

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...  
No extractable fcf data in found in CIF

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) xstr1688\_auto

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](#).  
Please wait while processing .... [Interpreting this report](#)

[Structure factor report](#)

Datablock: xstr1688\_auto

Bond precision: C-C = 0.0035 Å Wavelength=1.54184  
Cell: a=8.1570(1) b=13.1534(1) c=20.5029(2)  
alpha=90 beta=90 gamma=90  
Temperature: 151 K

	Calculated	Reported
Volume	2199.80(4)	2199.80(4)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C16 H36 Al2 Li N O5	C16 H36 Al2 Li N O5
Sum formula	C16 H36 Al2 Li N O5	C16 H36 Al2 Li N O5
Mr	383.36	383.37
Dx, g cm-3	1.158	1.158
Z	4	4
Mu (mm-1)	1.382	1.382
F000	832.0	836.0
F000'	835.84	
h,k,lmax	10,16,26	10,16,25
Nref	4763[ 2715]	4652
Tmin,Tmax	0.905,0.933	0.846,1.000
Tmin'	0.871	

Correction method= # Reported T Limits: Tmin=0.846 Tmax=1.000  
AbsCorr = MULTI-SCAN  
Data completeness= 1.71/0.98 Theta(max)= 78.840  
R(reflections)= 0.0416( 4266) wR2(reflections)= 0.1280( 4652)  
S = 1.032 Npar= 250

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](#)  
[STRVA01 ALERT 4 C](#) Flack test results are ambiguous.  
From the CIF: \_refine\_ls\_abs\_structure\_Flack 0.420  
From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 0.040  
[PLAT927 ALERT 1 C](#) Reported and Calculated wR2 Differ by ..... 0.0019 Check

[Alert level G](#)  
[PLAT033 ALERT 4 G](#) Flack x Value Deviates > 3.0 \* sigma from Zero . 0.420 Note  
[PLAT068 ALERT 1 G](#) Reported F000 Differs from Calcd (or Missing)... Please Check  
[PLAT142 ALERT 4 G](#) s.u. on b - Axis Small or Missing ..... 0.00010 Ang.  
[PLAT143 ALERT 4 G](#) s.u. on c - Axis Small or Missing ..... 0.00020 Ang.  
[PLAT720 ALERT 4 G](#) Number of Unusual/Non-Standard Labels ..... 59 Note

Al01	Al02	O003	O004	O005	O006	N008
C009	C00A	H00A	C00B	H00B	C00C	H00C
H00D	H00E	H00F	C00E	H00G	H00H	H00I
H00J	H00K	C00G	H00L	H00M	C00H	H00N
C00I	H00P	H00Q	C00J	H00R	H00S	H00T
H00U	H00V	C00L	H00W	H00X	H00Y	C00M
C00N	H00	Ha	C00O	Hb	Li0P	Hc
He	Hf	Hg				Hd

[PLAT769 ALERT 4 G](#) CIF Embedded Explicitly Supplied Scattering Data Please Note  
[PLAT791 ALERT 4 G](#) Model has Chirality at C00B (Sohncke SpGr) R Verify  
[PLAT912 ALERT 4 G](#) Missing # of FCF Reflections Above Sth/L= 0.600 45 Note  
[PLAT969 ALERT 5 G](#) The 'Henn et al.' R-Factor-gap value ..... 3.847 Note  
Predicted wR2: Based on Sigi\*\*2 3.33 or SHELX Weight 12.40  
[PLAT978 ALERT 2 G](#) Number C-C Bonds with Positive Residual Density. 0 Info  
[PLAT982 ALERT 1 G](#) The C-F'= 0.0192 Deviates from IT-value = 0.0181 Check  
And 2 other PLAT982 Alerts  
More ....  
[PLAT983 ALERT 1 G](#) The Al-F'= 0.2420 Deviates from IT-Value = 0.2455 Check  
[PLAT983 ALERT 1 G](#) The O-F'= 0.0338 Deviates from IT-Value = 0.0322 Check

- 0 ALERT level A = Most likely a serious problem - resolve or explain
  - 0 ALERT level B = A potentially serious problem, consider carefully
  - 2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  - 15 ALERT level G = General information/check it is not something unexpected
- 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 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  
8 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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 22/08/2024; check.def file version of 21/08/2024

**Datablock xstr1688\_auto - ellipsoid plot**



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