

# 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: b0988

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Bond precision:	C-C = 0.0025 A	Wavelength=0.71073
Cell:	a=21.4528(12)      b=17.1385(8)      c=20.4255(11)	alpha=90      beta=115.646(2)      gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	6770.0(6)	6770.0(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C20 H54 Li4 N O Si4, K	C40 H108 K2 Li8 N2 O2 Si8
Sum formula	C20 H54 K Li4 N O Si4	C40 H108 K2 Li8 N2 O2 Si8
Mr	503.86	1007.72
Dx,g cm-3	0.989	0.989
Z	8	4
Mu (mm-1)	0.309	0.309
F000	2208.0	2208.0
F000'	2212.58	
h,k,lmax	31,24,29	31,24,29
Nref	21582	21569
Tmin,Tmax	0.849,0.886	0.684,0.747
Tmin'	0.849	

Correction method= # Reported T Limits: Tmin=0.684 Tmax=0.747  
AbsCorr = MULTI-SCAN

Data completeness= 0.999      Theta(max)= 31.000

R(reflections)= 0.0421( 18107)      wR2(reflections)= 0.1162( 21569)

S = 1.044      Npar= 651

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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**

PLAT049_ALERT_1_B	Calculated Density Less Than 1.0 gcm-3 .....	0.9887	Check
PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density	2.19	eA-3
PLAT230_ALERT_2_B	Hirshfeld Test Diff for N2 --C22 .	9.6	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for N2 --C23 .	7.7	s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for N2 --C24 .	7.4	s.u.

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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.

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	3.70	Report
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C21 --C22 .	6.7	s.u.

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**Alert level G**

PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF .....		Please Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	2.00	Check
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	15	Note
PLAT303_ALERT_2_G	Full Occupancy Atom H17A with # Connections	2.00	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C9	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C13	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C29	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C33	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.59	Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF .... #	204	Check
	C29 -SI6 -LI7 1.555 1.555 1.555	44.80	Deg.
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2	Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
5 **ALERT level B** = A potentially serious problem, consider carefully  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
12 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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**PLATON version of 23/04/2018; check.def file version of 23/04/2018**

