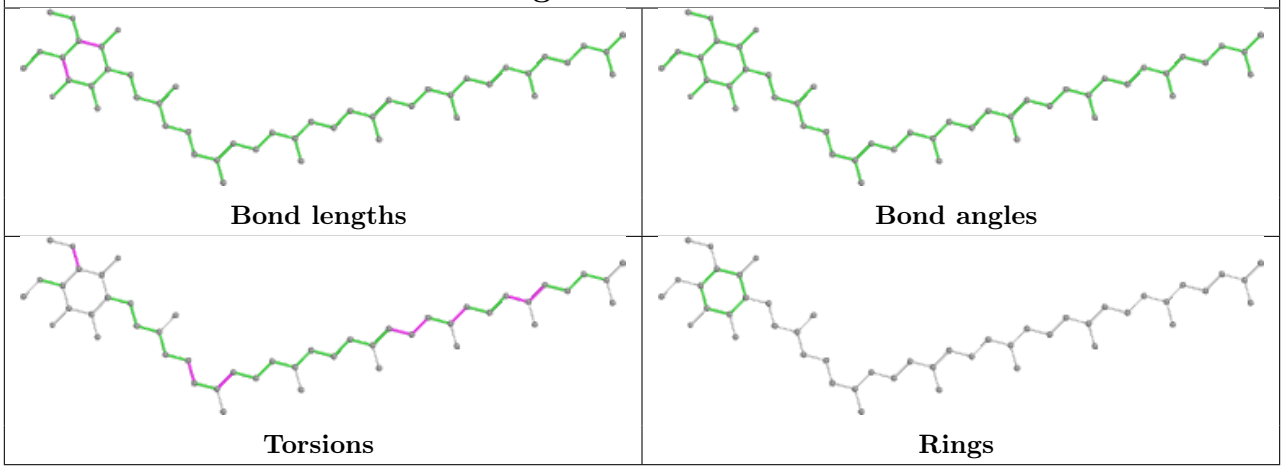


Rings

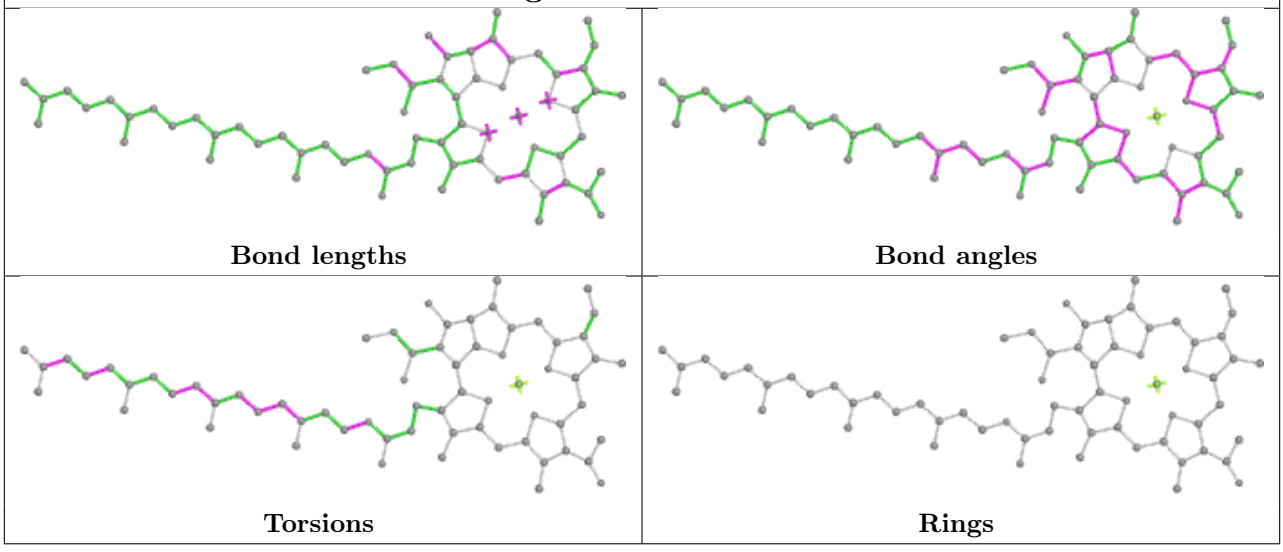
Ligand BCL Q 105



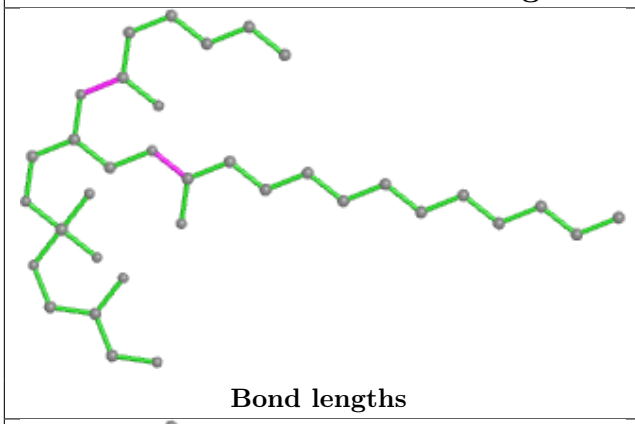
Ligand U10 L 303



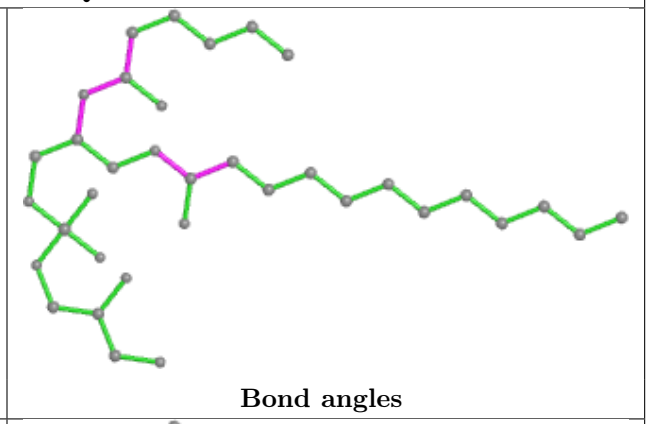
Ligand BCL K 102



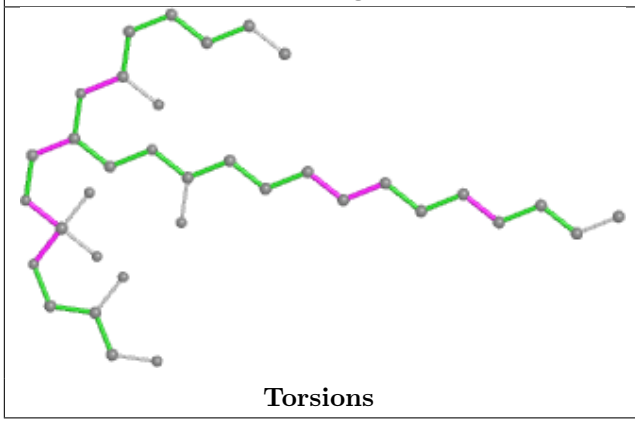
Ligand PGV Q 103



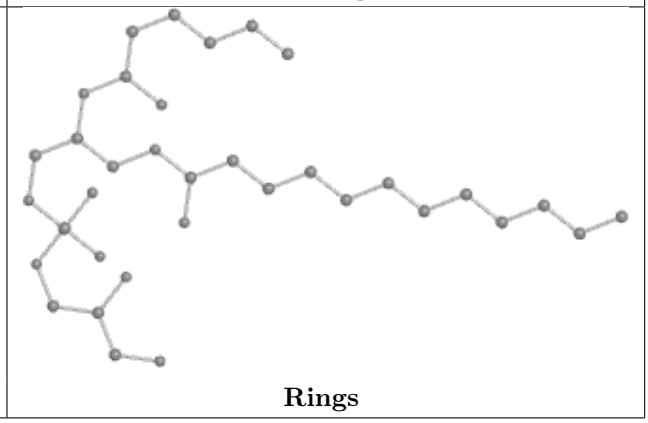
Bond lengths



Bond angles

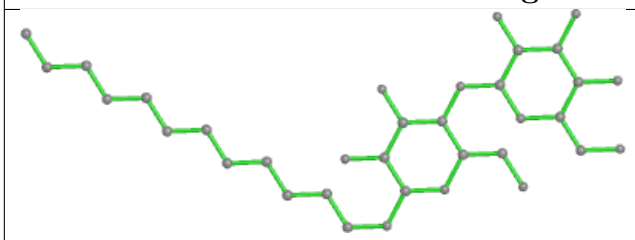


Torsions

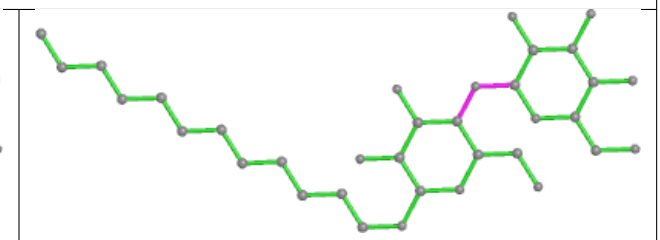


Rings

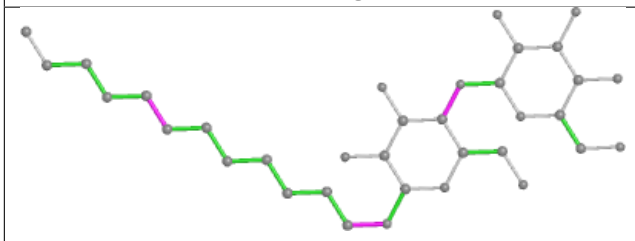
Ligand LMT K 101



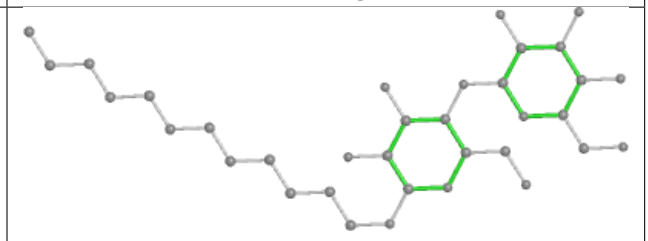
Bond lengths



Bond angles

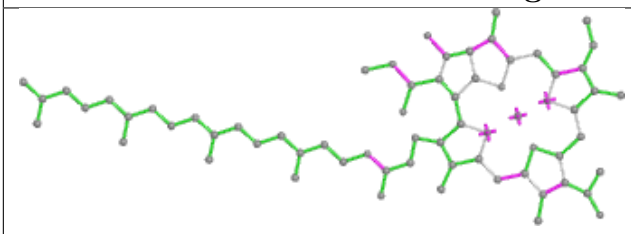


Torsions

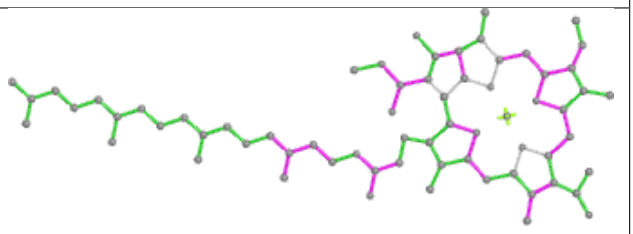


Rings

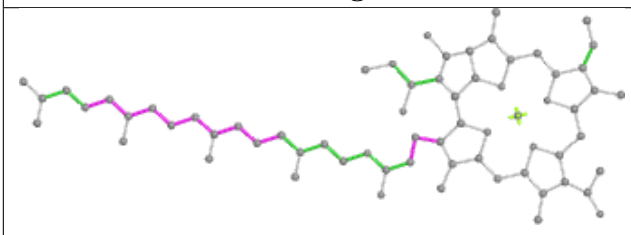
Ligand BCL D 102



Bond lengths



Bond angles



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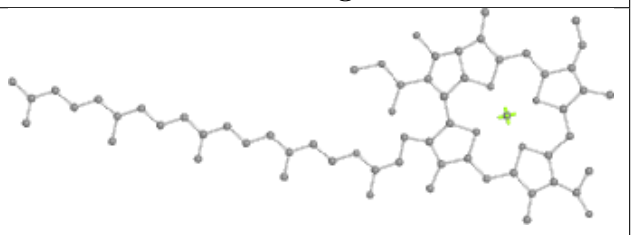
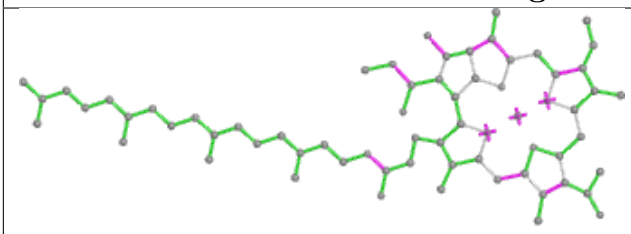
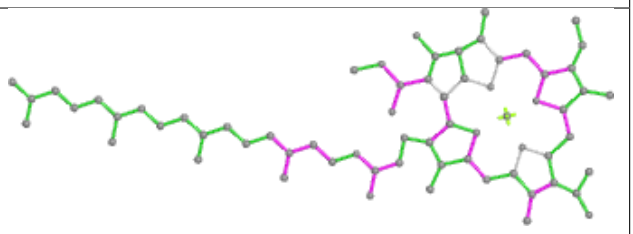


