

## 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: I

Bond precision: S-P = 0.0287 Å Wavelength=1.54056

Cell: a=10.51452(6) b=10.51452(6) c=6.59148(8)  
alpha=90 beta=90 gamma=120  
Temperature: 298 K

	Calculated	Reported
Volume	631.092(12)	631.092(10)
Space group	P 3 2 1	P 3 2 1
Hall group	P 3 2 "	P 3 2 "
Moiety formula	P2 S6, 4(Li)	P2 S6, 4(Li)
Sum formula	Li4 P2 S6	Li4 P2 S6
Mr	282.06	282.07
Dx, g cm <sup>-3</sup>	2.227	2.230
Z	3	3
Mu (mm <sup>-1</sup> )	17.600	17.929
F000	414.0	0.0
F000'	421.98	
h,k,lmax	13,13,8	8,8,6
Nref	971[ 565]	220
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.39/0.23 Theta(max)= 89.200

$$R(\text{reflections}) = \text{wR2}(\text{reflections}) =$$

S = Npar =

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

REFI015\_ALERT\_1\_C \_refine\_ls\_shift/su\_max is missing  
Maximum shift/s.u. ratio after final refinement cycle.  
The following tests will not be performed  
SHFSU\_01

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### 🟢 Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In,Ka	1.54056 Ang.
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elel	63 80 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elel	m 80 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elel	m 80 %Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elel	m 80 %Fit
PLAT113_ALERT_2_G	Suggests Possible Pseudo/New Space Group	P63mc Check
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	2 Units
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	4 Info
PLAT981_ALERT_1_G	No non-zero f" Anomalous Scattering Values Found	Please Check
PLAT986_ALERT_1_G	No non-zero f' Anomalous Scattering Values Found	Please Check

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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  
1 **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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
5 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  
2 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## checkCIF publication errors

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### 🟢 Alert level G

PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or empty.

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0 **ALERT level A** = Data missing that is essential or data in wrong format  
1 **ALERT level G** = General alerts. Data that may be required is missing

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## Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in *Acta Crystallographica Section C* or *E*, you should upload your CIF via the web. If you wish to submit your CIF for publication in *IUCrData* you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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### PLATON version of 23/04/2018; check.def file version of 23/04/2018

Datablock I - ellipsoid plot

