

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_li191b2\_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: mo\_li191b2\_0m

---

Bond precision:      C-C = 0.0061 Å      Wavelength=0.71073

Cell:                      a=10.1995 (5)                      b=12.2974 (6)                      c=31.3504 (16)  
                              alpha=79.558 (2)                      beta=86.966 (2)                      gamma=84.479 (2)  
Temperature:              100 K

	Calculated	Reported
Volume	3846.6 (3)	3846.6 (3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C150.52 H178.30 N16 O15, 0.5 (C2 H5 O), 0.24 (C2 H5), 0.5 (O) [+ s	C150.52 H178.3 N16 O15, 0.24 (C2 H5), 0.5 (C2 H5 O), 0.5 (O)
Sum formula	C152 H182 N16 O16 [+ solvent]	C152 H182 N16 O16
Mr	2489.15	2489.12
Dx, g cm <sup>-3</sup>	1.075	1.075
Z	1	1
Mu (mm <sup>-1</sup> )	0.070	0.070
F000	1334.0	1334.0
F000'	1334.54	
h, k, lmax		12, 14, 37
Nref		13372
Tmin, Tmax	0.990, 0.994	0.615, 0.745
Tmin'	0.989	

Correction method= # Reported T Limits: Tmin=0.615 Tmax=0.745  
AbsCorr = MULTII-SCAN

Data completeness=                      Theta (max)= 25.050

R(reflections)= 0.0978( 7256)

wR2(reflections)=  
0.3016( 13372)

S = 1.053

Npar= 859

The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.



### Alert level C

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75

The relevant atom site should be identified.

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25) .....	0.30	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	0.71	eA-3
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.6	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	4.8	Ratio
PLAT221_ALERT_2_C	Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range	5.1	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.5	Ratio
PLAT223_ALERT_4_C	Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range	6.2	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C01R	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang) .....	01	Check
PLAT329_ALERT_4_C	Carbon Atom Hybridisation Unclear for .....	C020	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00609	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	3.211	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.081	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & Sth/L= 0.596	232	Report
	-5 12 0, -4 12 0, 3-12 1, 4-12 1, 5-12 1, -9-10 1,		
	2 0 1, 2 1 1, -1 2 1, -4 12 1, -2 14 1, 1-14 2,		
	-4-13 2, 4-12 2, 2 0 2, -9 8 2, -2 14 2, 4-12 3,		
	5-12 3, 6-11 3, -1 -2 3, 2 -1 3, -2 2 3, 4-12 4,		
	5-12 4, 5-11 4, 6-11 4, 8 -7 4, 4-12 5, 5-12 5,		
	4-11 5, 5-11 5, 6-11 5, 7-10 5, 1 2 5, -4 13 5,		
	-2 14 5, -5-12 6, 4-12 6, 6-11 6, 7-10 6, 10 -4 6,		
	1 1 6, 9 10 6, -5 12 6, -4 12 6, -4 13 6, -2 13 6,		
	-2 14 6, 4-12 7, 4-11 7, 5-11 7, 6-11 7, 7-10 7,		
	0 2 7, -4 13 7, -2 13 7, -5-11 8, 5-11 8, 6-11 8,		
	7-10 8, -8 1 8, 9 5 8, 9 9 8, 10 9 8, 9 10 8,		
	-4 12 8, -4 13 8, -2 14 8, 4-12 9, -5-11 9, 5-11 9,		
	8 -7 9, -10 5 9, 9 5 9, 9 9 9, 10 9 9, 9 10 9,		
	-5 12 9, -4 13 9, 4-11 10, 5-11 10, -3-10 10, 6-10 10,		
	7 -9 10, 9 -5 10, 10 8 10, 8 9 10, 10 9 10, 9 10 10,		
	-5 12 10, -4 13 10, -4-11 11, 5-11 11, 6-10 11, 9 -4 11,		
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....	8	Note
	2 0 1, 2 1 1, -1 2 1, 2 0 2, 2 -1 3, -2 2 3,		
	1 2 5, 0 2 7,		



### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	62	Note
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
	Calc.: C150.52 H178.30 N16 O15, 0.5(C2 H5 O), 0.24(C2 H5), 0.5(O)		
	Rep.: C150.52 H178.30 N16 O15, 0.24(C2 H5), 0.5(C2 H5 O), 0.5(O)		
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.15	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	10	Report

[illegible]

[illegible]

[illegible]

PLAT300_ALERT_4_G	Atom Site Occupancy of H37C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C43	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C02O	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43A	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43B	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43C	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02V	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H02W	Constrained at	0.12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2O	Constrained at	0.25	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )		35%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4 )		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 1 )		359.82	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3 )		0.84	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 4 )		0.25	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O2O	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O004 .		105.3	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O02L .		107.8	Degree
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H00G ..H41B .		1.99	Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H014 ..H33D .		1.99	Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H018 ..H34F .		1.91	Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H010 ..H41B .		1.93	Ang.
		x,y,z =	1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H02N ..H37C .		1.75	Ang.
		x,l+y,z =	1_565	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C02D ..C37 .		3.20	Ang.
		x,l+y,z =	1_565	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure .....			! Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		148	Note
	O001 O002 O003 O004 C005 C006 C007 H007			
	C008 C009 C00A O00B N00C C00D C00E H00A			
	H00B C00G H00G C00H H00H C00I H00I C00J			
	C00K C00L C00M H00M C00N C00O H00C H00D			
	C00P C00Q H00Q C00R C00S H00E H00F C00T			
	C00U C00V N00W C00X H00J H00K C00Y H00L			
	H00N C00Z H00O H00P C010 N011 C012 C013			
	C014 H014 C015 C016 H01A H01B H01C C017			
	C018 H018 N0 C01B C01C H01D O01E C01F			
	H01E H01F H01G N01H C01I H01H H01I H01J			
	C01J H01K H01L H01M C01L H01N H01O H01P			
	C01P H01Q H01R H01S C01R H01W H01X H01Y			
	H01T H01U H01V C0 C01X C020 H02C H02D			
	H02A H02B C023 H02E H02F H02G N025 C027			
	H02H H02I H02J C02C H02K H02L H02M C02D			
	H02N H02O C02I H02P H02Q C02J H02S H02R			
	O02L C02M H02T H02U C02O H02V H02W H1AA			
	H1AB H1BA H1BB H1DA H1DB H1KA H1KB H1KC			
	H1LA H1LB H1MA H1MB			
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		26	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....			! Info
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers		9	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		83	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed			! Info

PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta (Min).	2 Note
	0 0 1, 0 0 2,	
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.4 Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.1 Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	7 Info

---

0	<b>ALERT level A</b>	= Most likely a serious problem - resolve or explain
0	<b>ALERT level B</b>	= A potentially serious problem, consider carefully
16	<b>ALERT level C</b>	= Check. Ensure it is not caused by an omission or oversight
213	<b>ALERT level G</b>	= General information/check it is not something unexpected
4	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
18	ALERT type 2	Indicator that the structure model may be wrong or deficient
25	ALERT type 3	Indicator that the structure quality may be low
180	ALERT type 4	Improvement, methodology, query or suggestion
2	ALERT type 5	Informative message, check

---

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

