

## 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

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Bond precision:	C-C = 0.0061 A	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

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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.

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### ● 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) .....	O1	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,		

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### ● 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 H178.3 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









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). 0 0 1, 0 0 2,	2 Note
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

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
213 **ALERT level G** = 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

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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.

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**PLATON version of 14/11/2023; check.def file version of 14/09/2023**