Rings

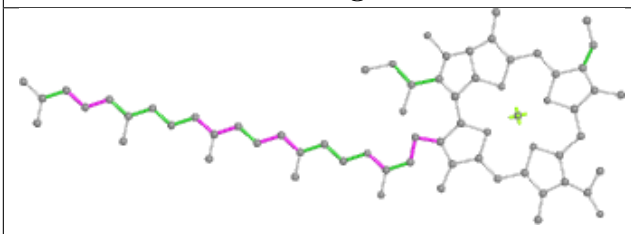
Ligand BCL J 101



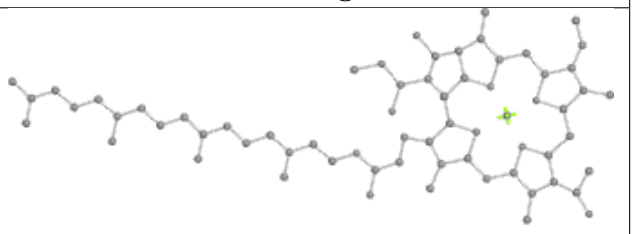
Bond lengths



Bond angles

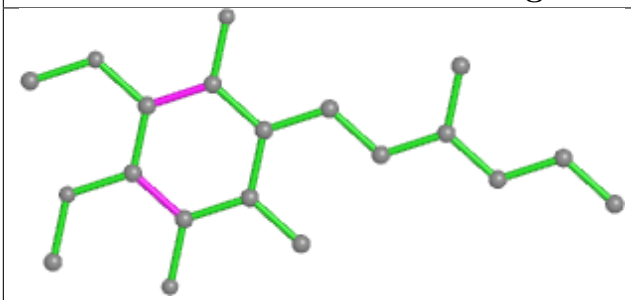


Torsions

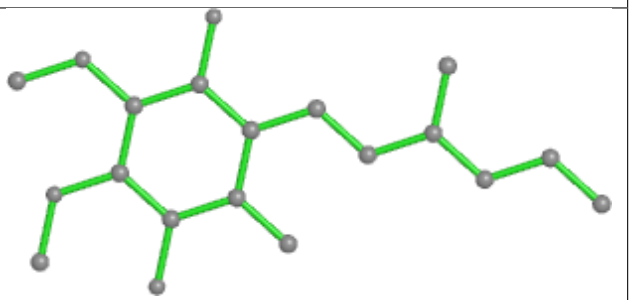


Rings

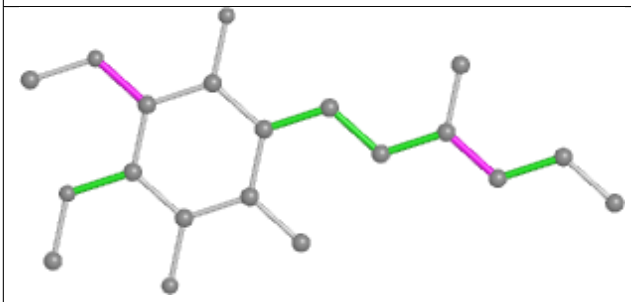
Ligand U10 M 401



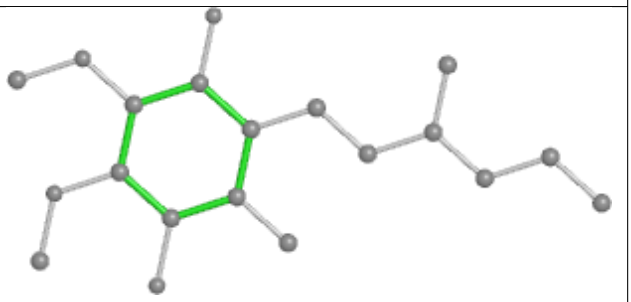
Bond lengths



Bond angles

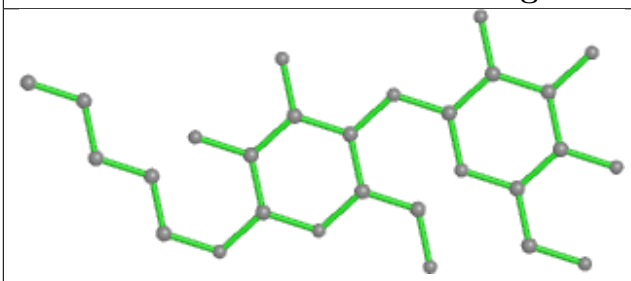


Torsions

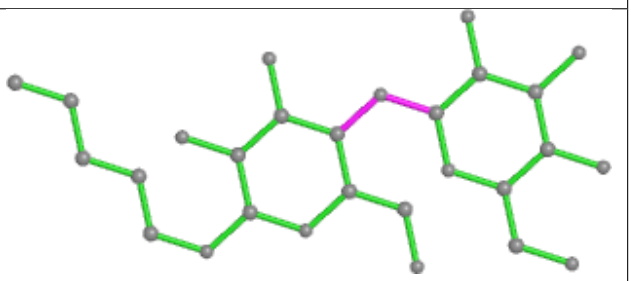


Rings

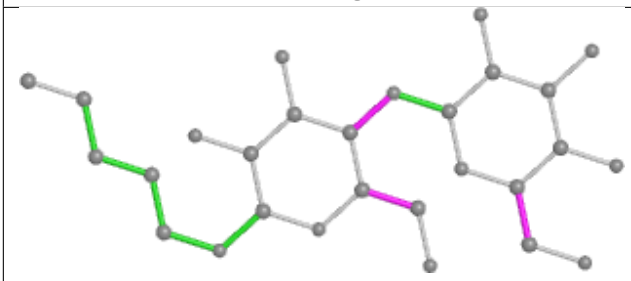
Ligand LMT Y 101



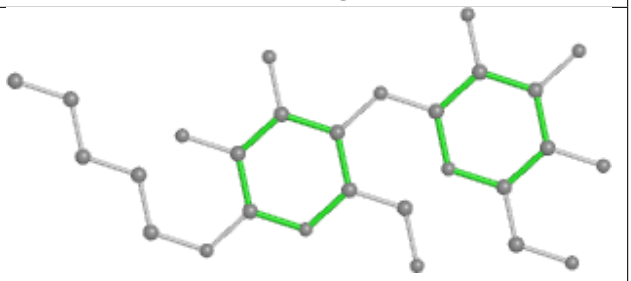
Bond lengths



Bond angles

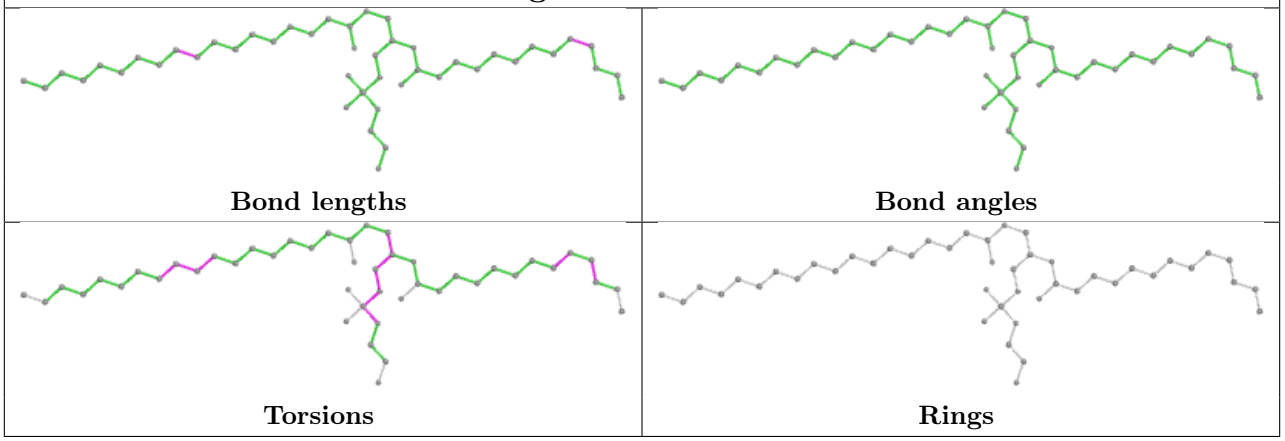


Torsions

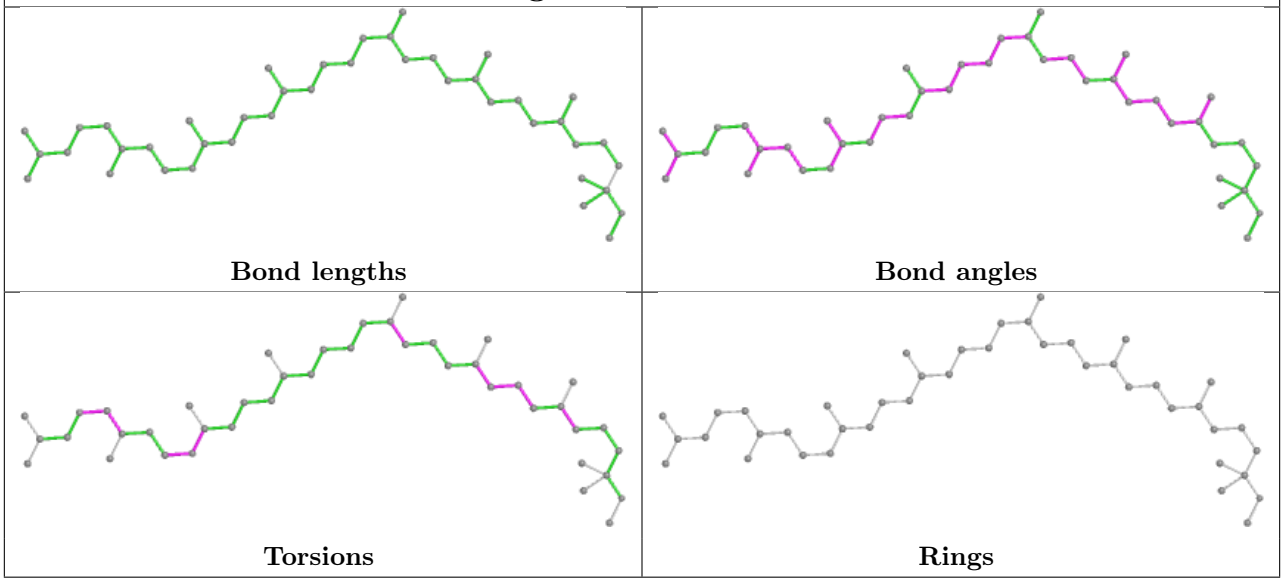


Rings

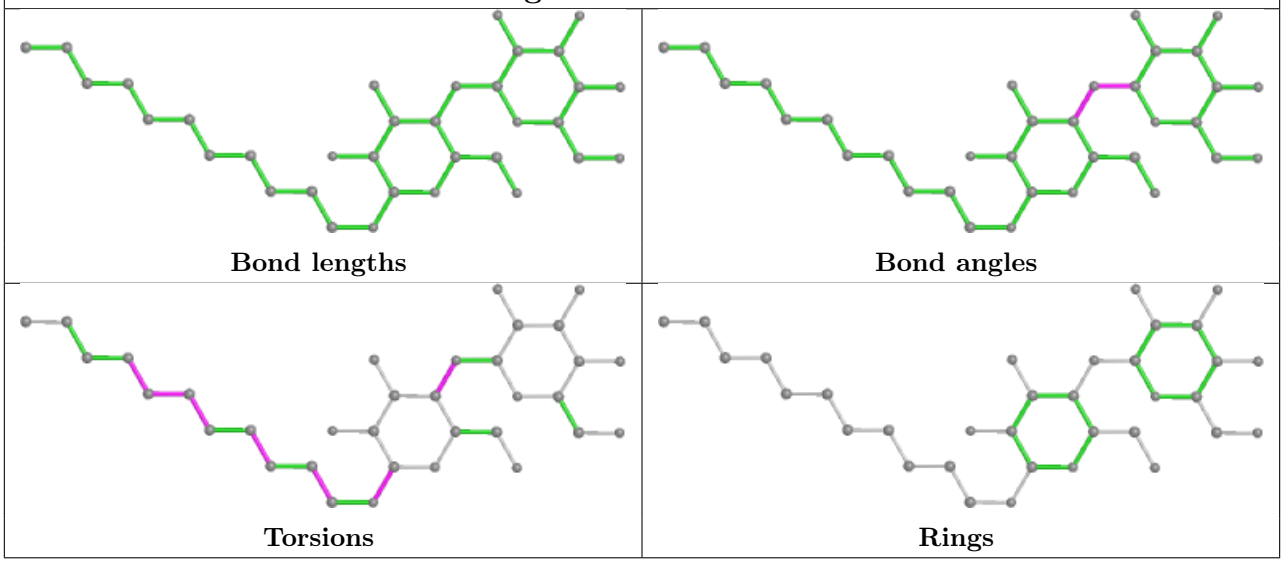
Ligand PEE L 306



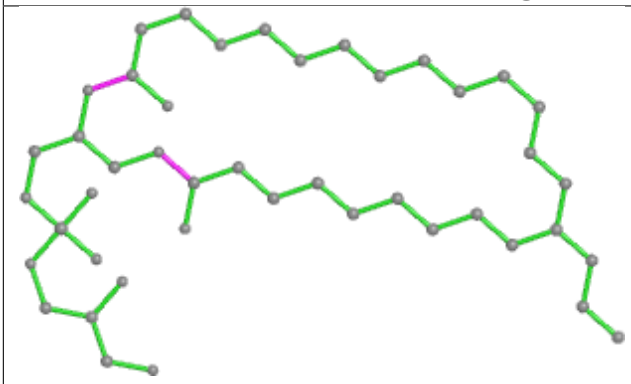
Ligand SPO E 101



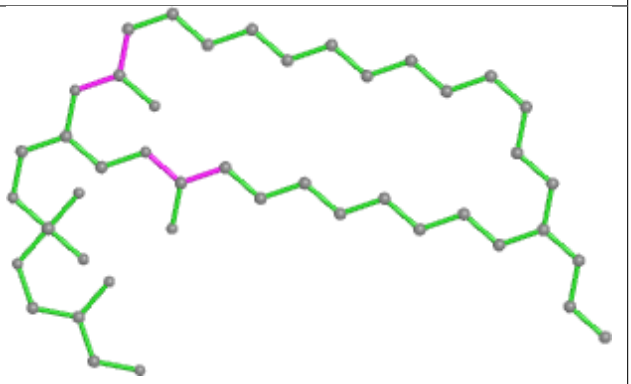
Ligand LMT L 309



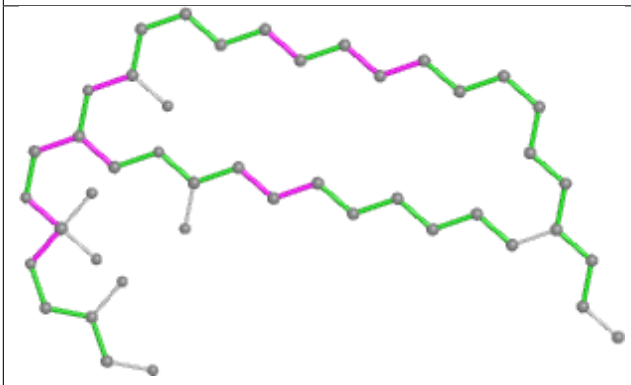
Ligand PGV M 413



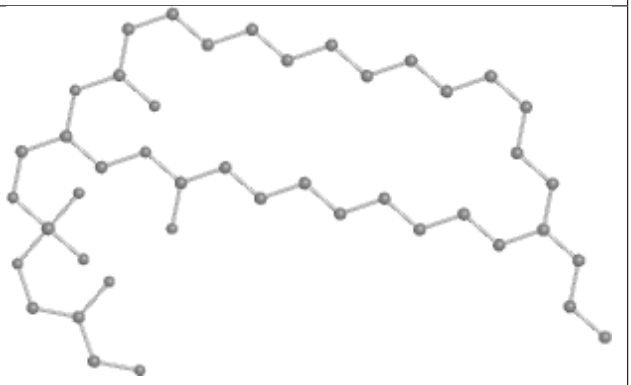
Bond lengths



Bond angles

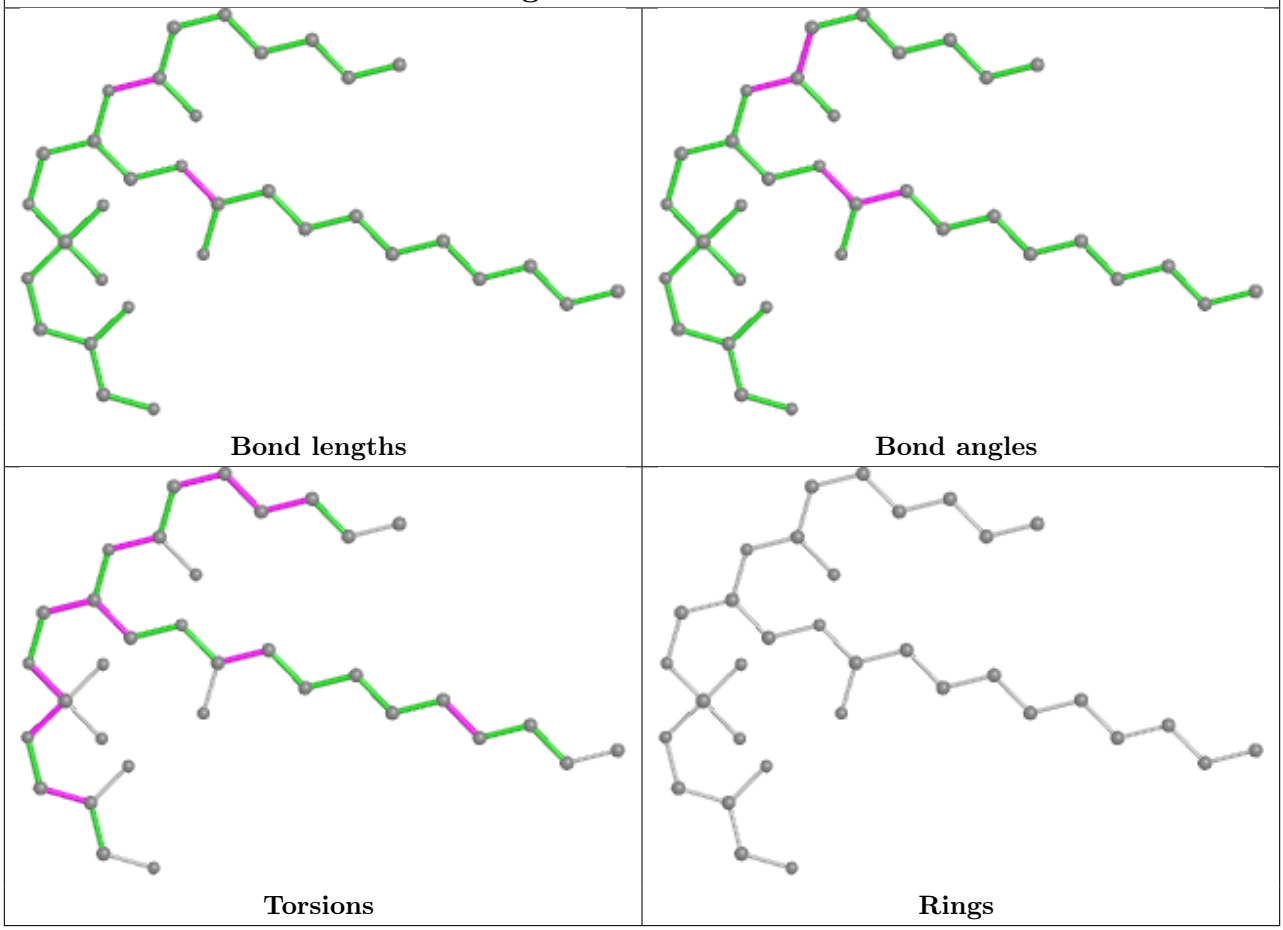


Torsions

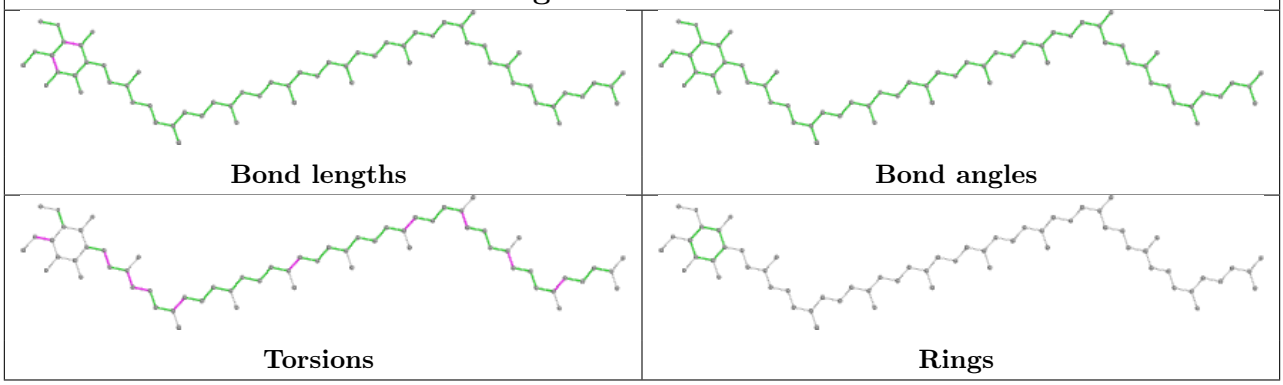


Rings

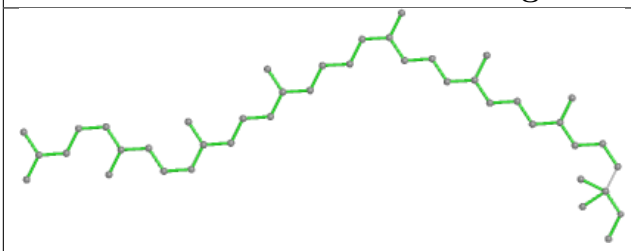
Ligand PGV H 304



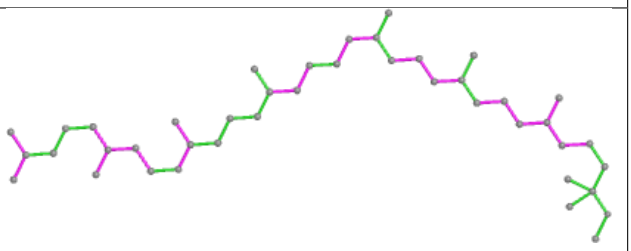
Ligand U10 L 304



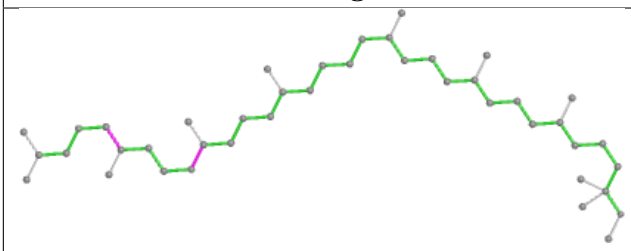
Ligand SPO M 408



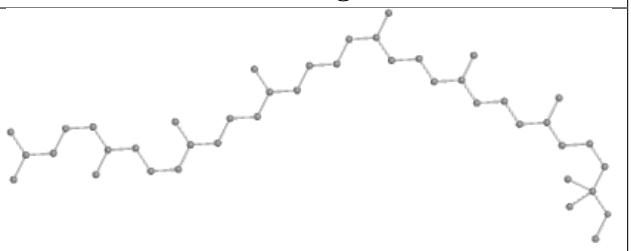
Bond lengths



Bond angles

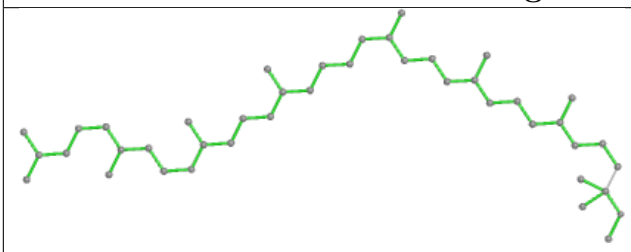


Torsions

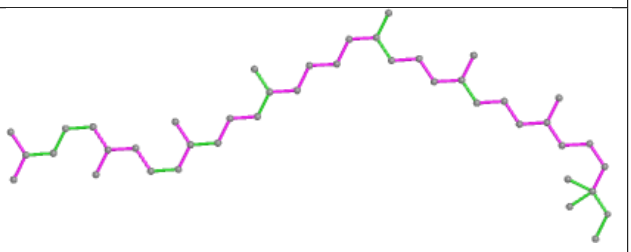


Rings

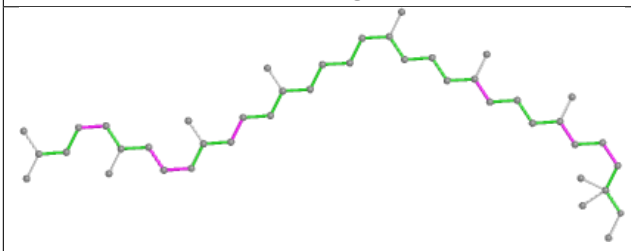
Ligand SPO N 101



Bond lengths



Bond angles



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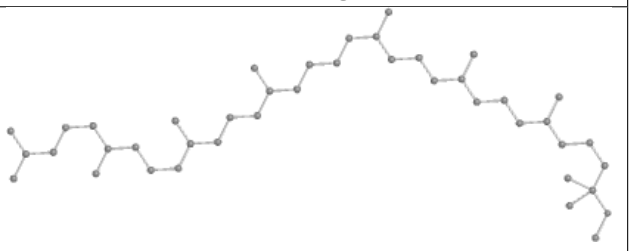
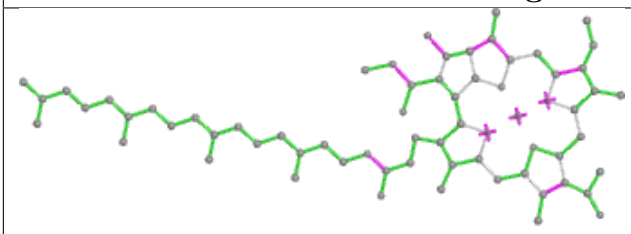
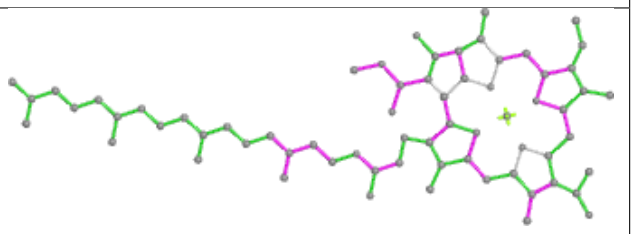


Rings

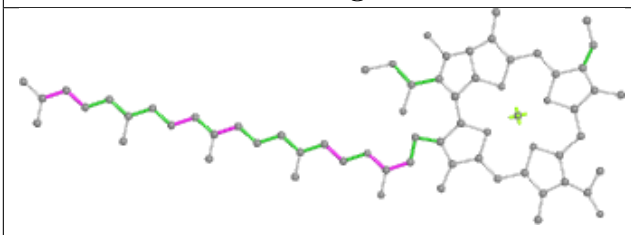
Ligand BCL B 101



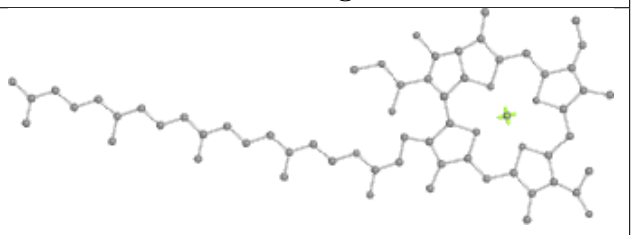
Bond lengths



Bond angles

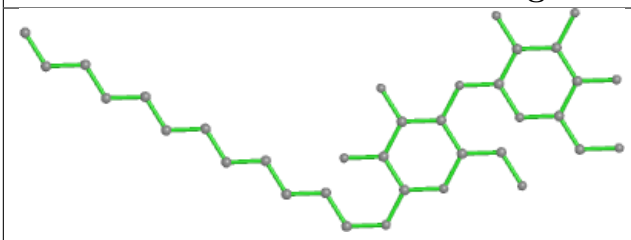


Torsions

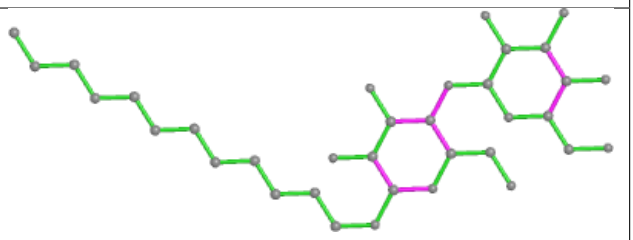


Rings

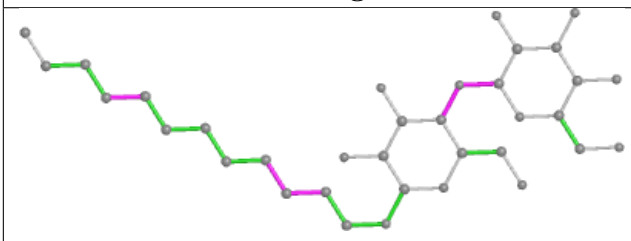
Ligand LMT I 101



Bond lengths



Bond angles



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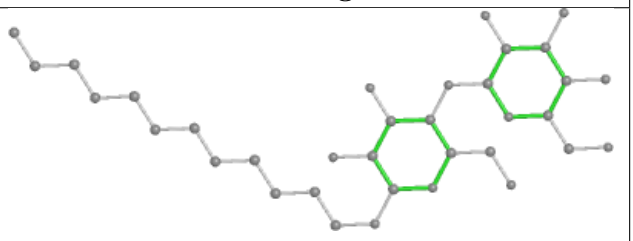
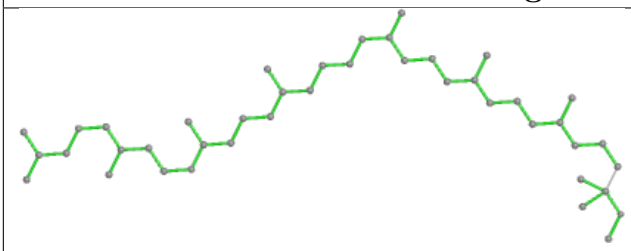
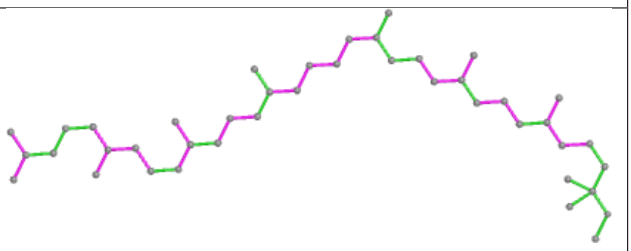


Rings

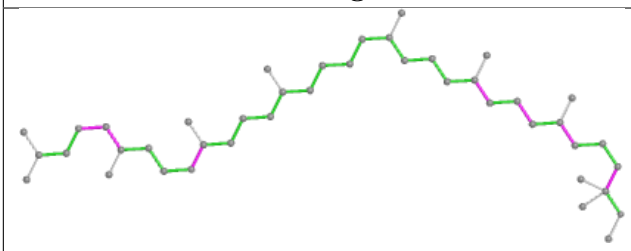
Ligand SPO G 102



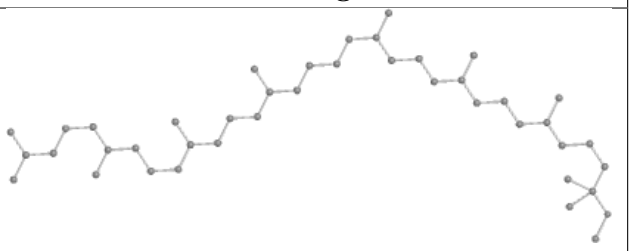
Bond lengths



Bond angles

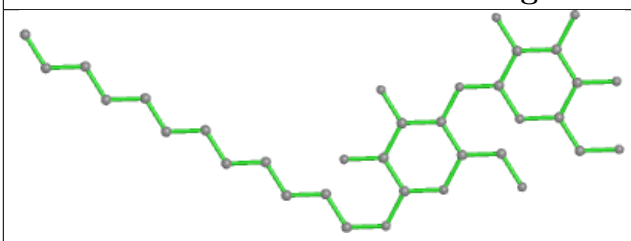


Torsions



Rings

Ligand LMT Q 101



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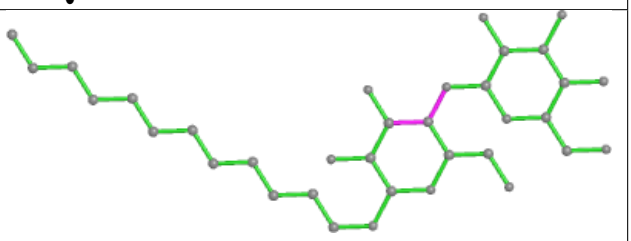
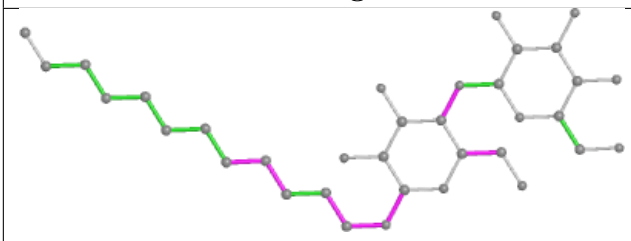
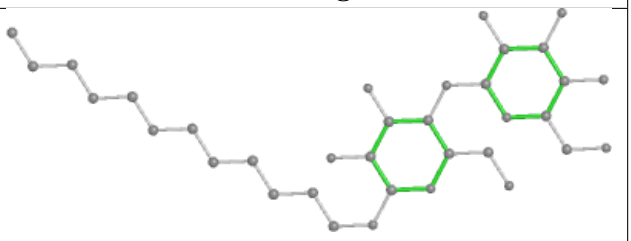


Bond angles

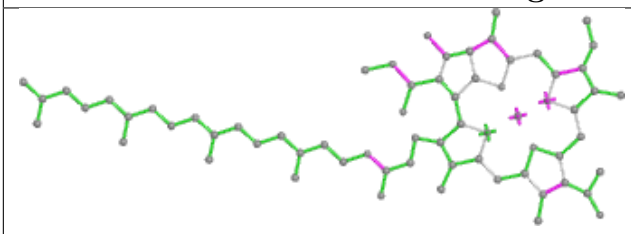


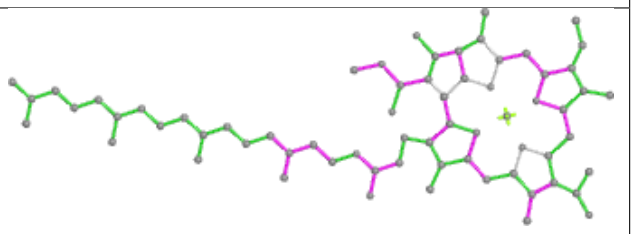
Torsions

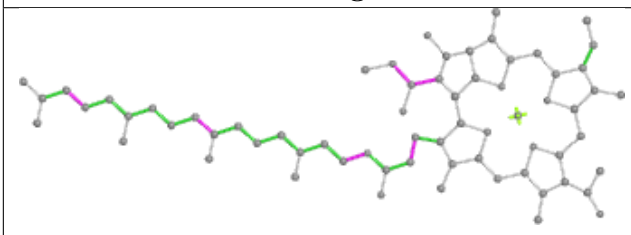


Rings

Ligand BCL L 301


Bond lengths


Bond angles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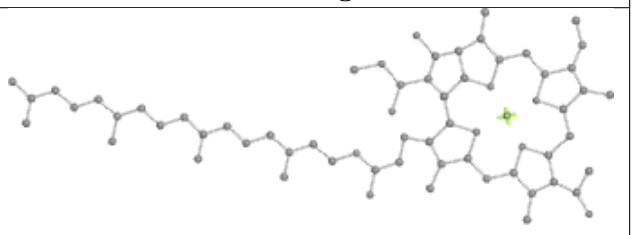
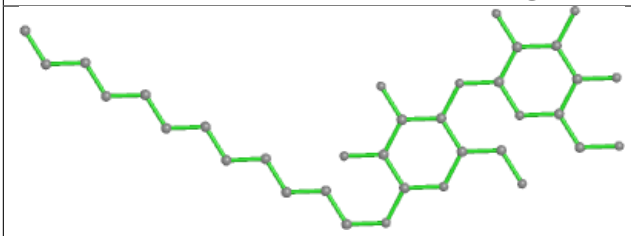
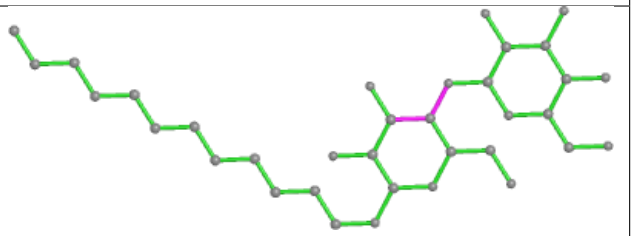
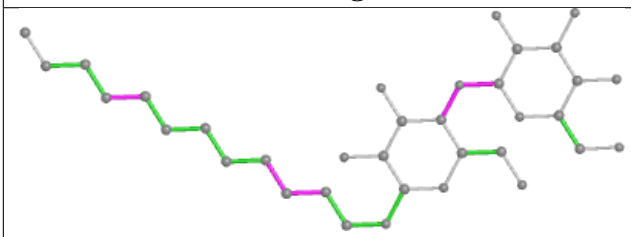
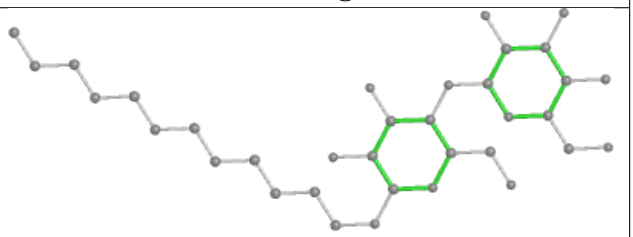

