

## checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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\_b0483\_0m

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Bond precision:    C-C = 0.0018 A                      Wavelength=0.71073

Cell:                      a=16.8564(9)              b=19.0045(15)              c=20.4178(12)  
                                    alpha=90                      beta=90                      gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	6540.8(7)	6540.8(7)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C26 H58 Li4 N2 O6	C26 H58 Li4 N2 O6
Sum formula	C26 H58 Li4 N2 O6	C26 H58 Li4 N2 O6
Mr	522.50	522.50
Dx,g cm-3	1.061	1.061
Z	8	8
Mu (mm-1)	0.071	0.071
F000	2304.0	2304.0
F000'	2304.96	
h,k,lmax	21,24,26	21,24,26
Nref	7146	7136
Tmin,Tmax	0.986,0.989	0.695,0.746
Tmin'	0.966	

Correction method= # Reported T Limits: Tmin=0.695 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.999                      Theta(max)= 27.000

R(reflections)= 0.0390( 5474)              wR2(reflections)= 0.1020( 7136)

S = 1.026                      Npar= 386

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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 G

PLAT303_ALERT_2_G	Full Occupancy H-Atom H21	with # Connections	2.00	Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C21	Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C24	Check
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C21 - C22 ..	1.53 Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C21 - C23 ..	1.53 Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C24 - C25 ..	1.53 Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond	C24 - C26 ..	1.53 Ang.
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.	1.18	Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #		40	Check
	O3 -C8 -LI1	1.555 1.555 1.555	44.59	Deg.
PLAT793_ALERT_4_G	The Model has Chirality at N1	(Centro SPGR)		S Verify
PLAT933_ALERT_2_G	Number of OMIT records in Embedded RES .....			5 Note

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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  
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
11 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
8 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
0 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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