

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3182

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: 3182

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Bond precision:	C-C = 0.0083 A	Wavelength=0.71073
Cell:	a=20.3421(14)      b=10.7413(5)      c=21.0670(16)	
	alpha=90      beta=112.664(9)      gamma=90	
Temperature:	173 K	
	Calculated	Reported
Volume	4247.7(6)	4247.7(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C28 H68 Li4 O8 Si4	C28 H68 Li4 O8 Si4
Sum formula	C28 H68 Li4 O8 Si4	C28 H68 Li4 O8 Si4
Mr	672.94	672.94
Dx,g cm-3	1.052	1.052
Z	4	4
Mu (mm-1)	0.176	0.176
F000	1472.0	1472.0
F000'	1473.84	
h,k,lmax	24,12,25	24,12,25
Nref	7471	7469
Tmin,Tmax		0.619,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.619 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.000      Theta(max)= 25.000

R(reflections)= 0.0710( 5669)      wR2(reflections)= 0.2057( 7469)

S = 1.134      Npar= 409

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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 B**

PLAT934\_ALERT\_3\_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 2 Check

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**Alert level C**

PLAT053\_ALERT\_1\_C Minimum Crystal Dimension Missing (or Error) ... Please Check  
PLAT054\_ALERT\_1\_C Medium Crystal Dimension Missing (or Error) ... Please Check  
PLAT055\_ALERT\_1\_C Maximum Crystal Dimension Missing (or Error) ... Please Check  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C18 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Si4 Check  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00833 Ang.  
PLAT790\_ALERT\_4\_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note  
C28 H68 Li4 O8 Si4  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 7.388 Check  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 2.017 Check  
PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check  
PLAT978\_ALERT\_2\_C Number C-C Bonds with Positive Residual Density 0 Note

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**Alert level G**

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 6.78 Why ?  
PLAT764\_ALERT\_4\_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.12 Ratio  
PLAT909\_ALERT\_3\_G Percentage of Observed Data at Theta(Max) Still 51 %  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min) 2 Note  
PLAT955\_ALERT\_1\_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
1 **ALERT level B** = A potentially serious problem, consider carefully  
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
5 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
4 ALERT type 2 Indicator that the structure model may be wrong or deficient  
7 ALERT type 3 Indicator that the structure quality may be low  
2 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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**PLATON version of 06/05/2016; check.def file version of 05/05/2016**