Rings

Ligand LMT L 311

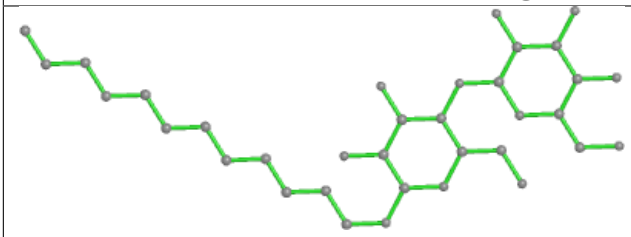

Bond lengths


Bond angles


Torsions


Rings

Ligand LMT M 411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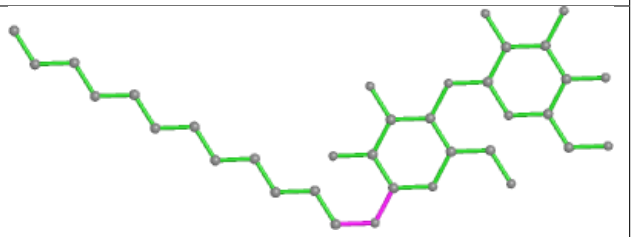
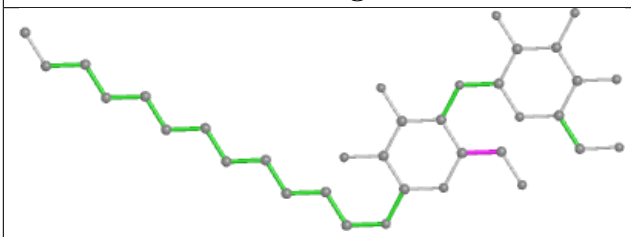

Bond angles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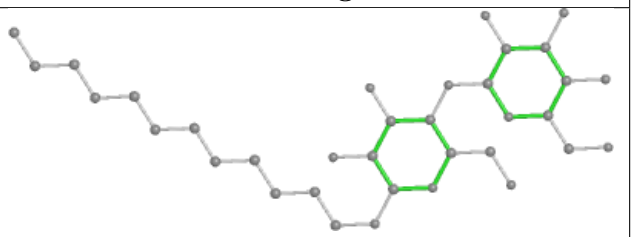
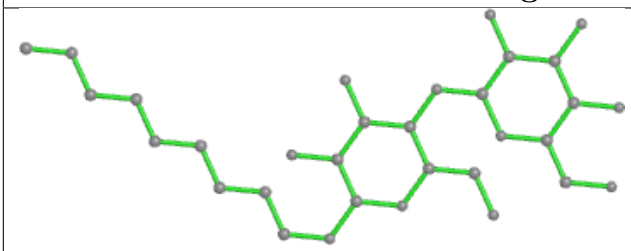
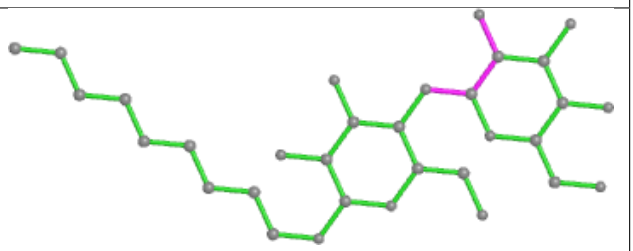

Rings

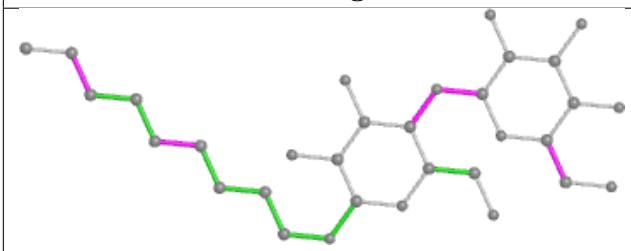
Ligand LMT A 102



Bond lengths



Bond angles



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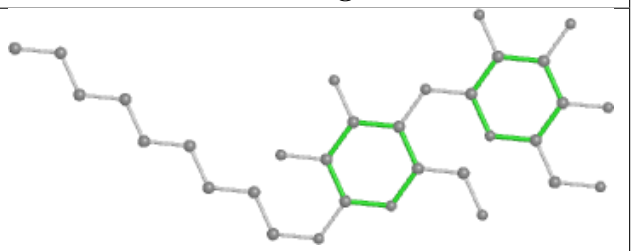
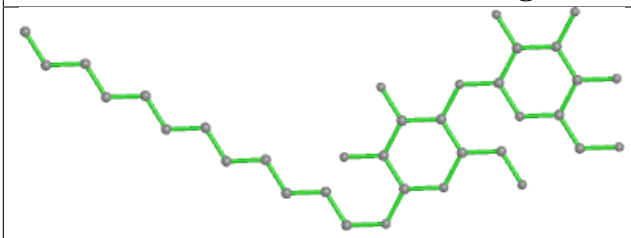
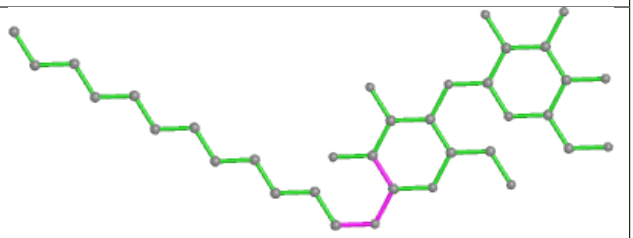


Rings

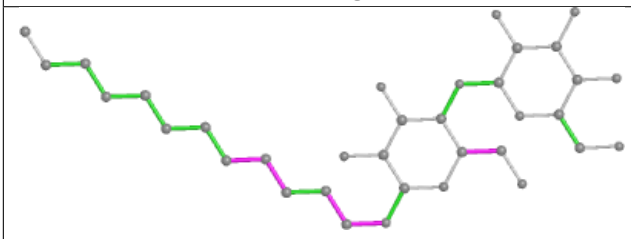
Ligand LMT M 410



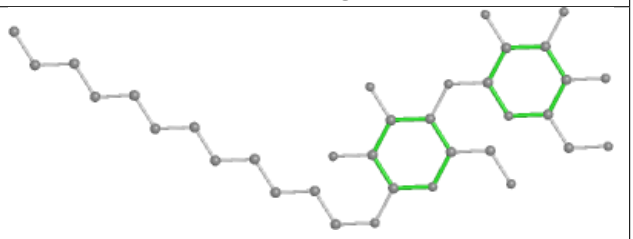
Bond lengths



Bond angles

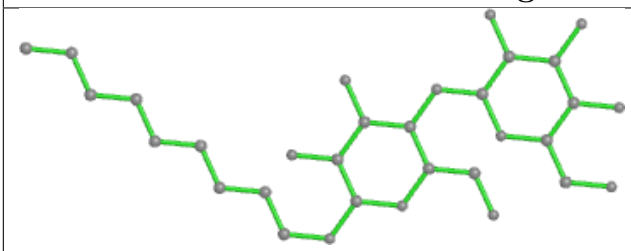


Torsions

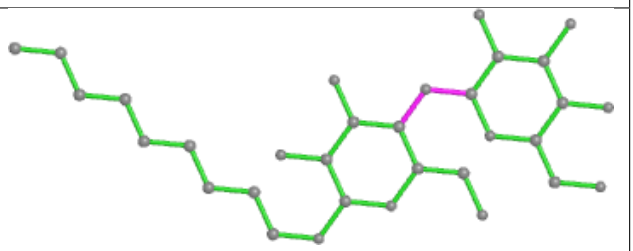


Rings

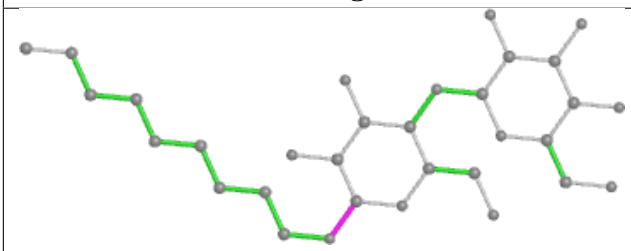
Ligand LMT M 412



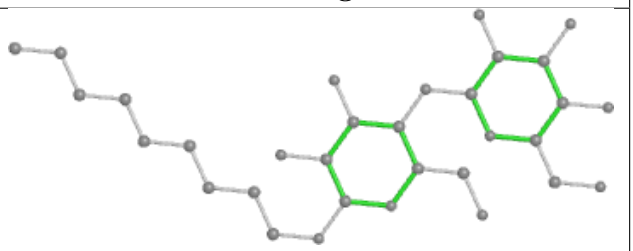
Bond lengths



Bond angles

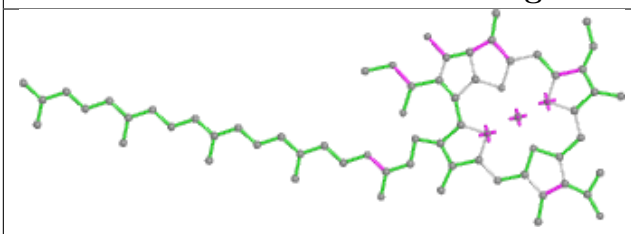


Torsions



Rings

Ligand BCL O 102



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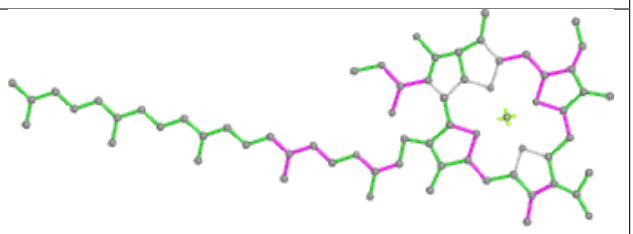
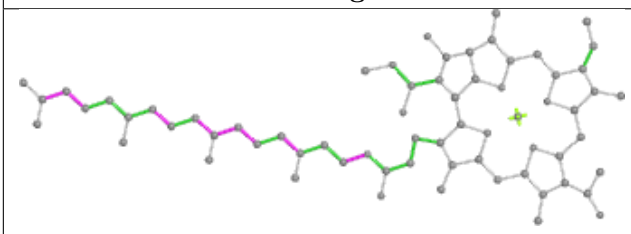


Bond angles



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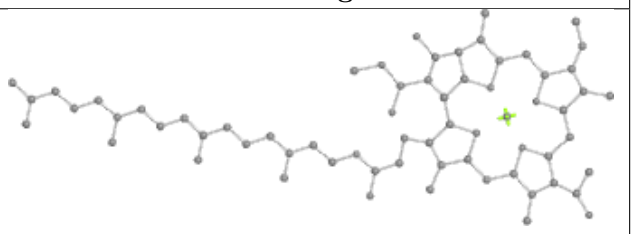
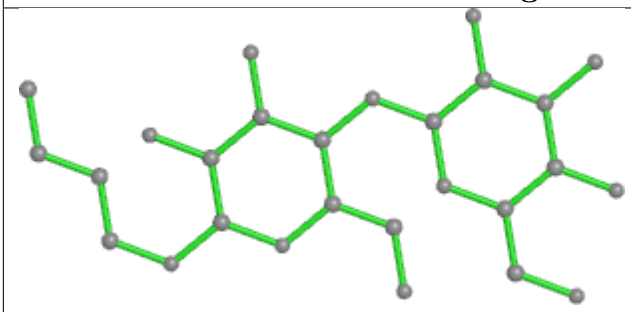


Rings

Ligand LMT Y 103



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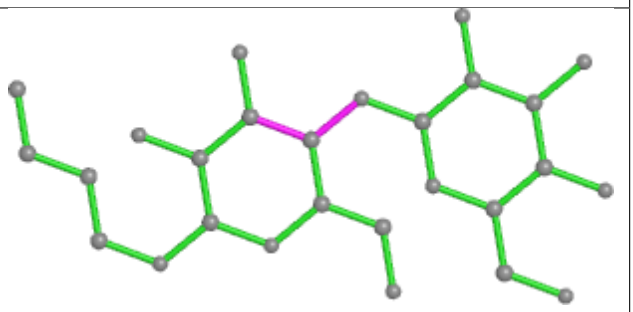
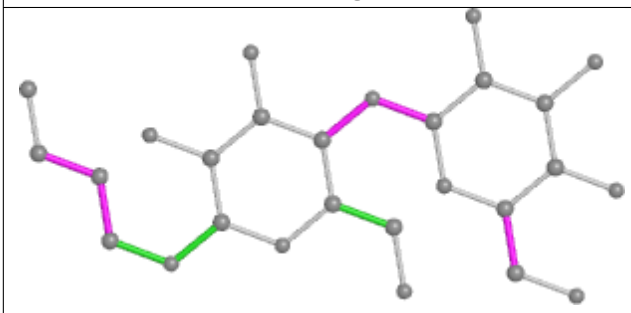


Bond angles



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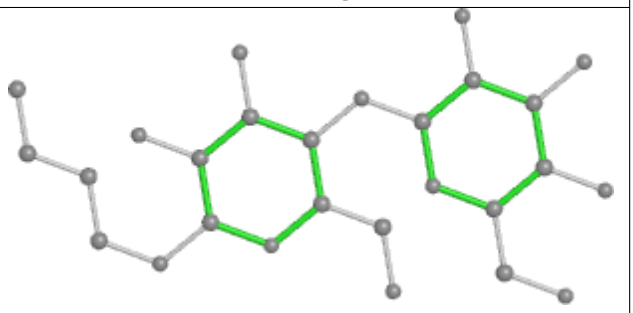
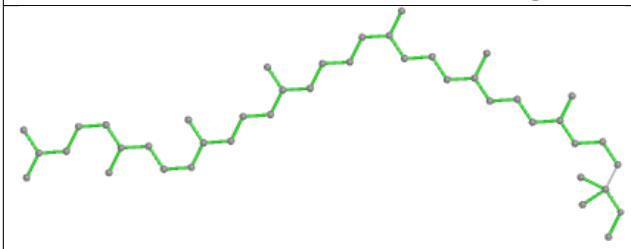


Rings

Ligand SPO P 101



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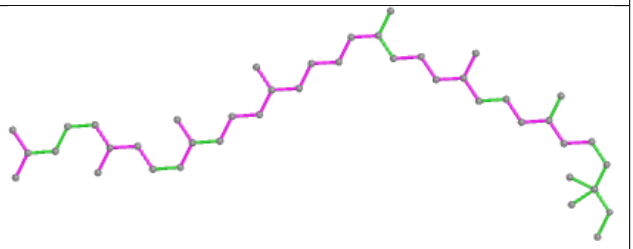
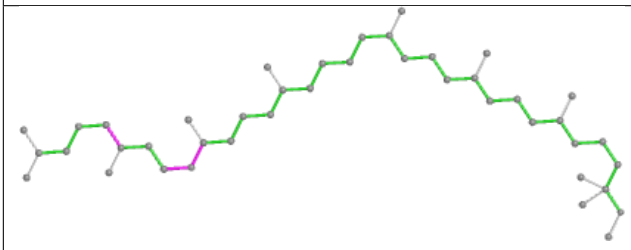


Bond angles



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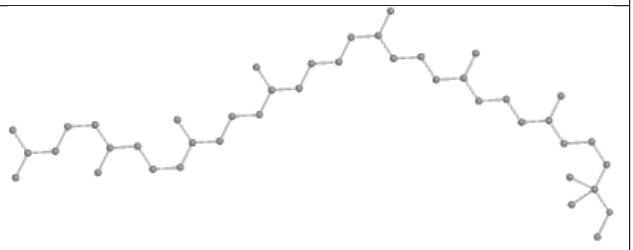
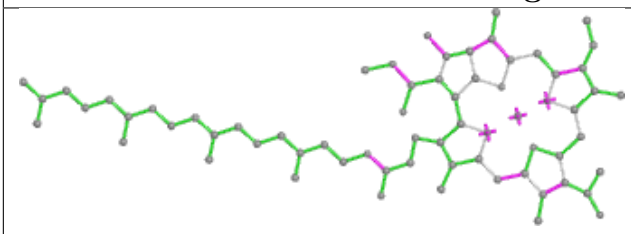


Rings

Ligand BCL G 101



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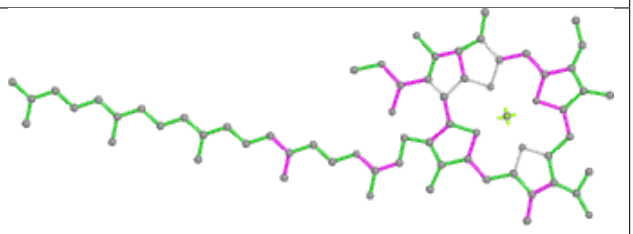
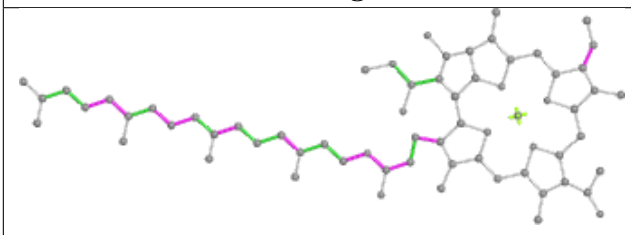


Bond angles



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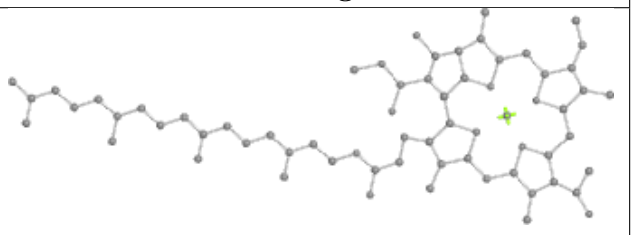
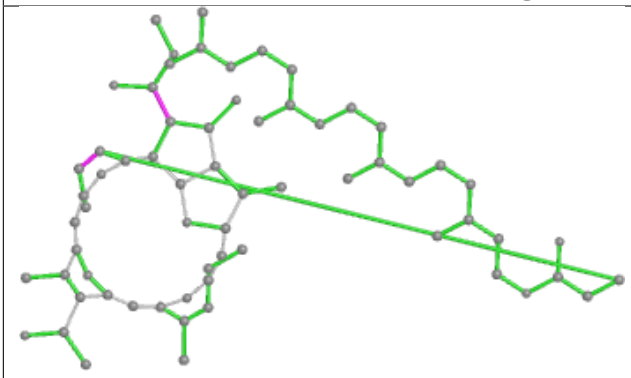


Rings

Ligand BPH M 405



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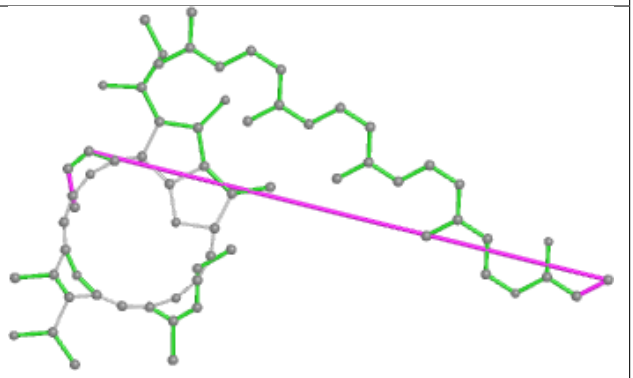
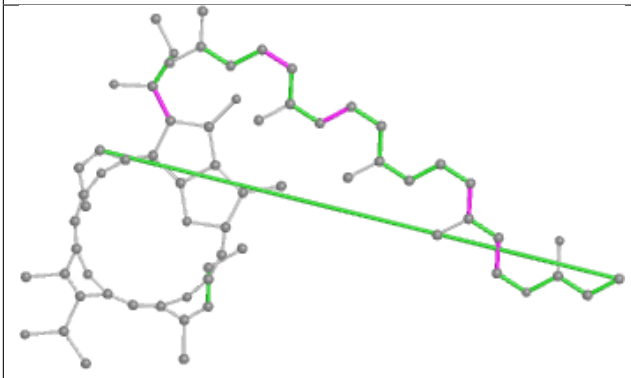


Bond angles



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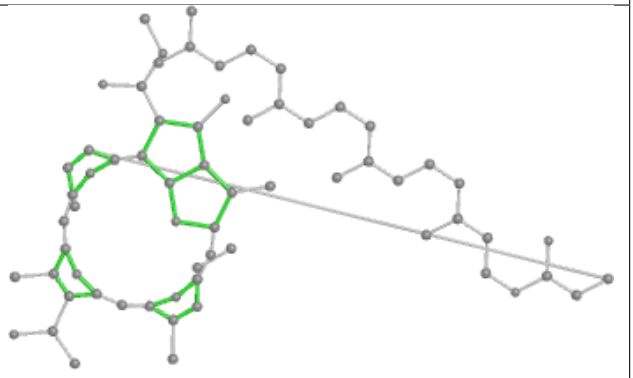
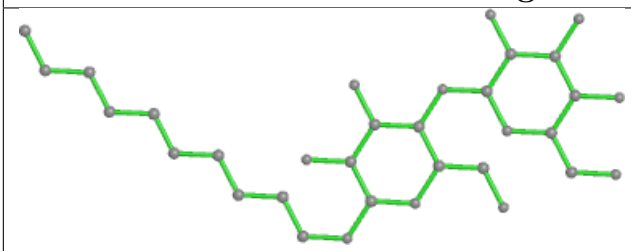


Rings

Ligand LMT M 417



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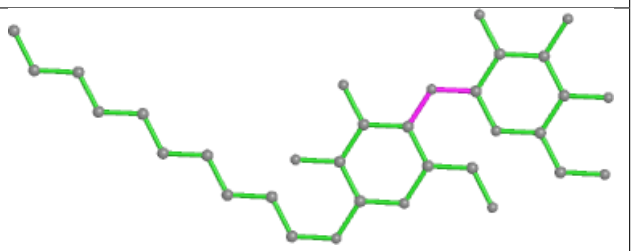
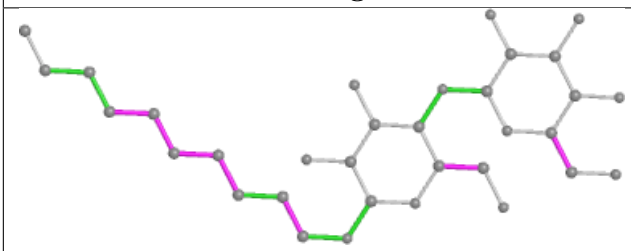


Bond angles



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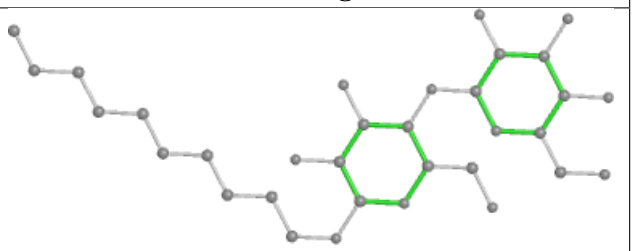
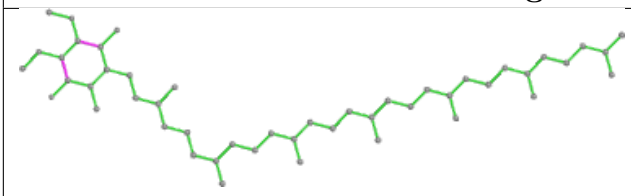


Rings

Ligand U10 M 407



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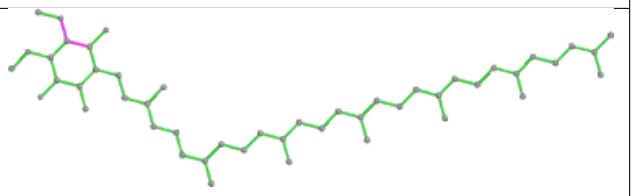
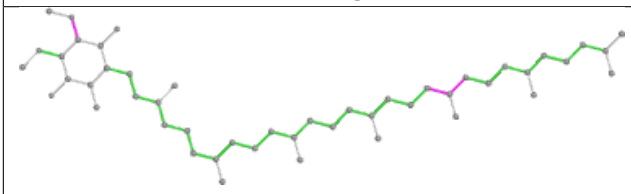


Bond angles



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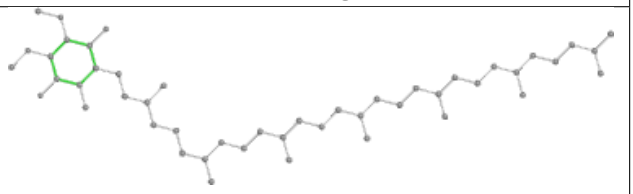
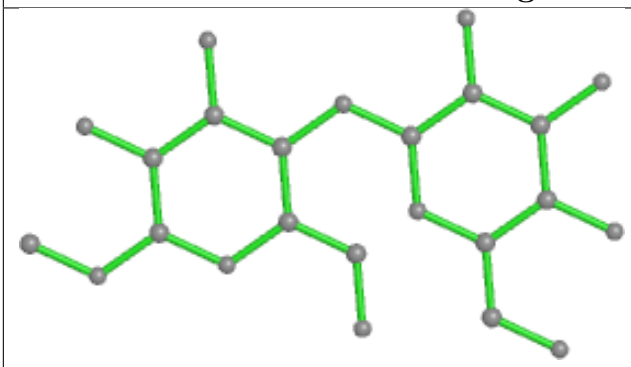


Rings

Ligand LMT M 409



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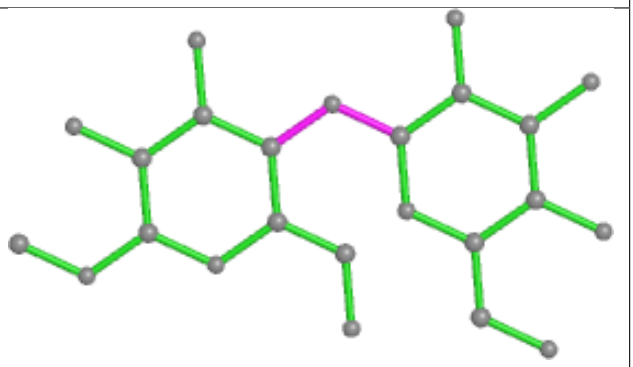

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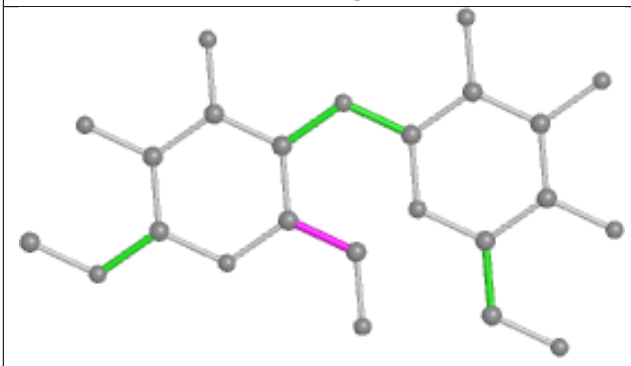

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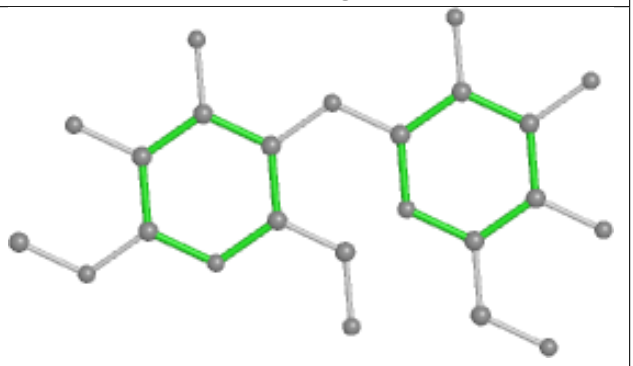
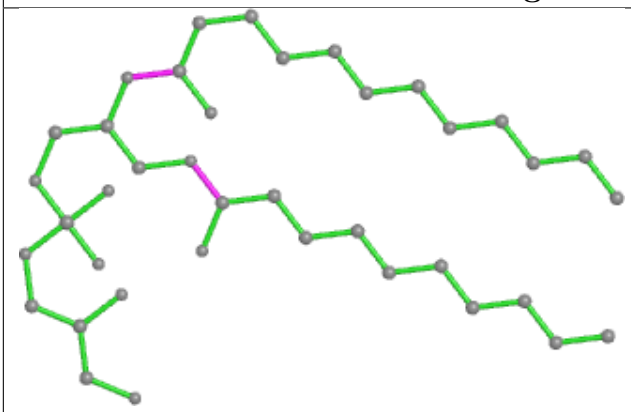


Rings

Ligand PGV L 305



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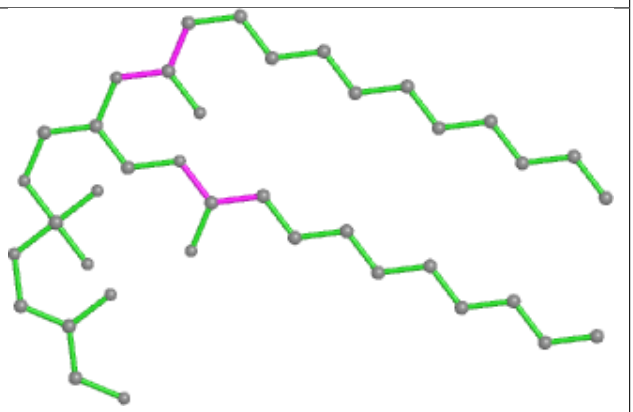
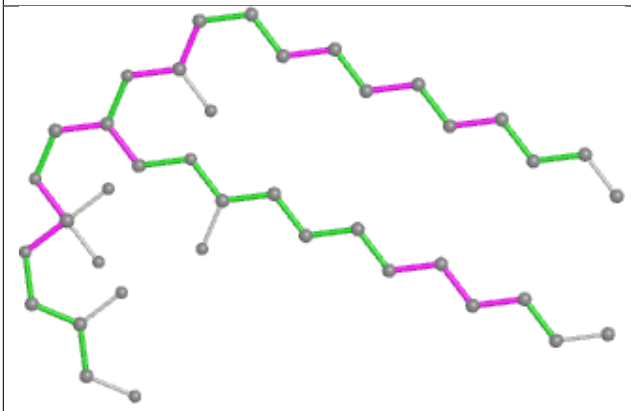


Bond angles



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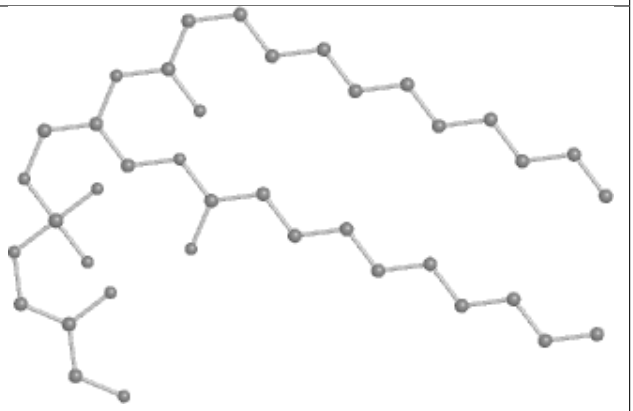
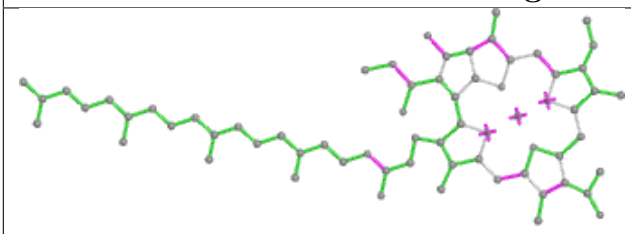


Rings

Ligand BCL V 101



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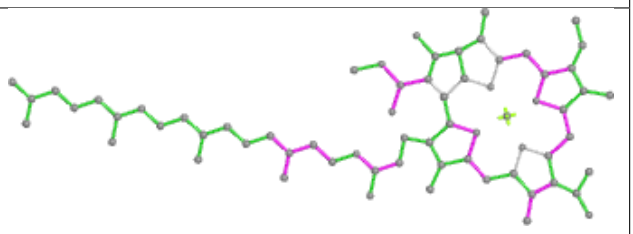
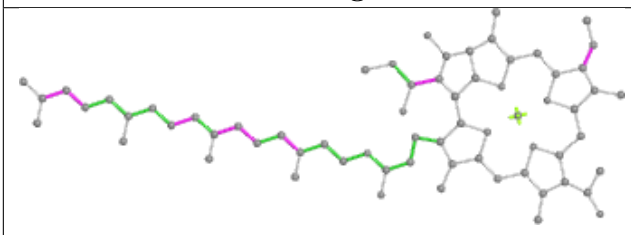


Bond angles



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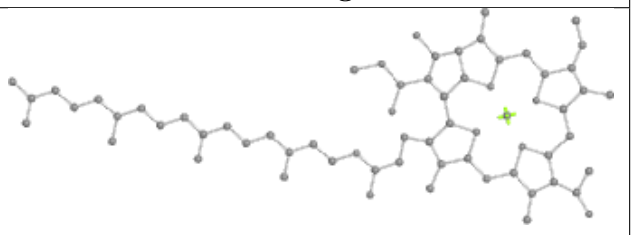
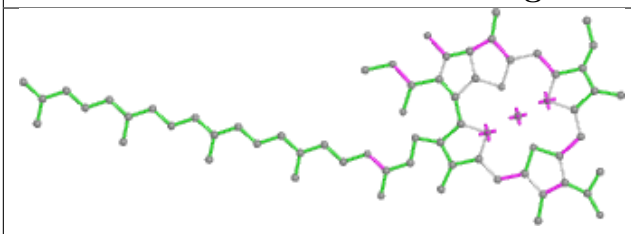


Rings

Ligand BCL Y 102



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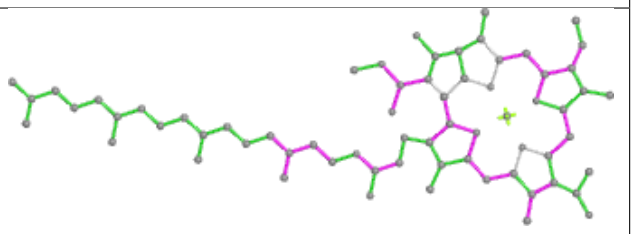
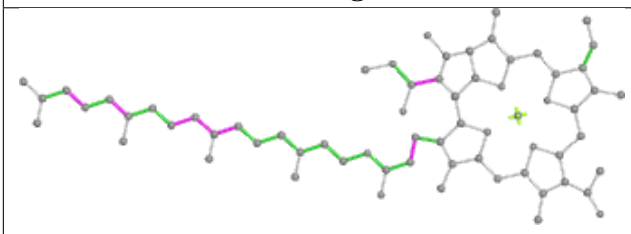


Bond angles



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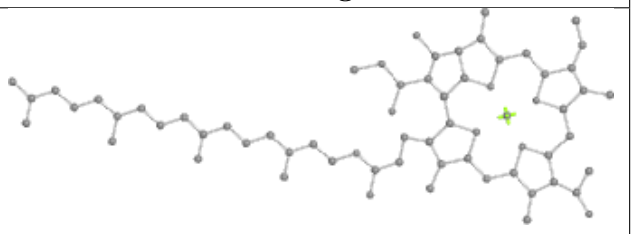
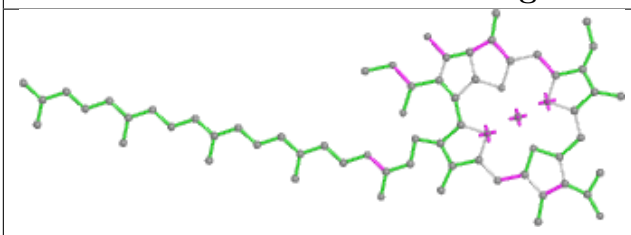


Rings

Ligand BCL W 102



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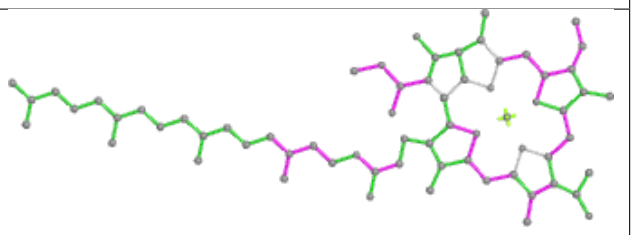
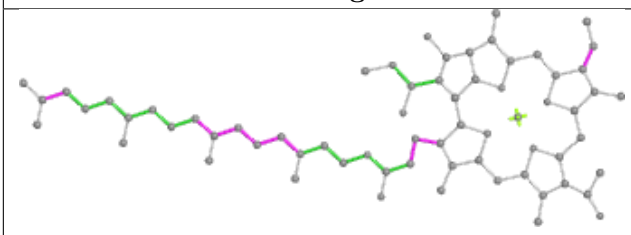


Bond angles



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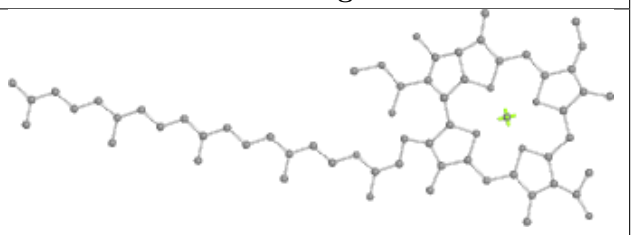
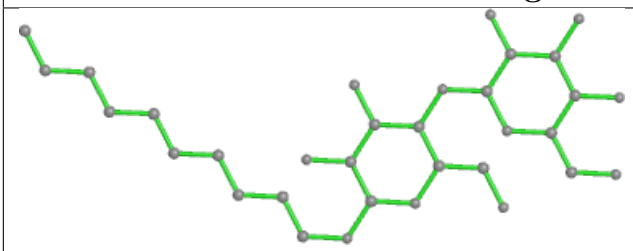


Rings

Ligand LMT S 102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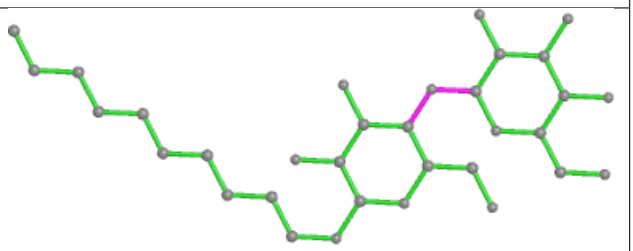
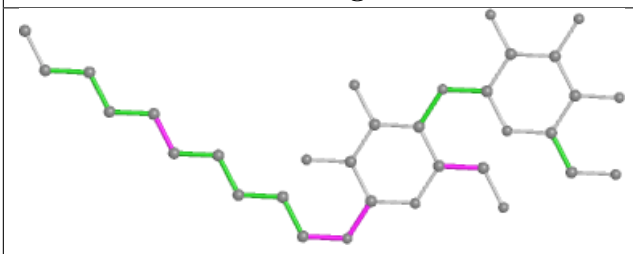

Bond angles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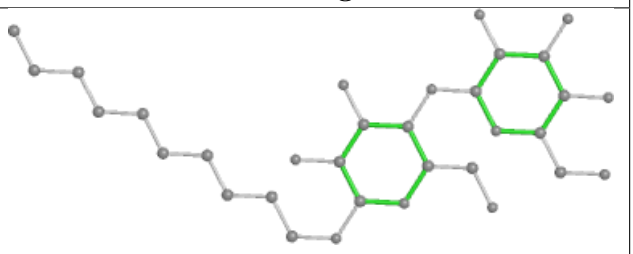
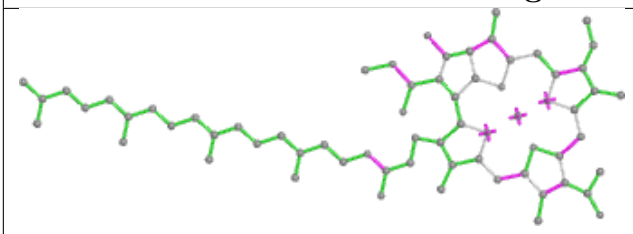
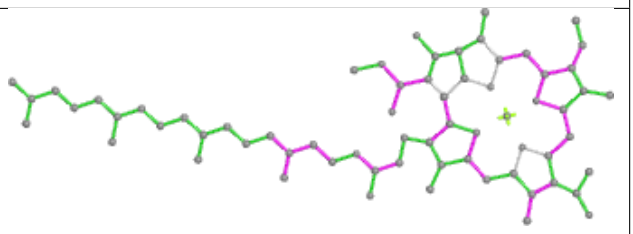
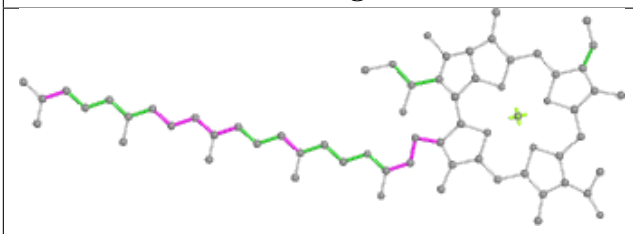
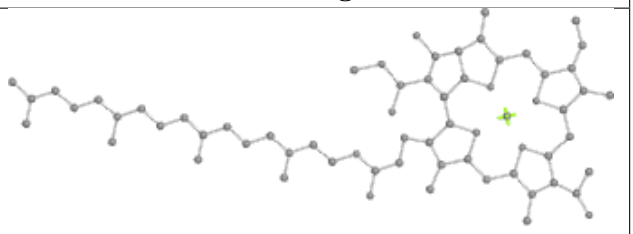

Rings

Ligand BCL R 102

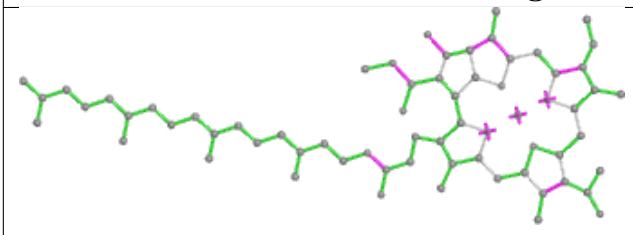

Bond lengths


Bond angles


Torsions


Rings

Ligand BCL F 103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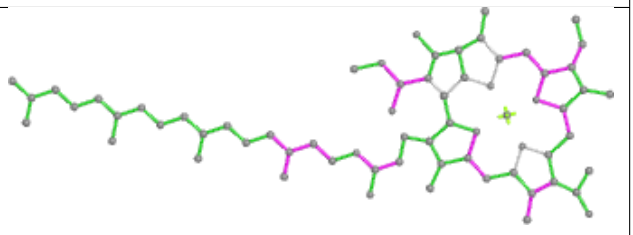
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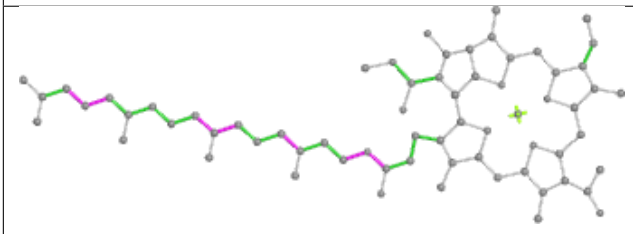
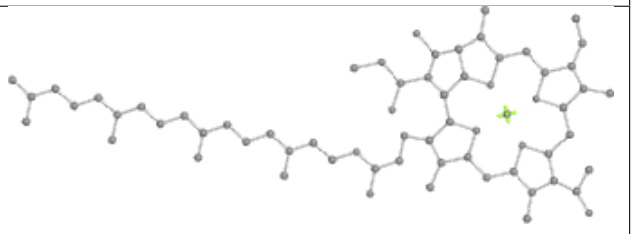
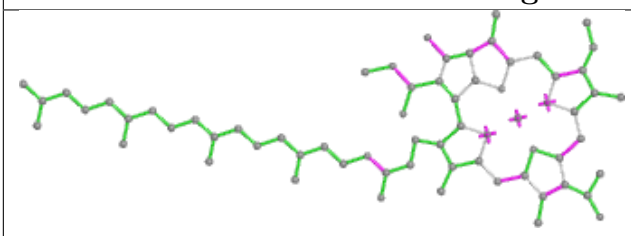
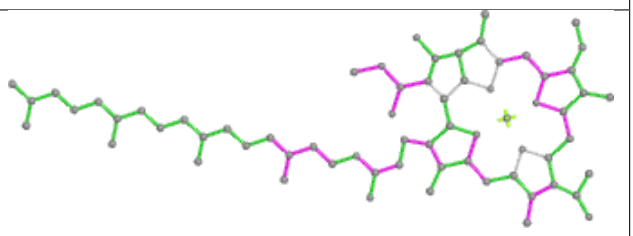

Torsions


Rings

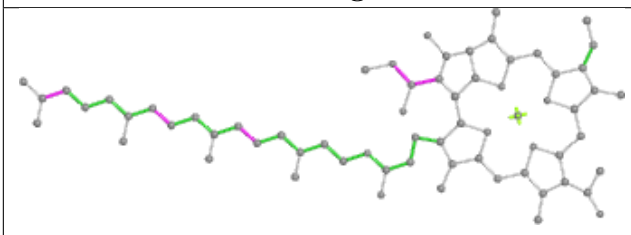
Ligand BCL M 404



Bond lengths



Bond angles



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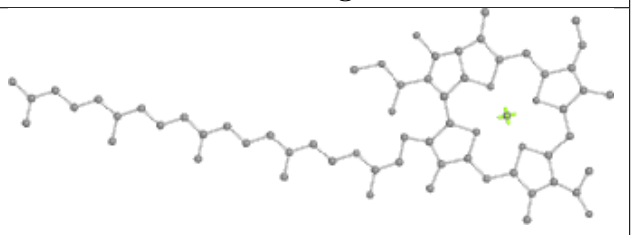
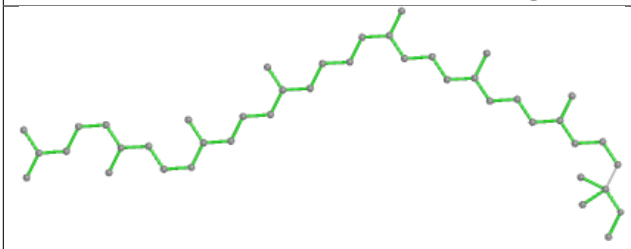


Rings

Ligand SPO D 101



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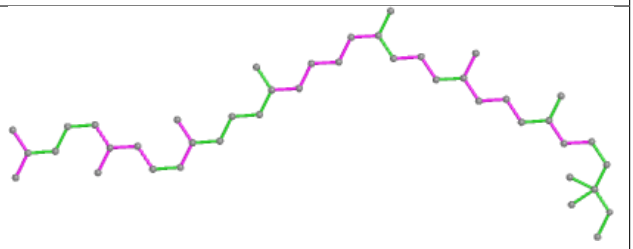
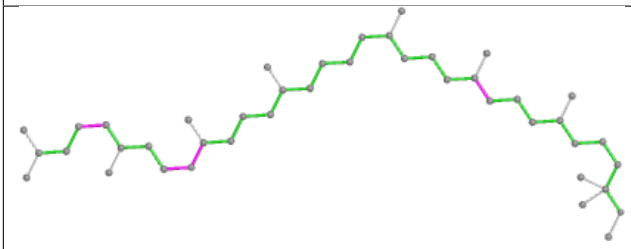


Bond angles



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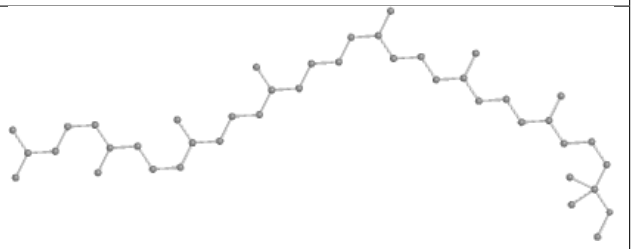
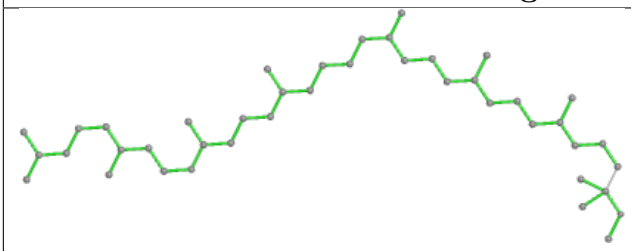


Rings

Ligand SPO W 101



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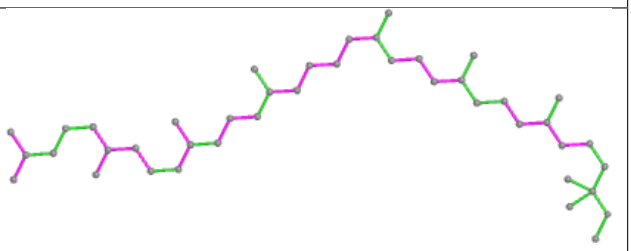
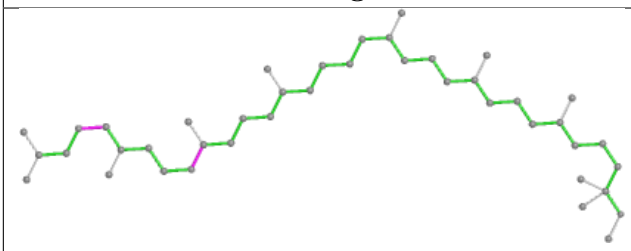


Bond angles



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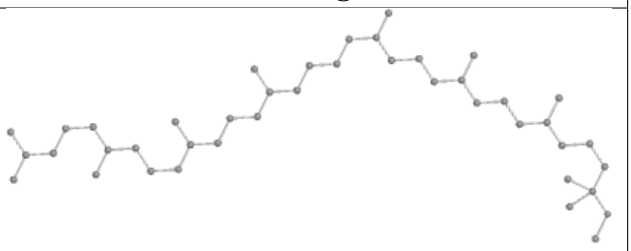
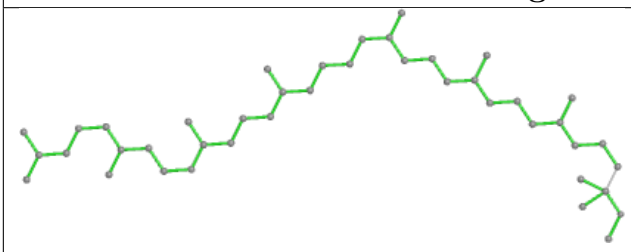


Rings

Ligand SPO S 105



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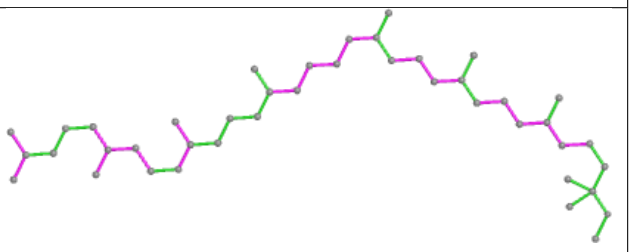
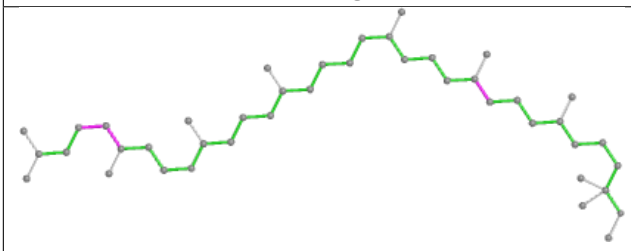


Bond angles



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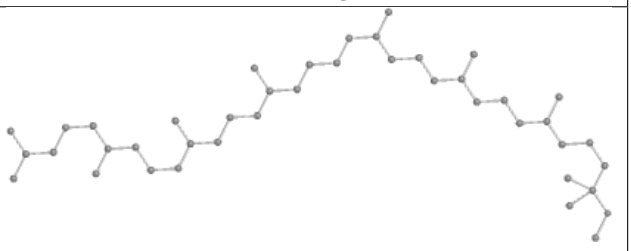
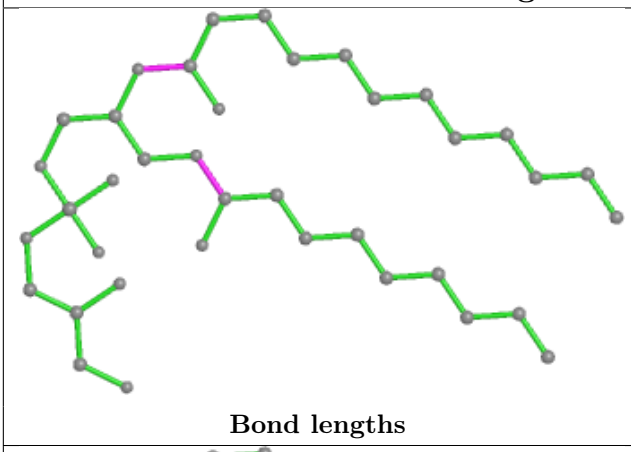


Rings

Ligand PGV M 415



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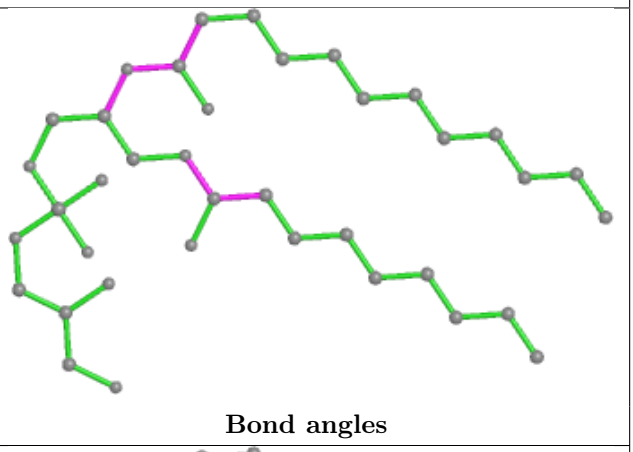
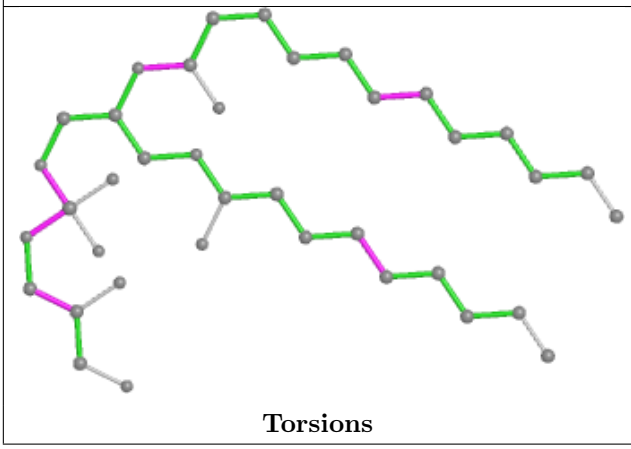


Bond angles



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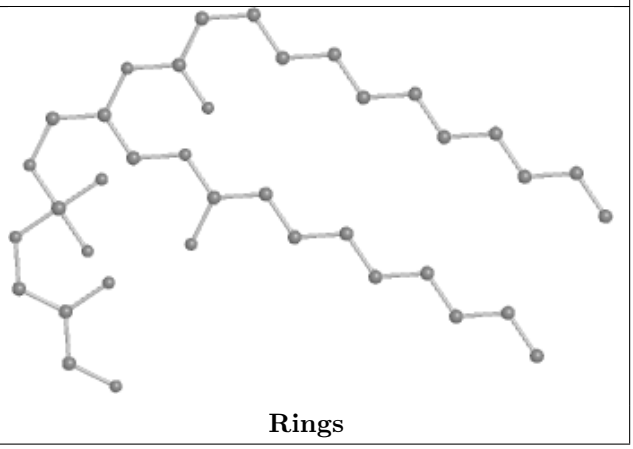
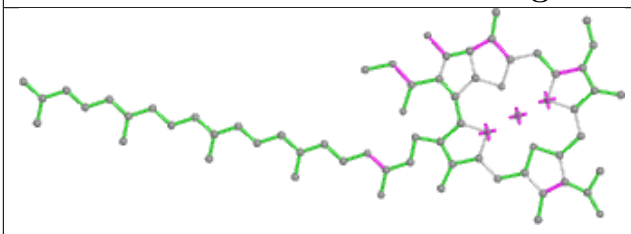


Rings

Ligand BCL I 102



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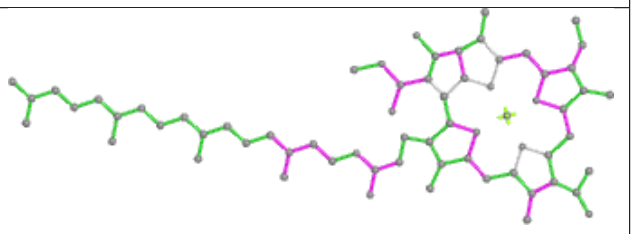
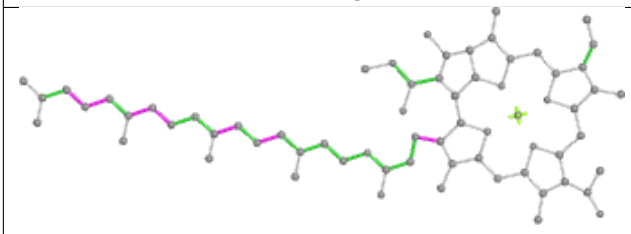


Bond angles



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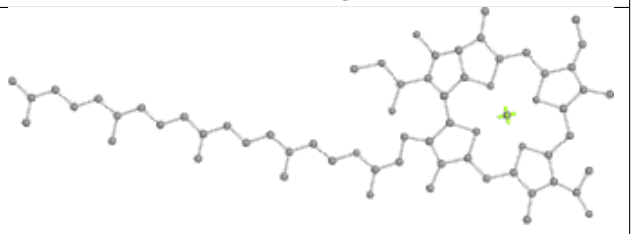
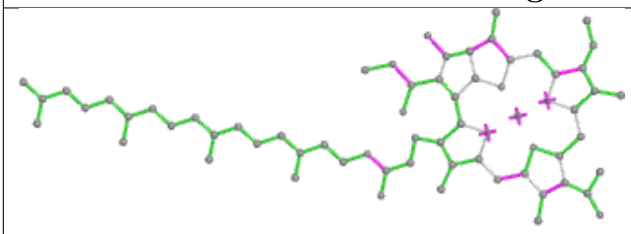


Rings

Ligand BCL E 102



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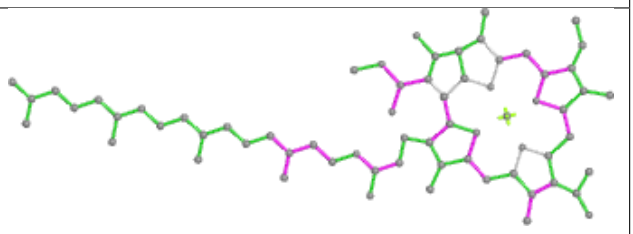
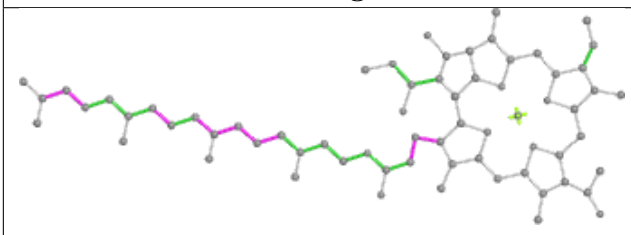


Bond angles



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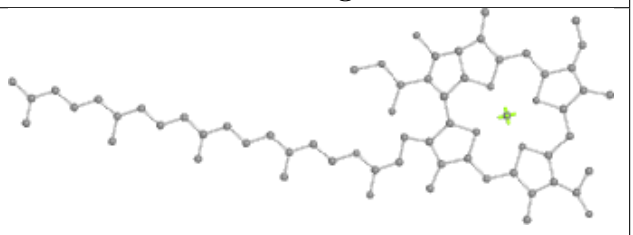
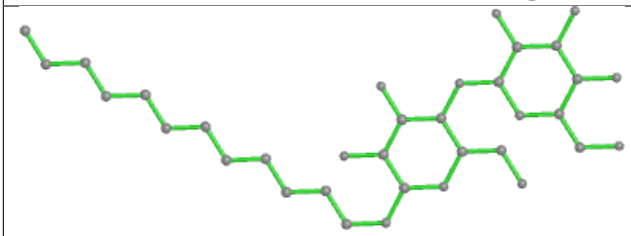


Rings

Ligand LMT L 308



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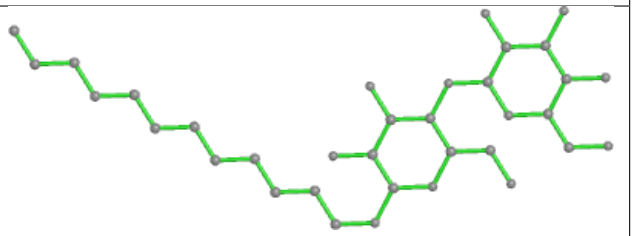

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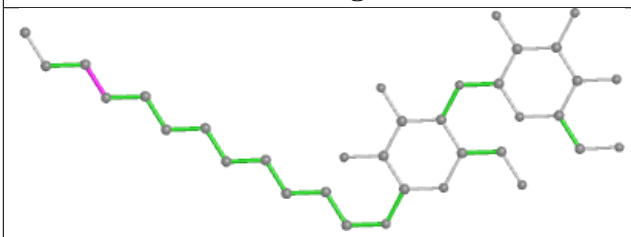

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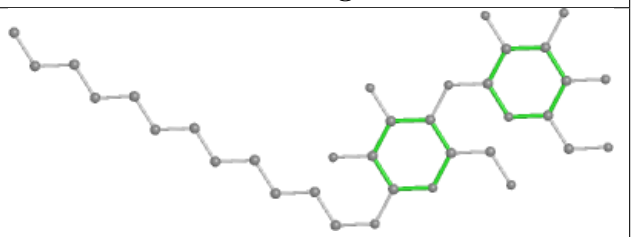
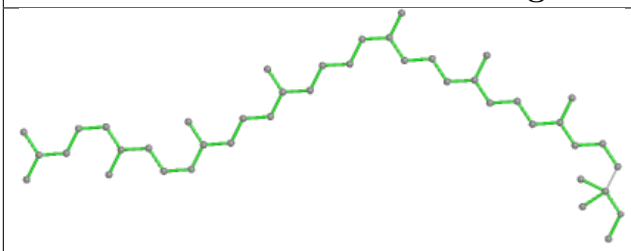


Rings

Ligand SPO F 104



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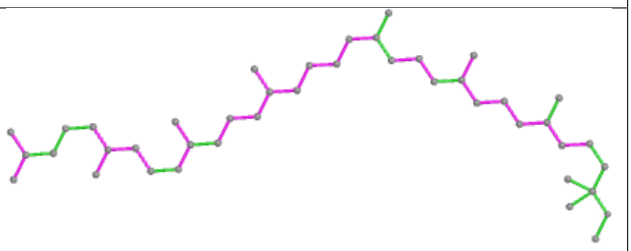
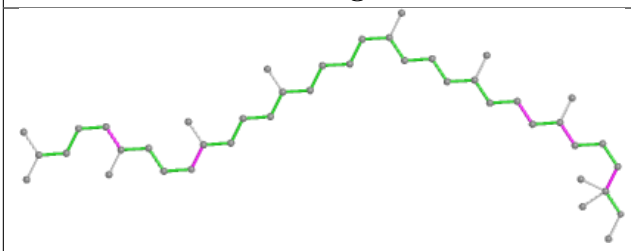


Bond angles



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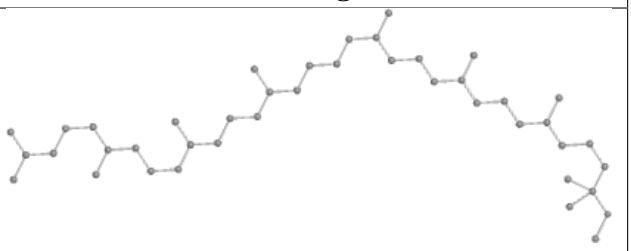
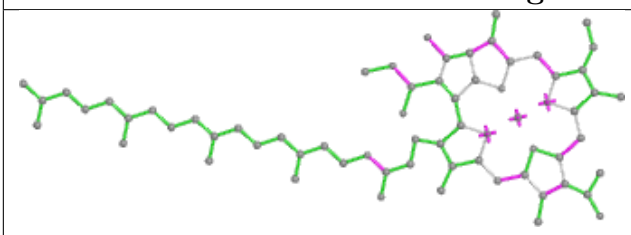


Rings

Ligand BCL F 101



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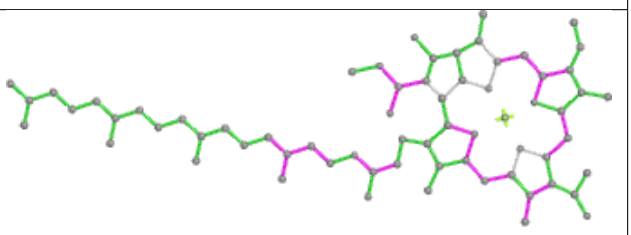
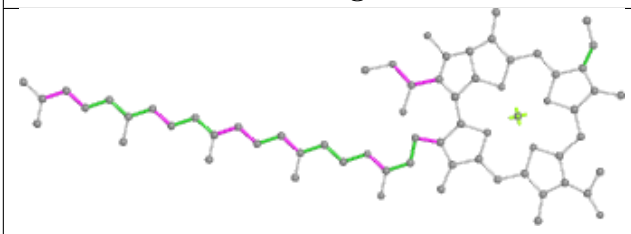


Bond angles



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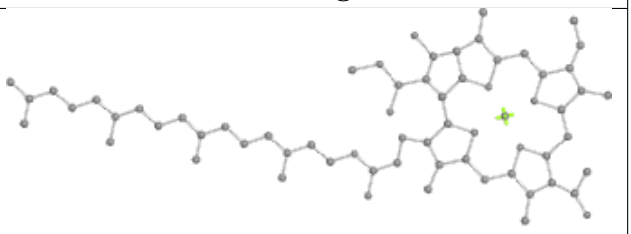
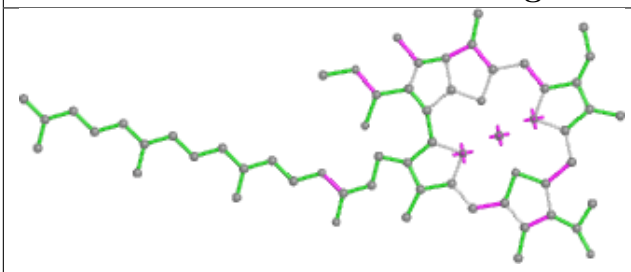


Rings

Ligand BCL A 101



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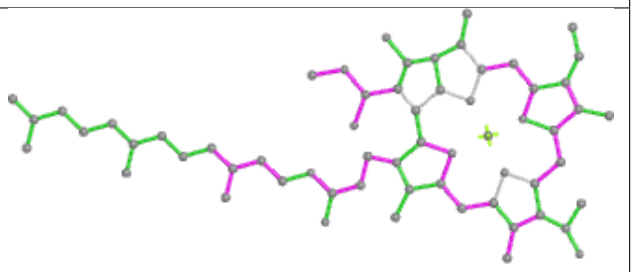
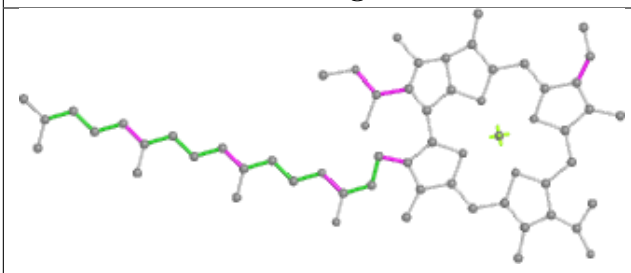
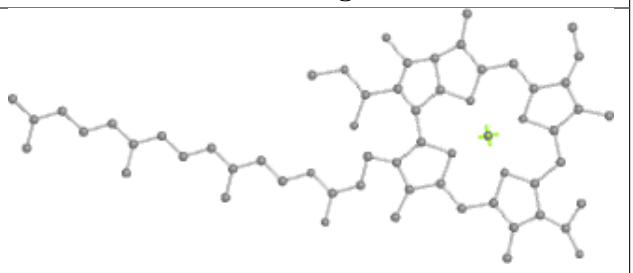


Bond angles

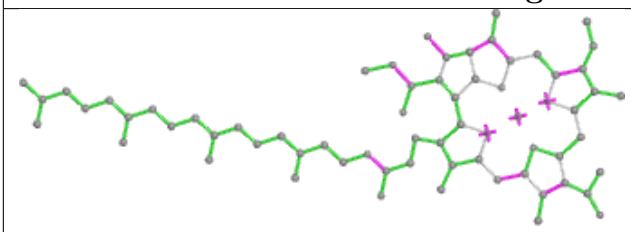


Torsions



Rings

Ligand BCL P 102



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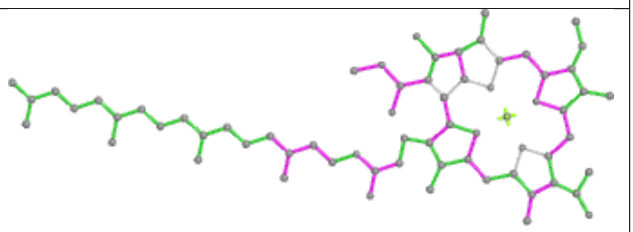
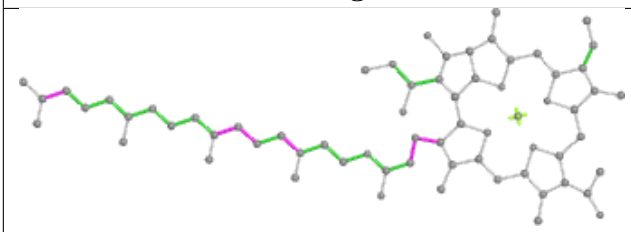


Bond angles



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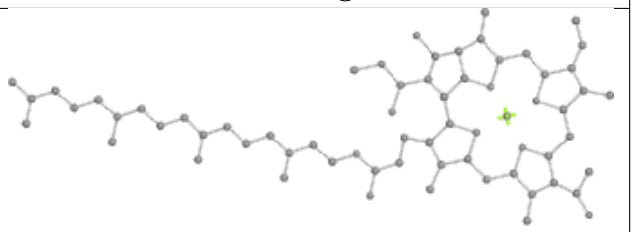
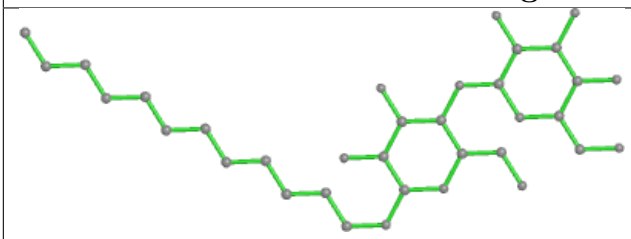
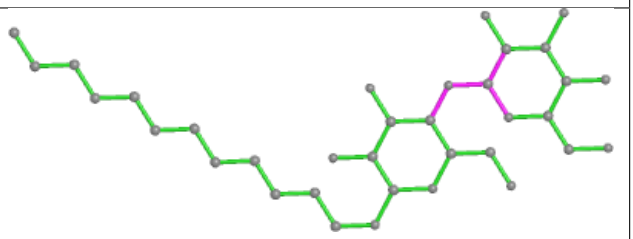


Rings

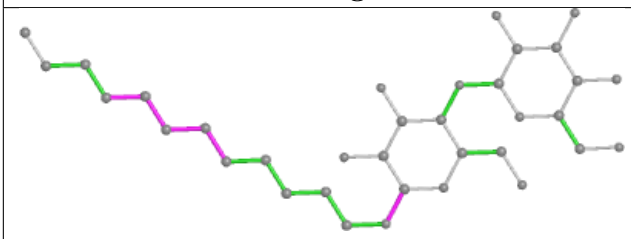
Ligand LMT X 101



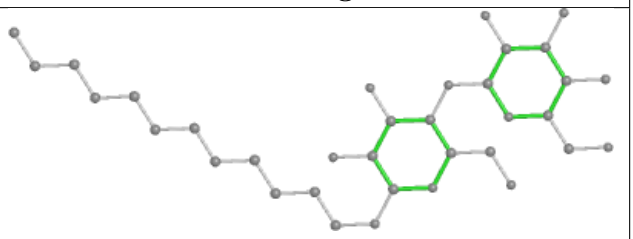
Bond lengths



Bond angles

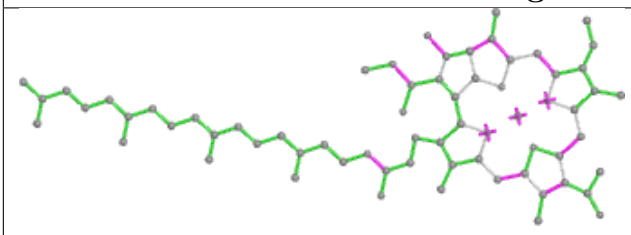


Torsions

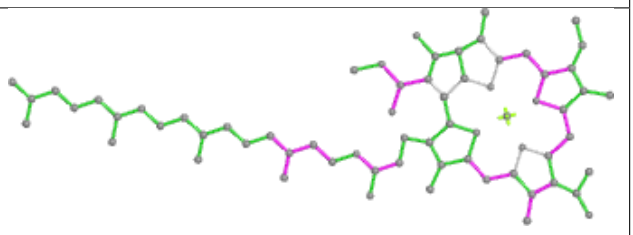


Rings

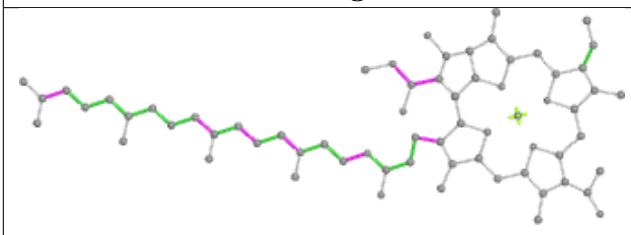
Ligand BCL Z 101



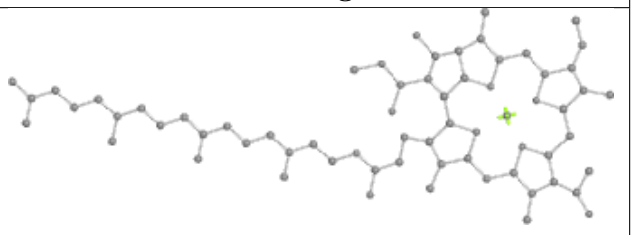
Bond lengths



Bond angles

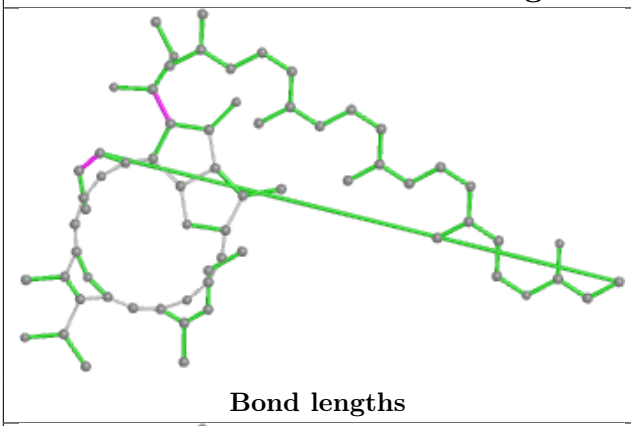


Torsions

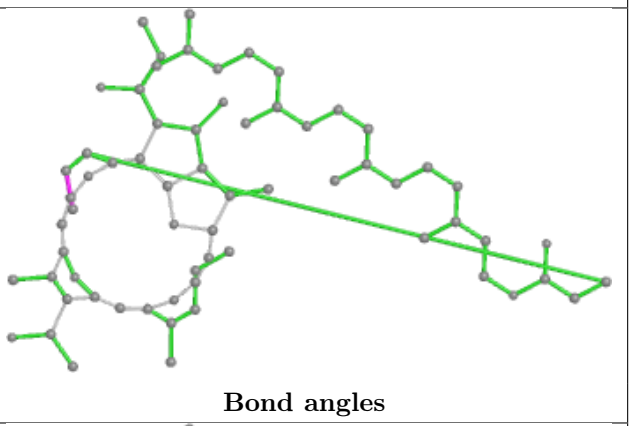


Rings

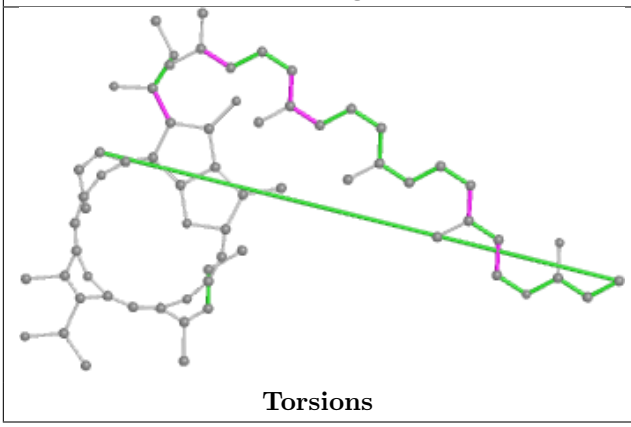
Ligand BPH L 302



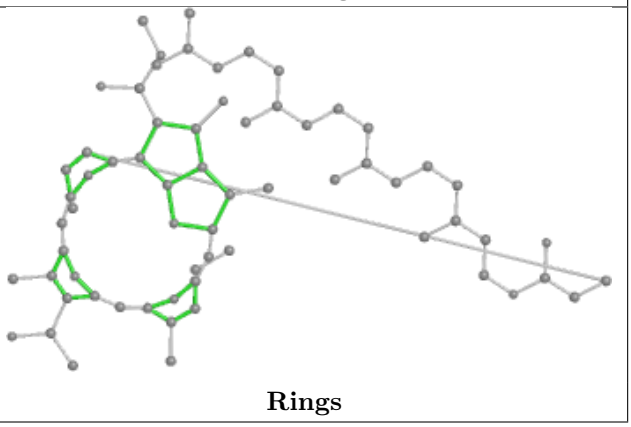
Bond lengths



Bond angles

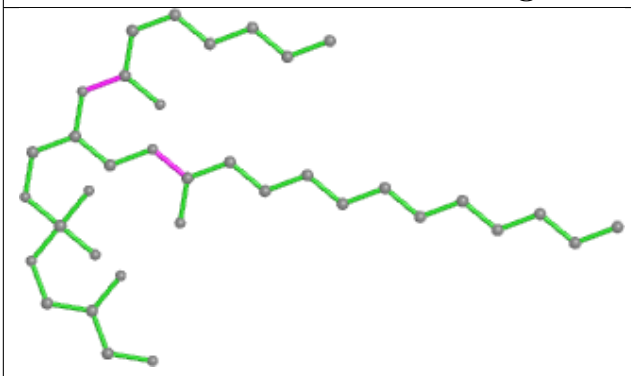


Torsions

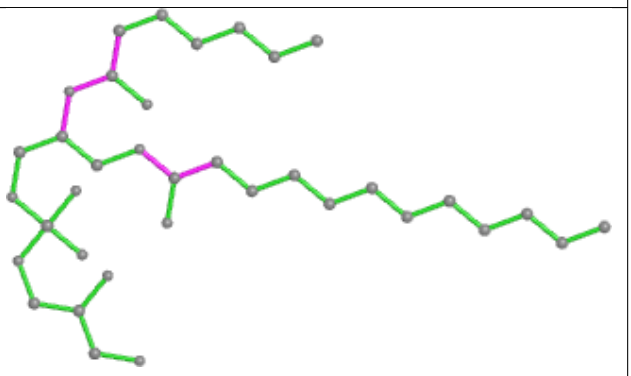


Rings

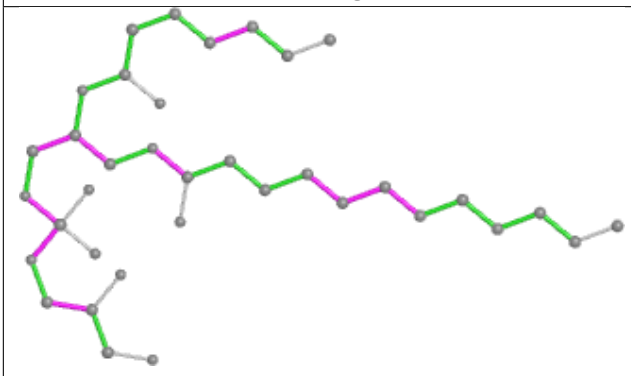
Ligand PGV M 402



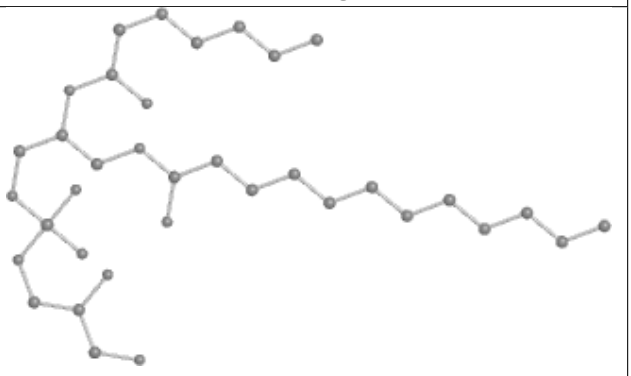
Bond lengths



Bond angles

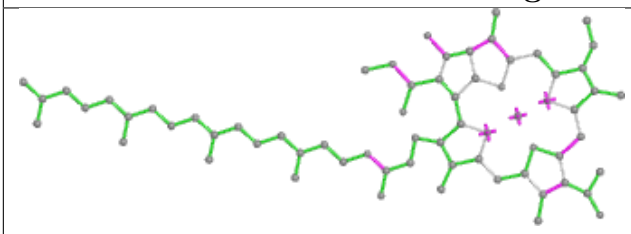


Torsions



Rings

Ligand BCL N 102



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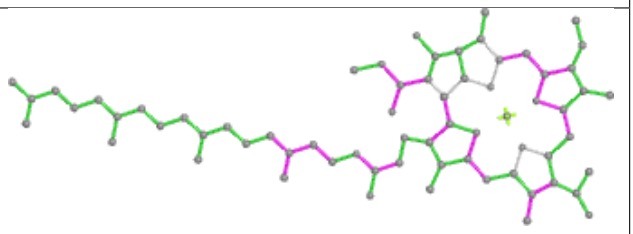
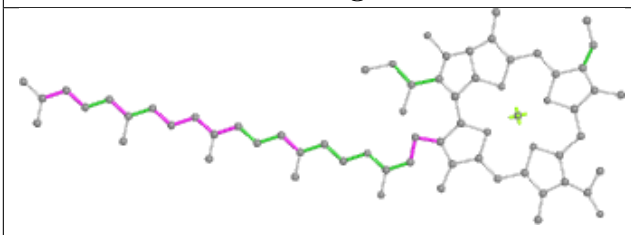
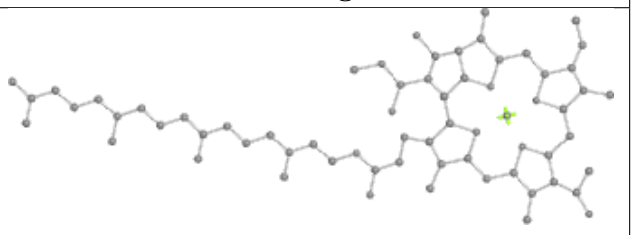


Bond angles

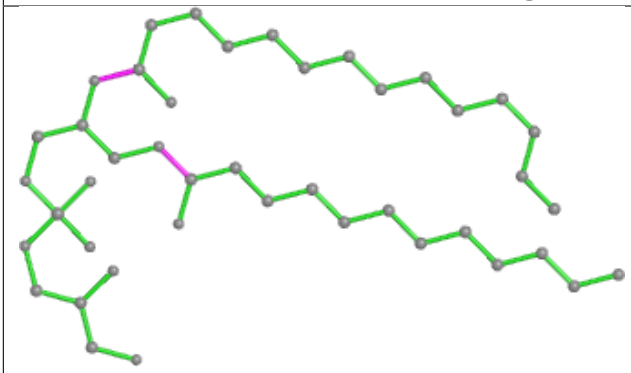


Torsions

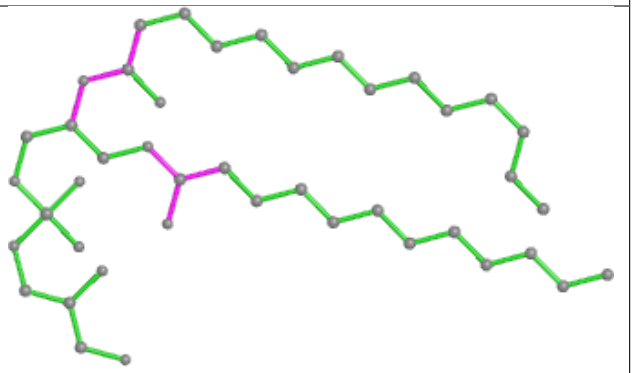


Rings

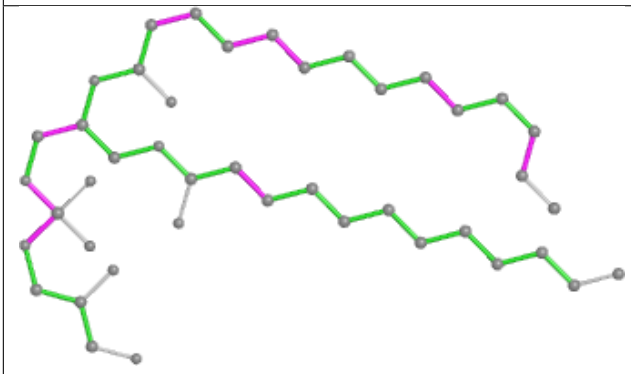
Ligand PGV H 303



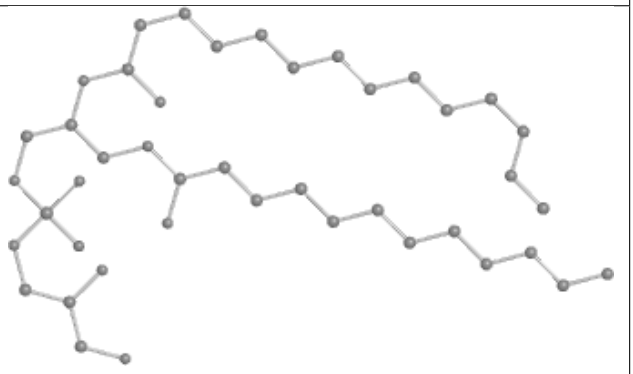
Bond lengths



Bond angles

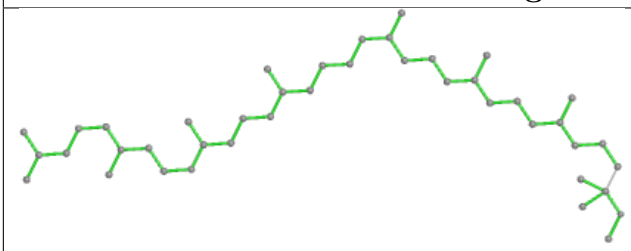


Torsions

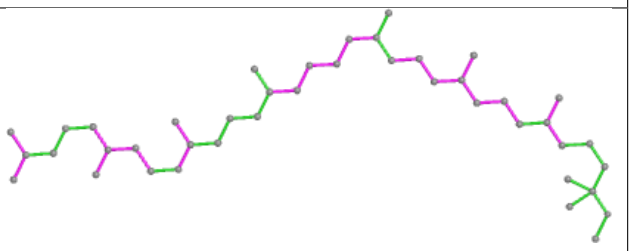


Rings

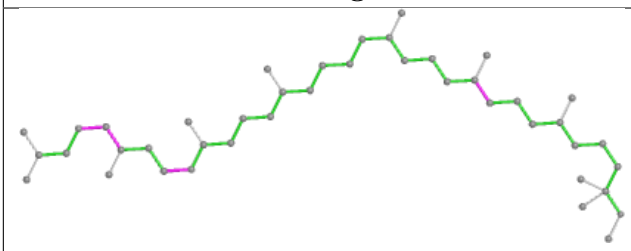
Ligand SPO D 103



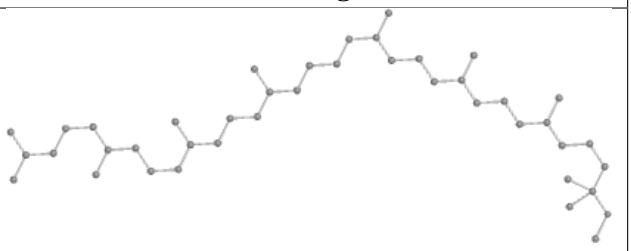
Bond lengths



Bond angles

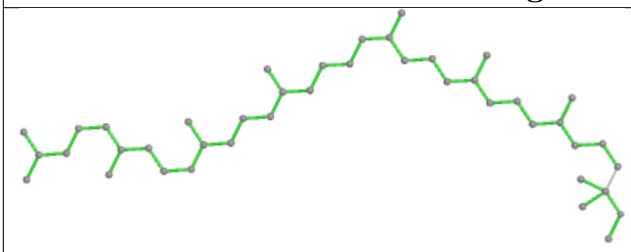


Torsions

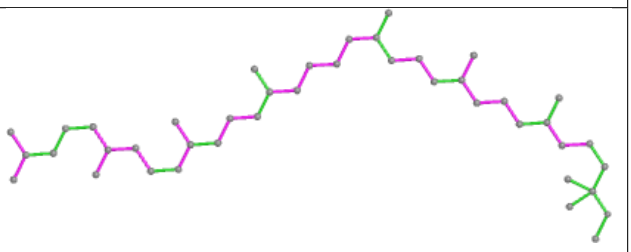


Rings

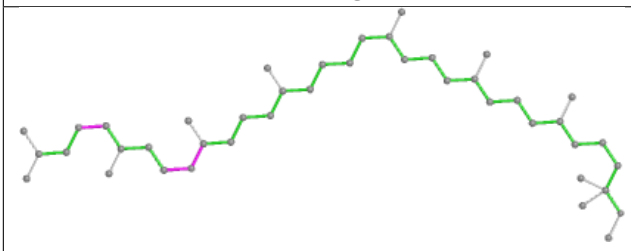
Ligand SPO T 101



Bond lengths



Bond angles



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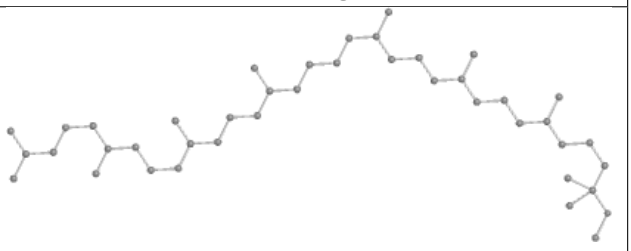
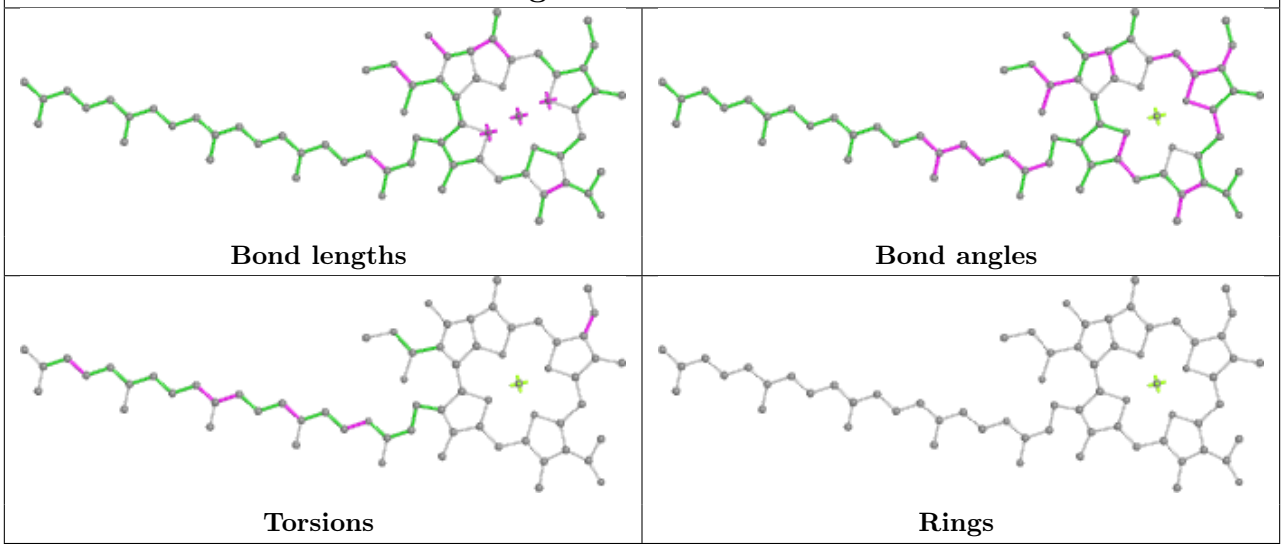
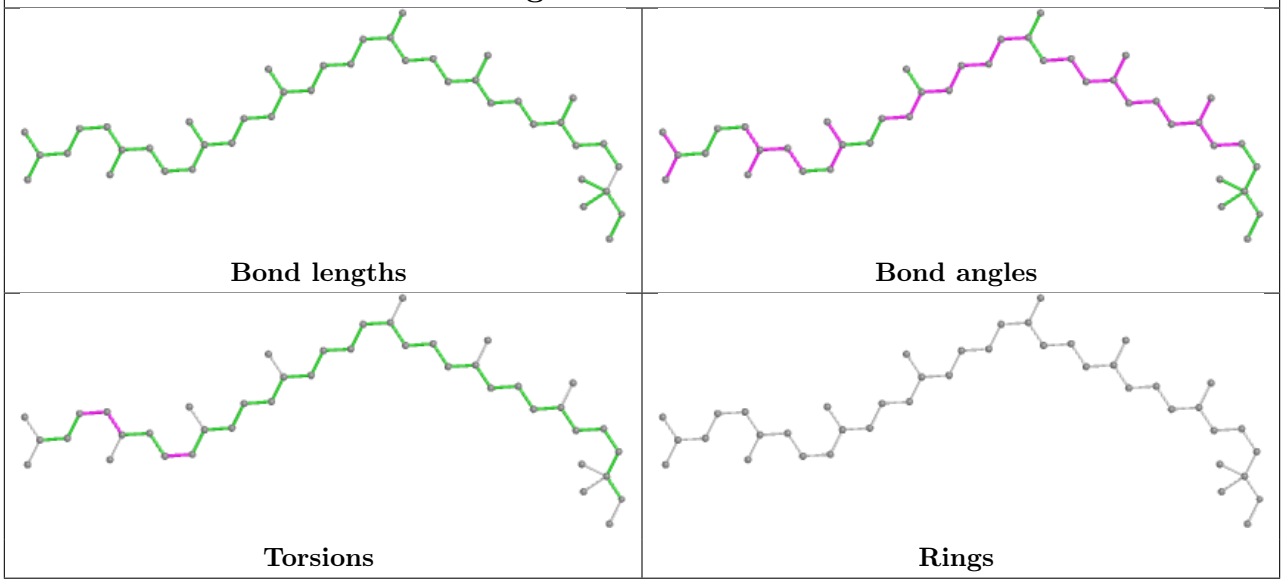


Rings

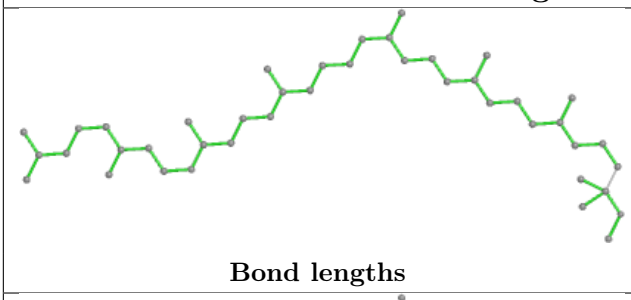
Ligand BCL S 103



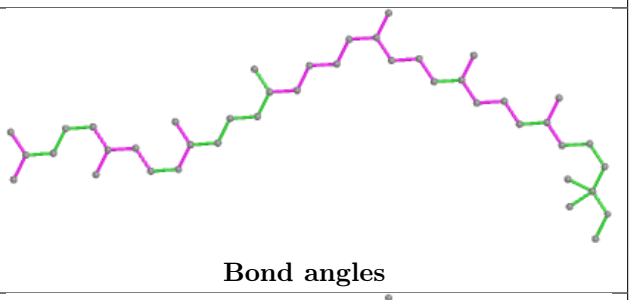
Ligand SPO O 104



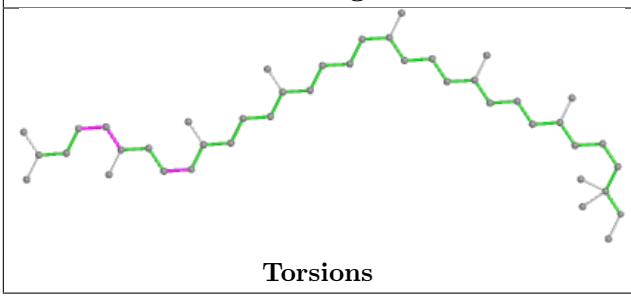
Ligand SPO I 103



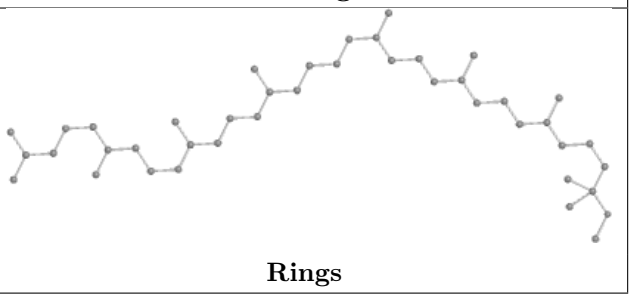
Bond lengths



Bond angles

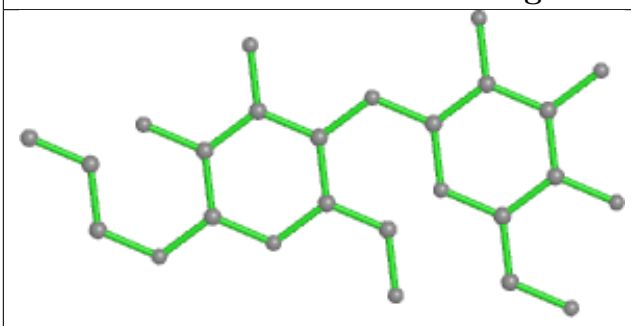


Torsions

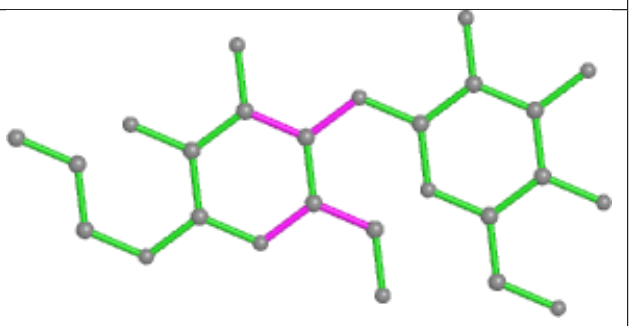


Rings

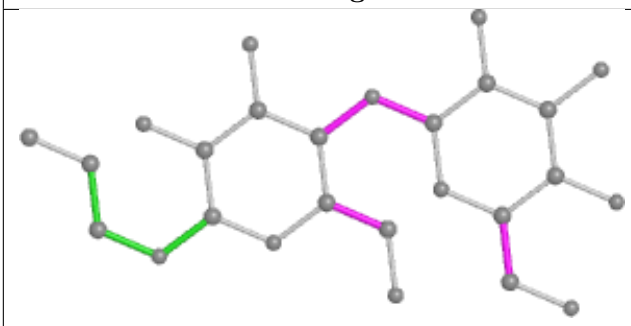
Ligand LMT S 101



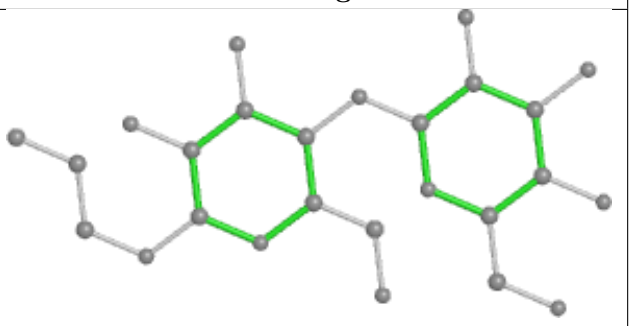
Bond lengths



Bond angles

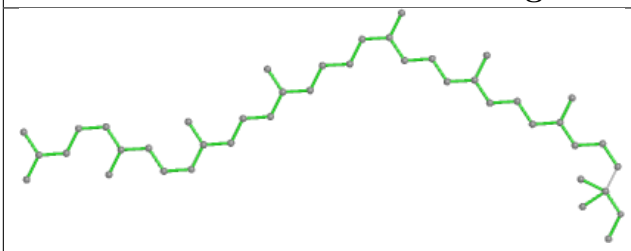


Torsions

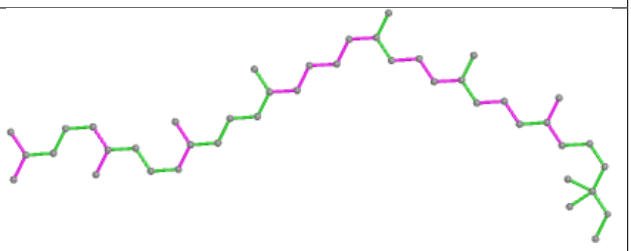


Rings

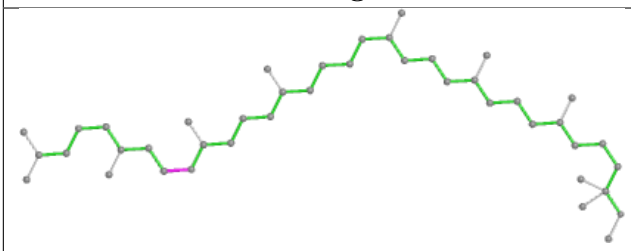
Ligand SPO O 103



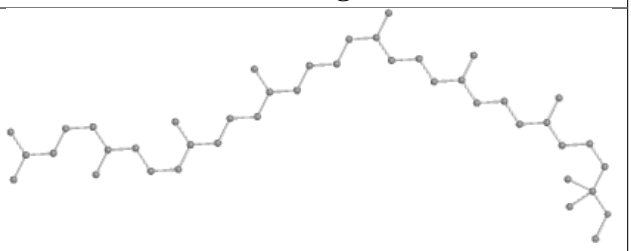
Bond lengths



Bond angles

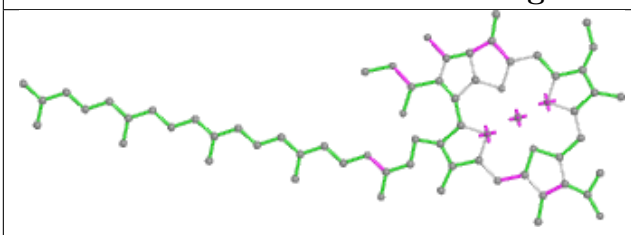


Torsions

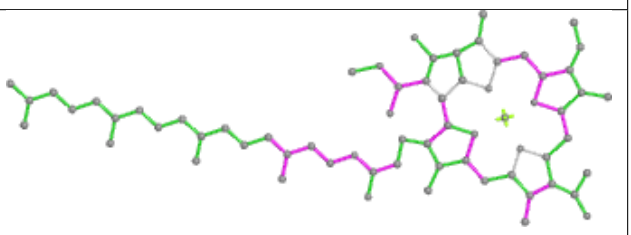


Rings

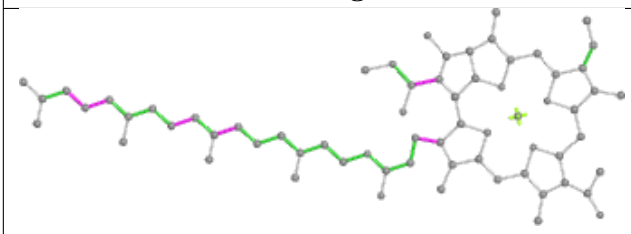
Ligand BCL L 310



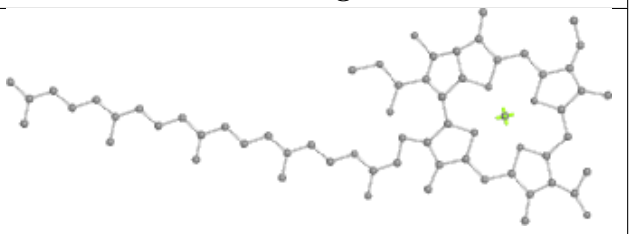
Bond lengths



Bond angles

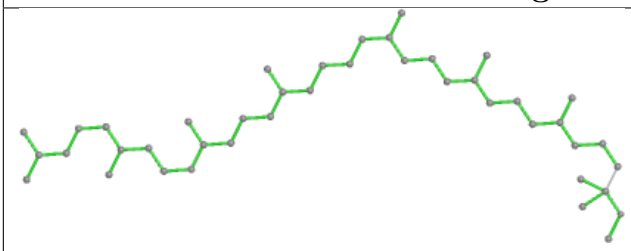


Torsions

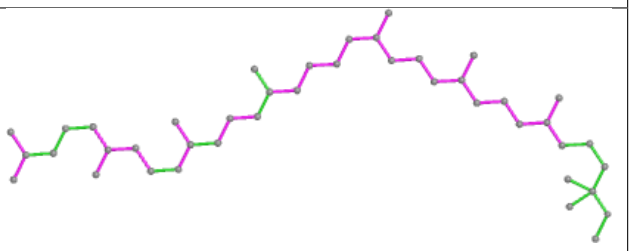


Rings

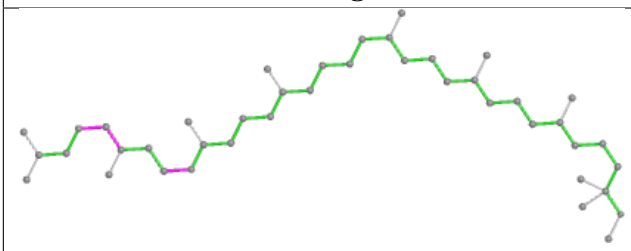
Ligand SPO I 104



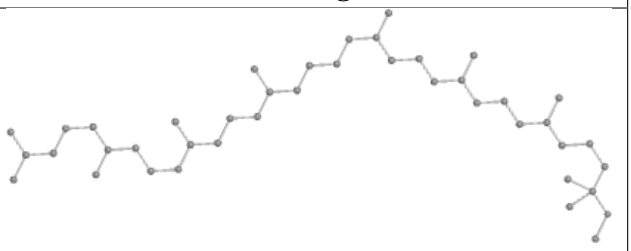
Bond lengths



Bond angles

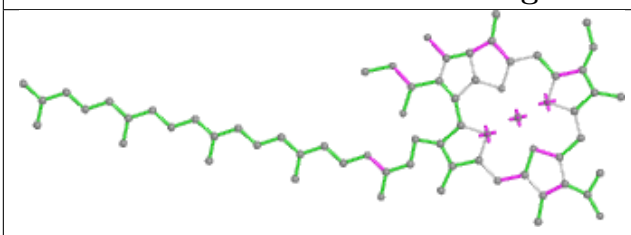


Torsions

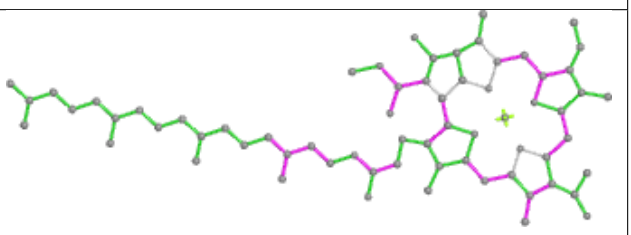


Rings

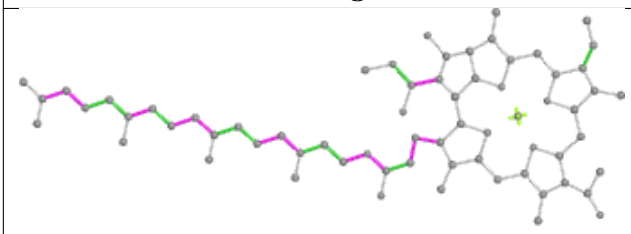
Ligand BCL M 403



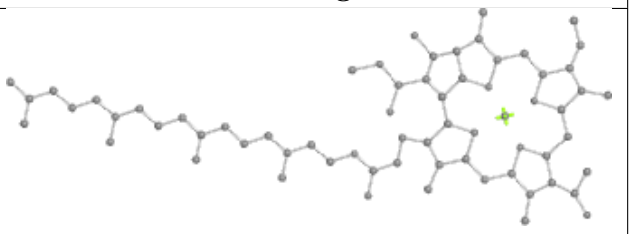
Bond lengths



Bond angles

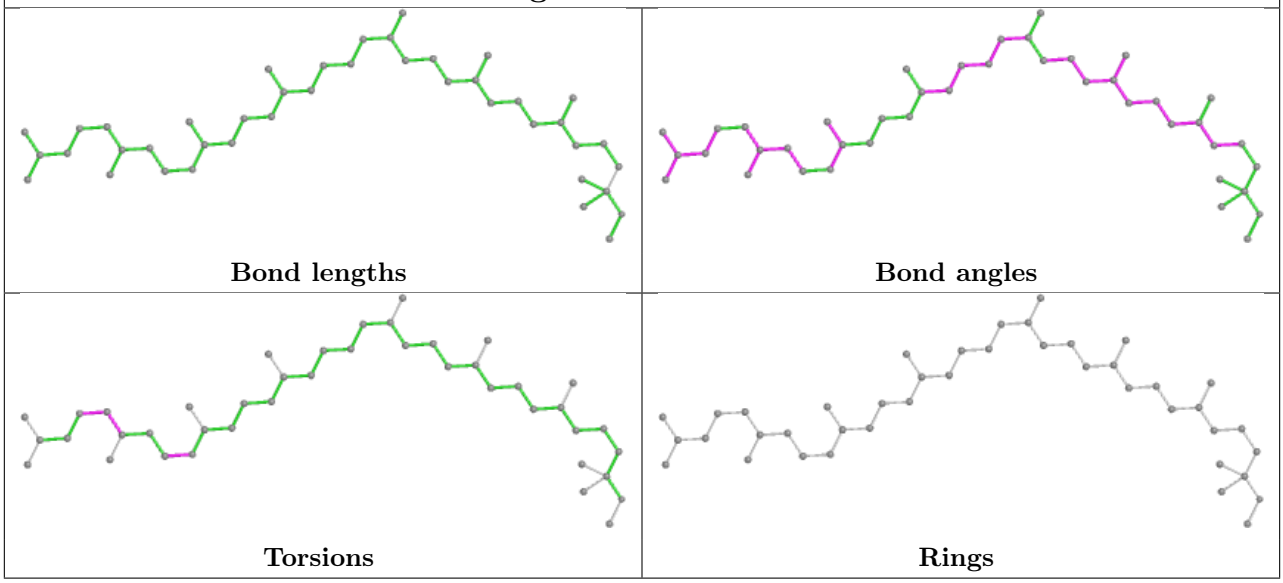


Torsions

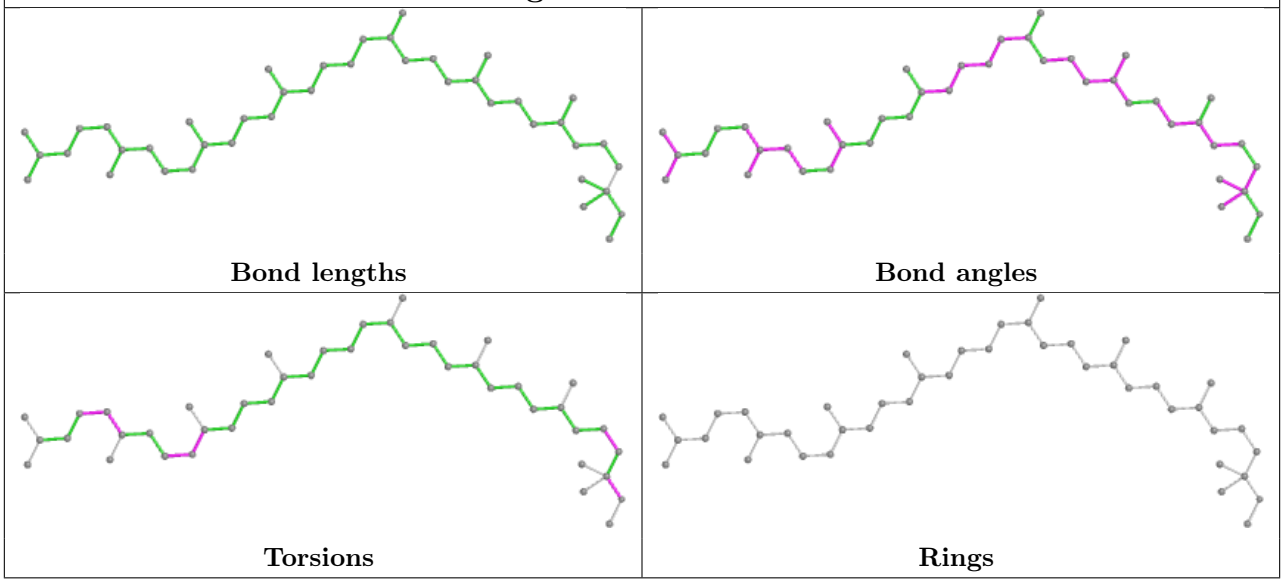


Rings

Ligand SPO S 104



Ligand SPO R 101



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.

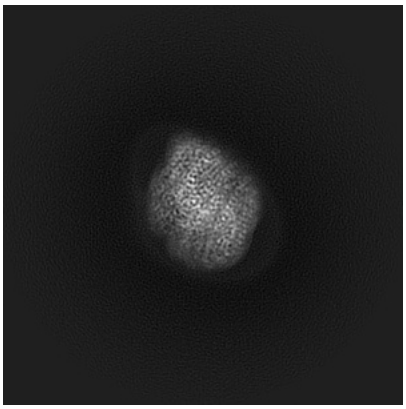
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33931. These allow visual inspection of the internal detail of the map and identification of artifacts.

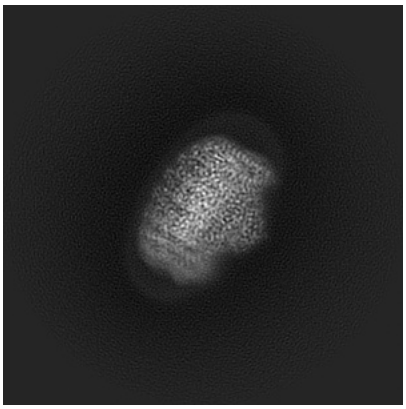
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

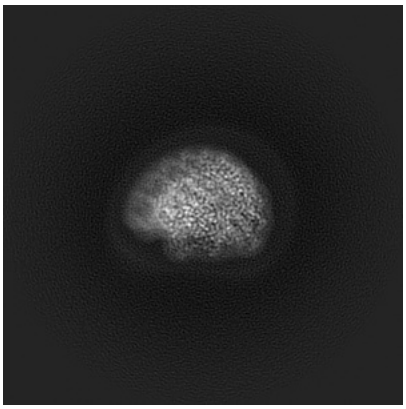
6.1.1 Primary map



X

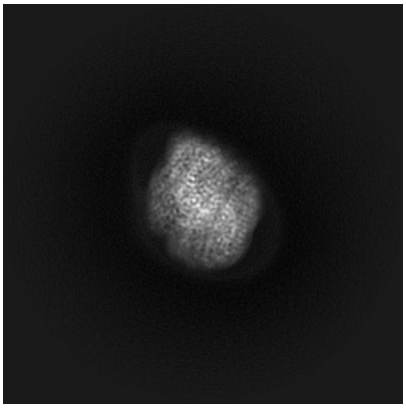


Y

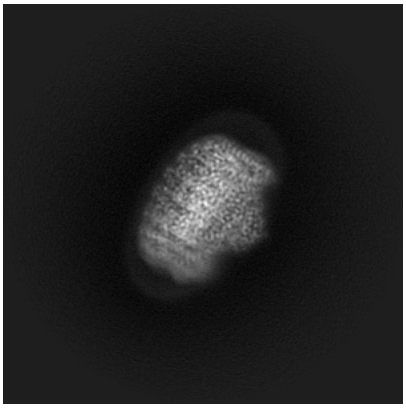


Z

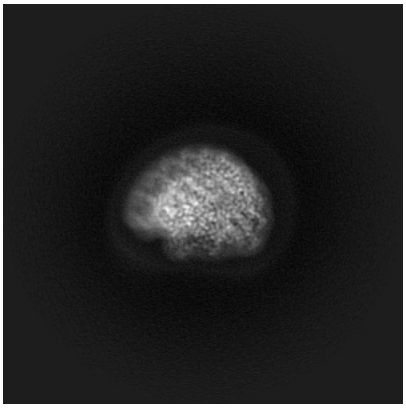
6.1.2 Raw map



X



Y

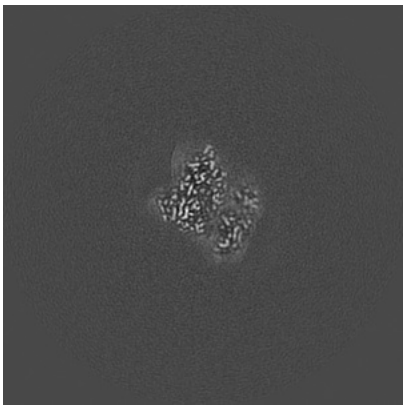


Z

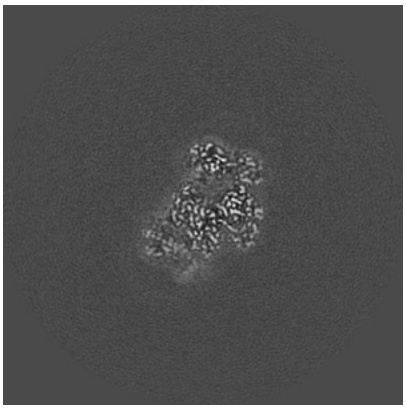
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

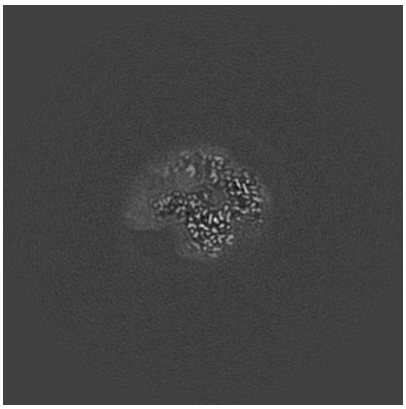
6.2.1 Primary map



X Index: 200

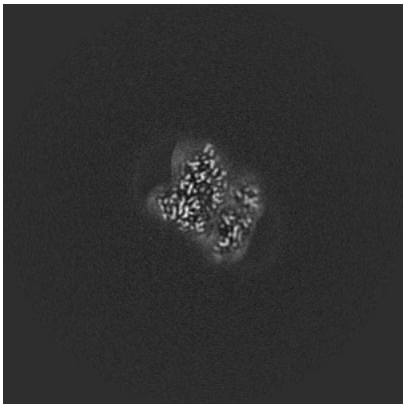


Y Index: 200

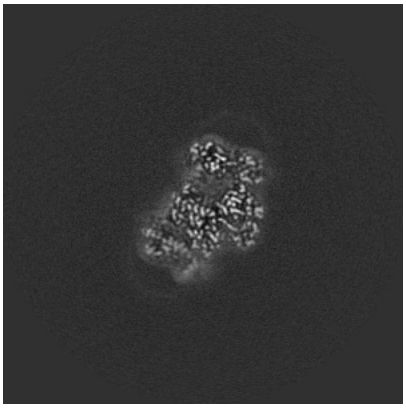


Z Index: 200

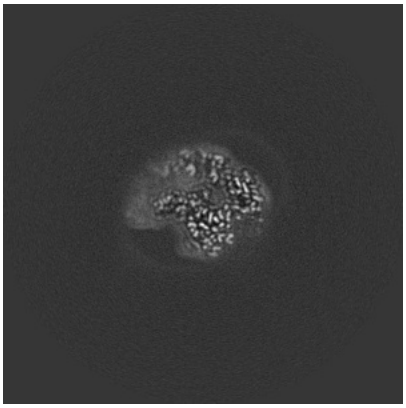
6.2.2 Raw map



X Index: 200



Y Index: 200

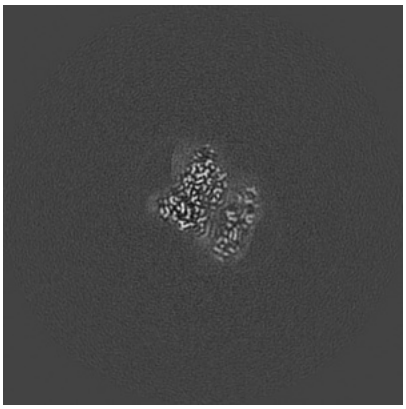


Z Index: 200

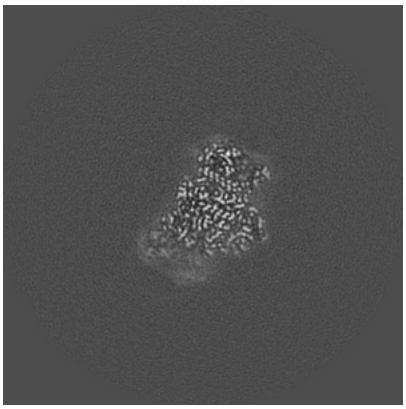
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

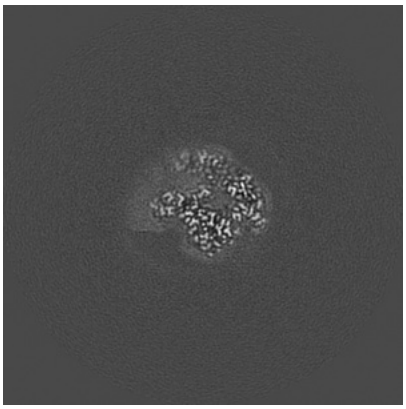
6.3.1 Primary map



X Index: 198

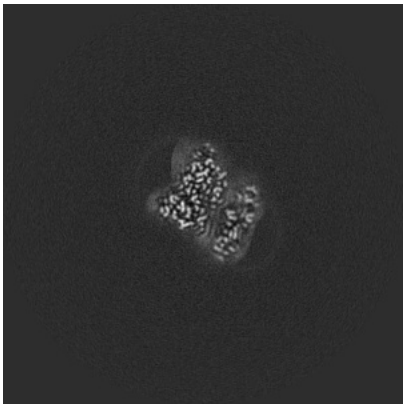


Y Index: 190

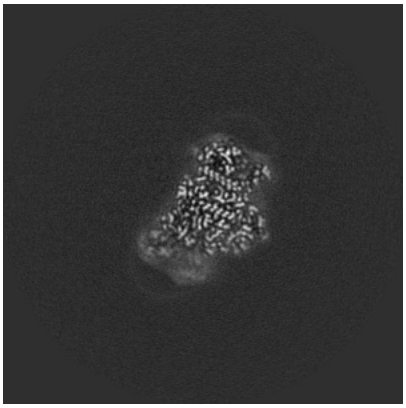


Z Index: 203

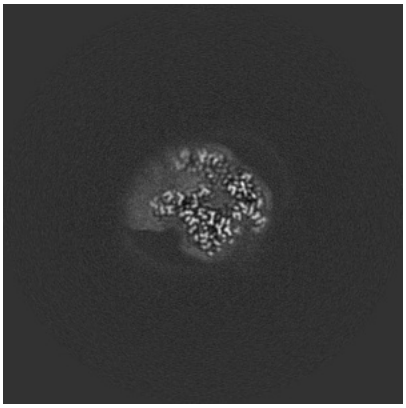
6.3.2 Raw map



X Index: 198



Y Index: 190

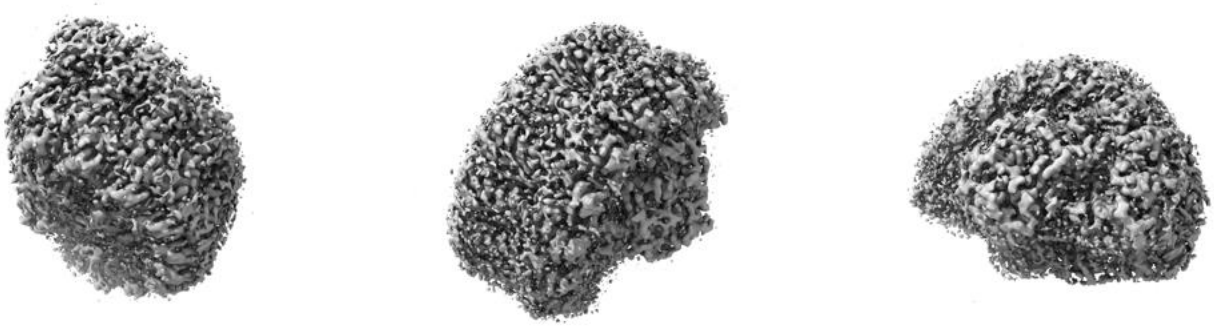


Z Index: 203

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

6.4 Orthogonal surface views (i)

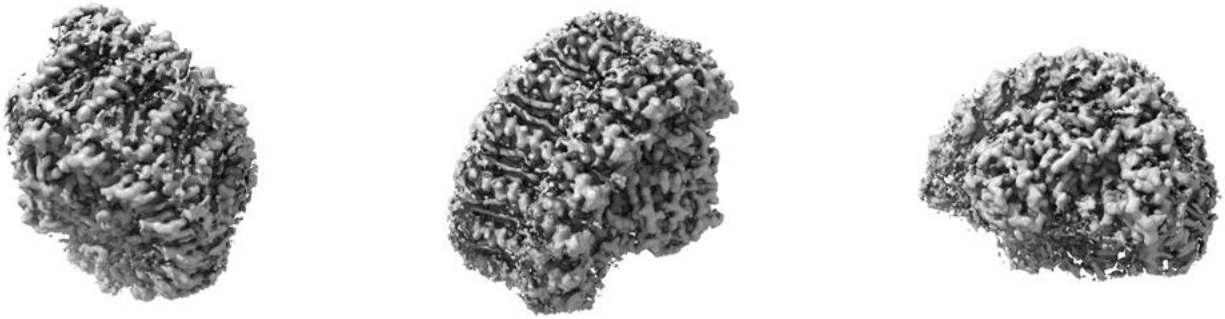
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

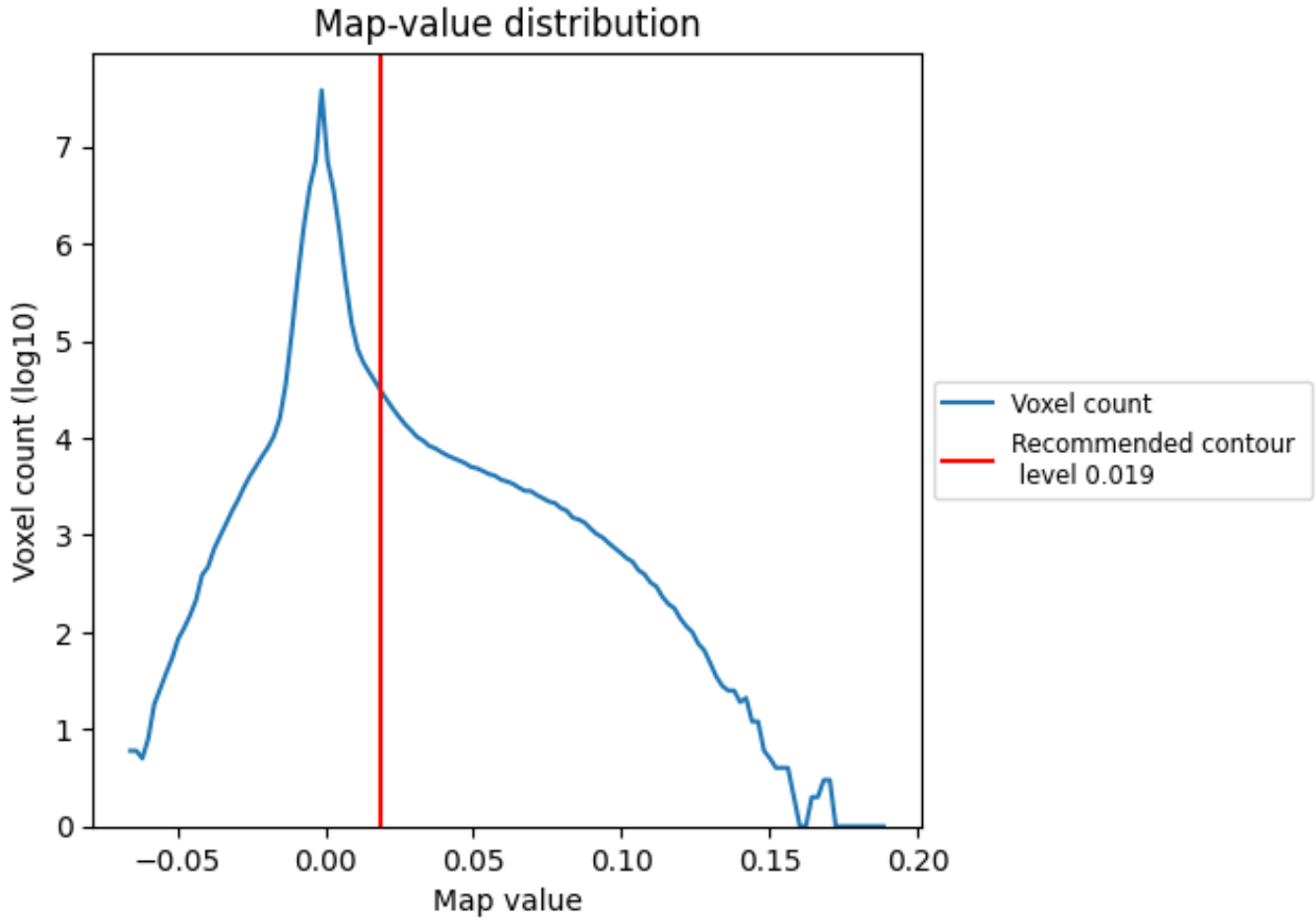
6.5 Mask visualisation (i)

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

7 Map analysis

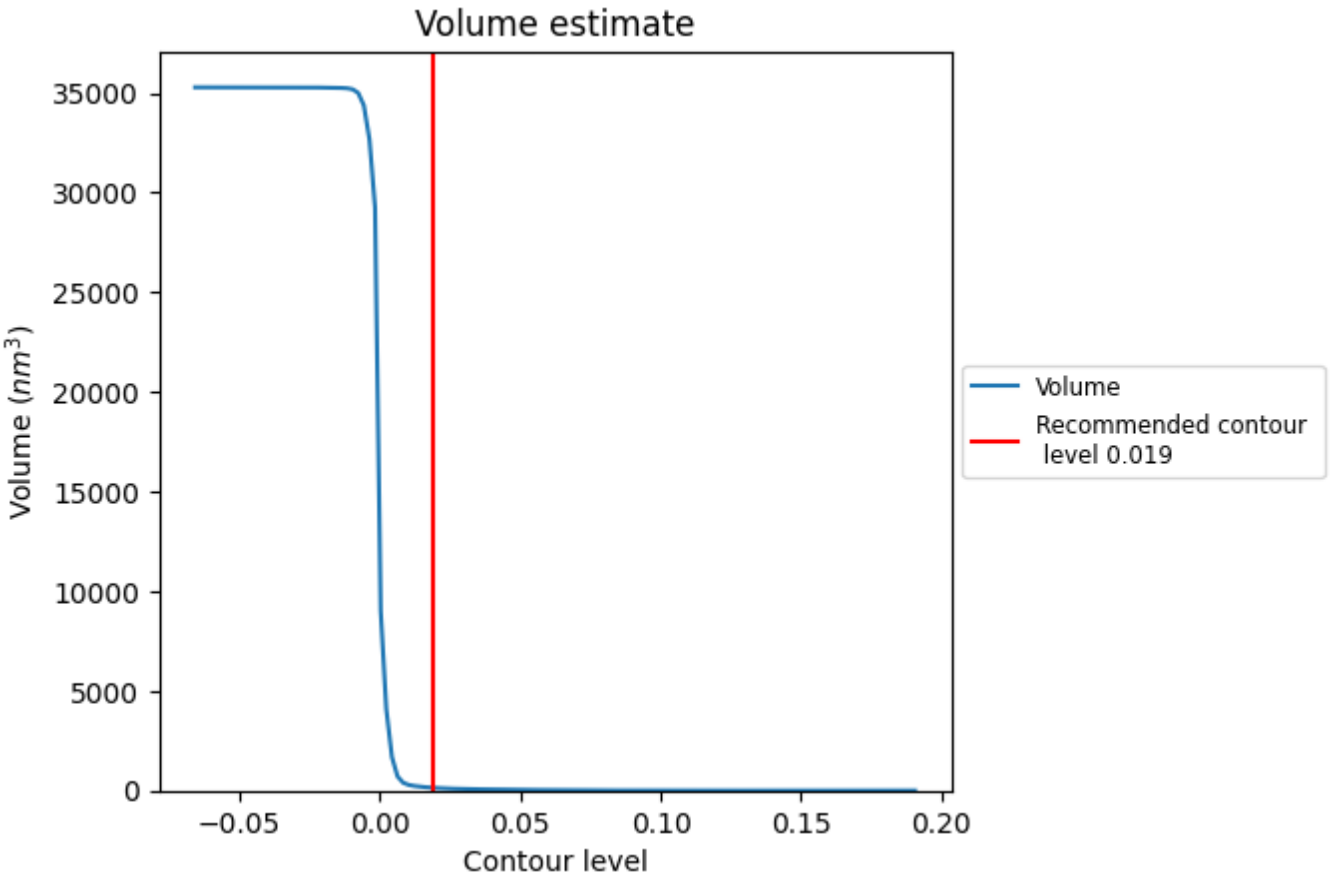
This section contains the results of statistical analysis of the map.

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.

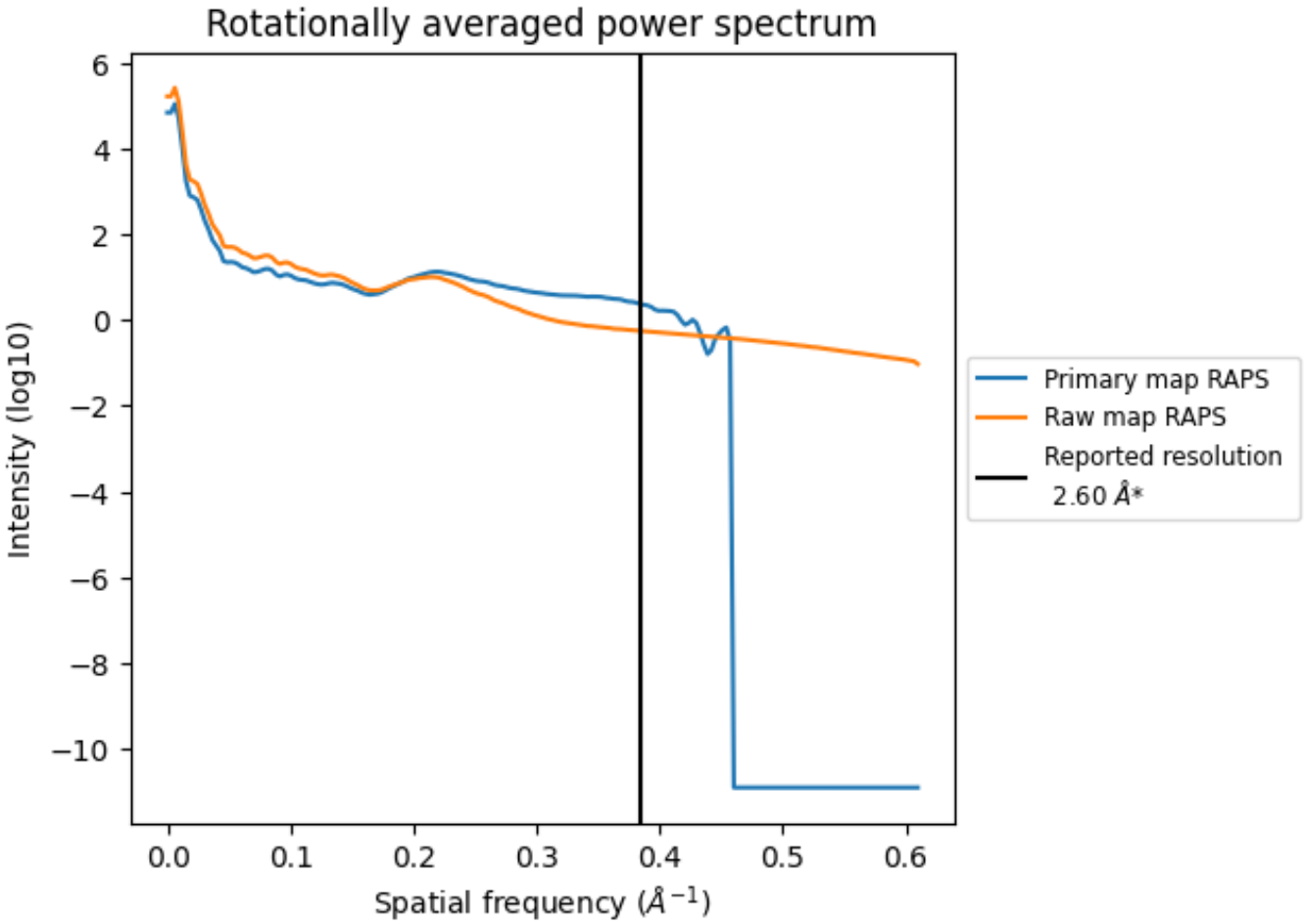
7.2 Volume estimate



The volume at the recommended contour level is 139 nm^3; this corresponds to an approximate mass of 125 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)

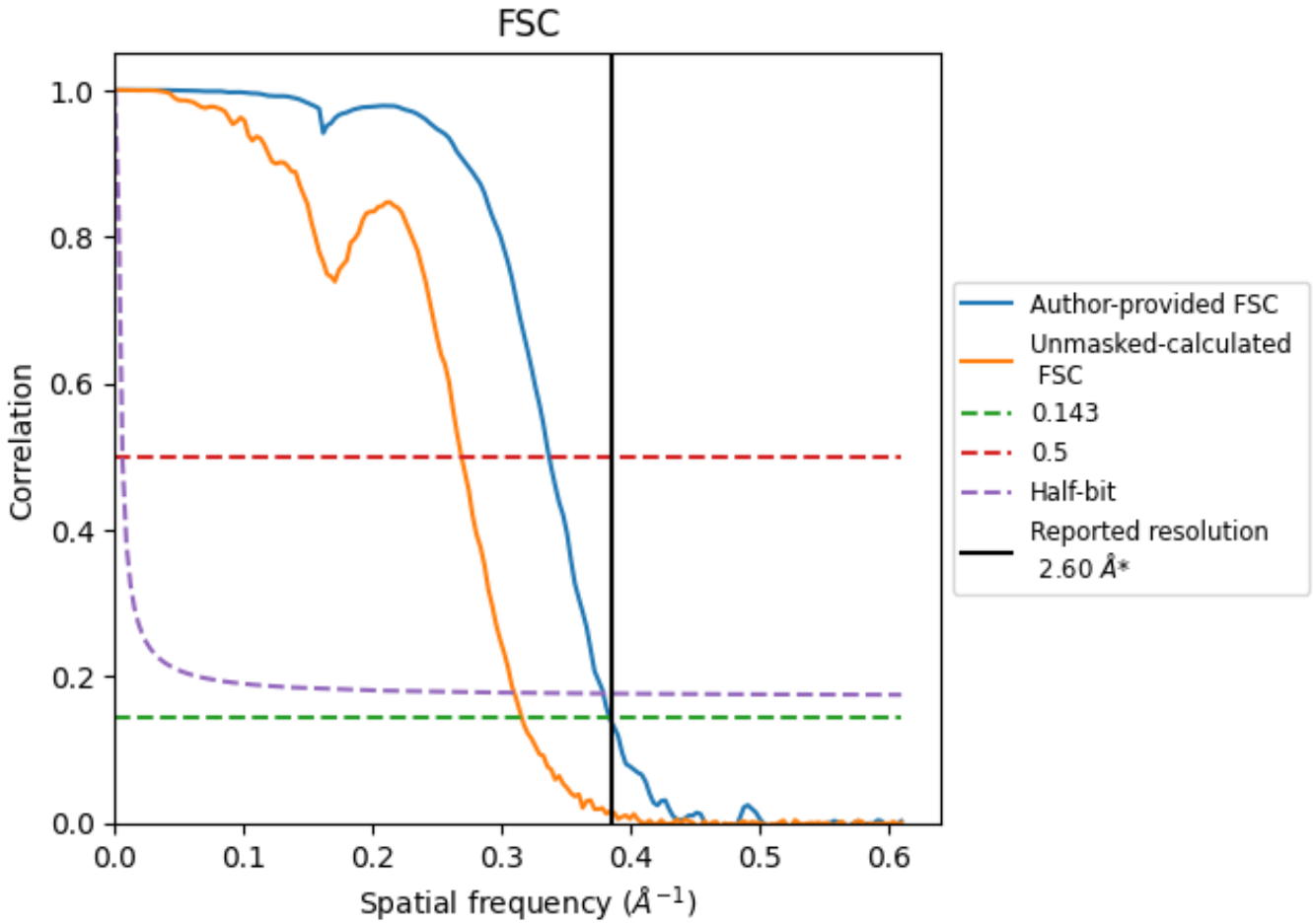


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

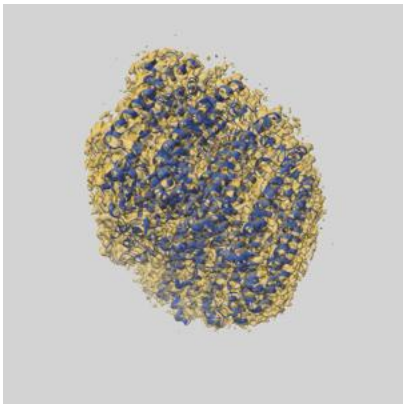
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	2.97	2.64
Unmasked-calculated*	3.17	3.72	3.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.17 differs from the reported value 2.6 by more than 10 %

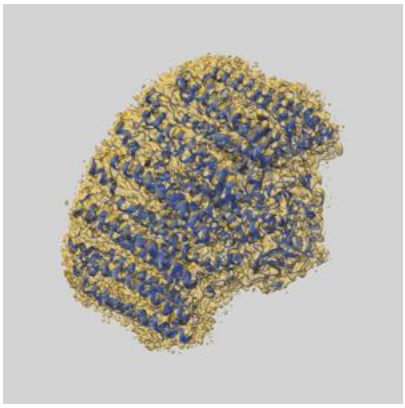
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33931 and PDB model 7YML. Per-residue inclusion information can be found in section 3 on page 15.

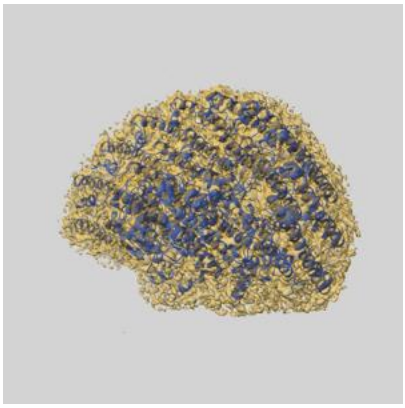
9.1 Map-model overlay



X



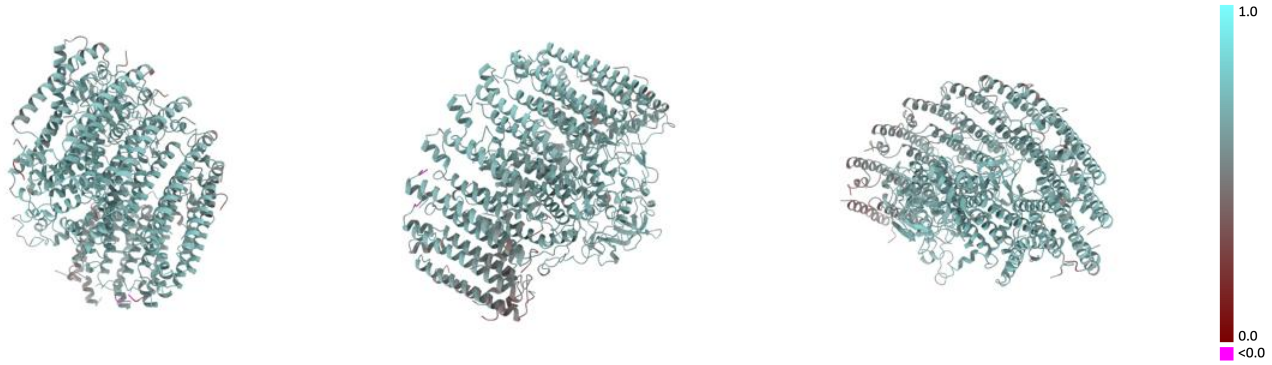
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 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.

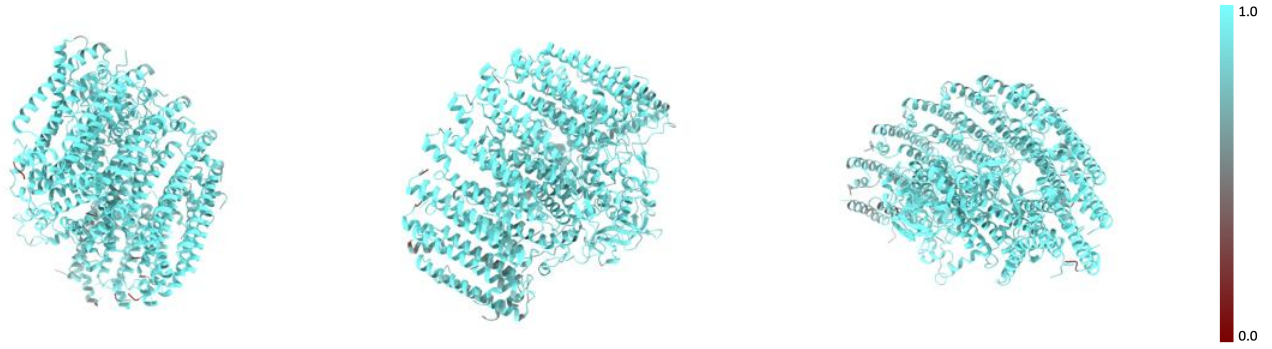
9.2 Q-score mapped to coordinate model



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.

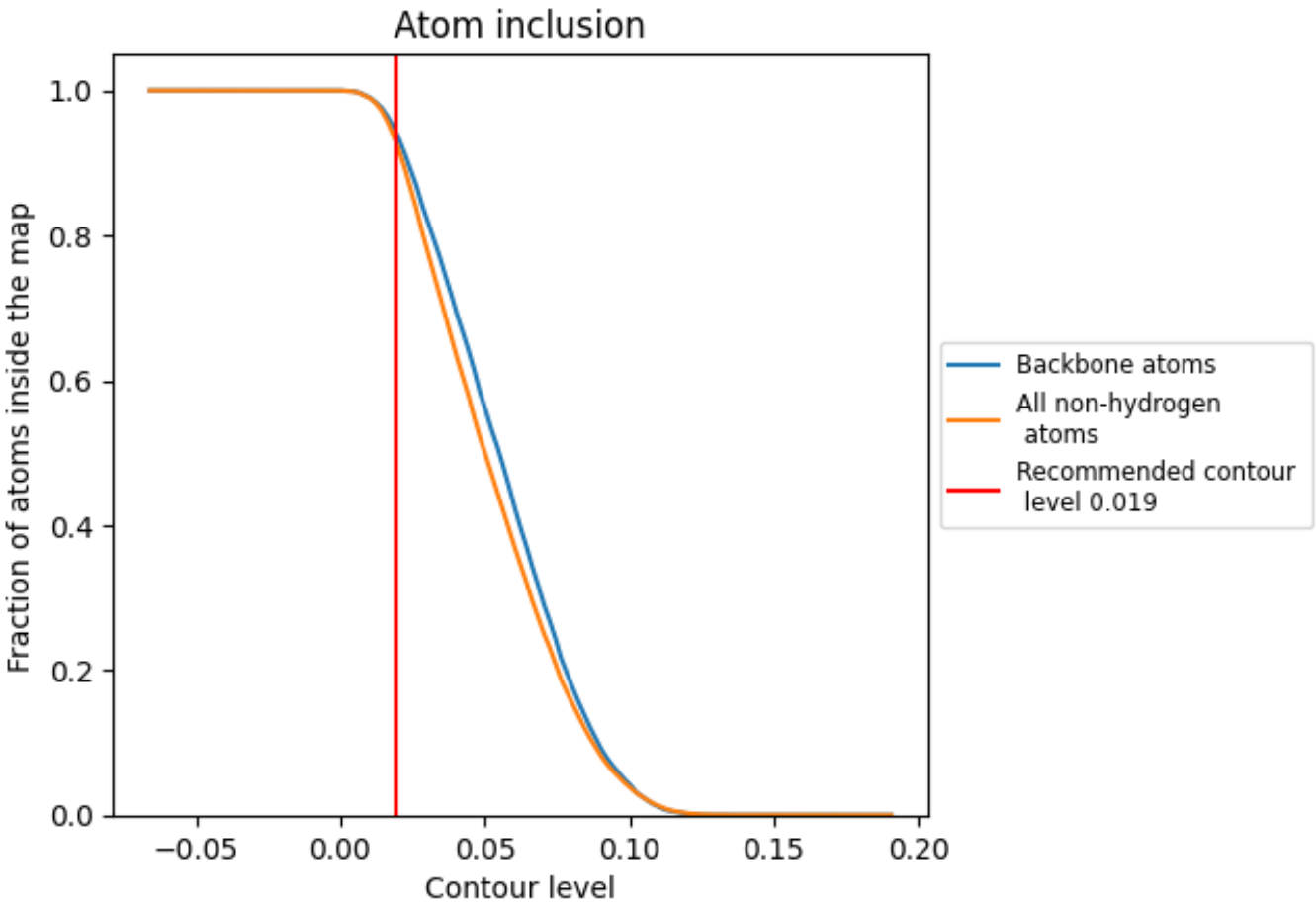
9.3 Atom inclusion mapped to coordinate model



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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9316	0.6130
A	0.9605	0.6030
B	0.9355	0.5990
D	0.9525	0.6350
E	0.9483	0.6210
F	0.9726	0.6430
G	0.9657	0.6390
H	0.9476	0.6270
I	0.9381	0.6340
J	0.9553	0.6250
K	0.9649	0.6230
L	0.9632	0.6550
M	0.9585	0.6470
N	0.9314	0.6180
O	0.9357	0.6260
P	0.9314	0.6000
Q	0.8920	0.5800
R	0.9192	0.5840
S	0.8879	0.5580
T	0.9039	0.5780
V	0.8532	0.5280
W	0.8603	0.5320
X	0.9325	0.6100
Y	0.7175	0.4540
Z	0.6655	0.3590