

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: 3207\_twin1\_hklf4

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Bond precision:    C-C = 0.0098 Å

Wavelength=0.71073

Cell:                a=9.3542(8)                b=9.9397(8)                c=22.1527(17)  
                      alpha=79.942(7)            beta=78.411(7)            gamma=70.771(7)  
Temperature:        173 K

	Calculated	Reported
Volume	1892.0(3)	1892.0(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H58 Fe2 Li2 N2 O Si2	C36 H58 Fe2 Li2 N2 O Si2
Sum formula	C36 H58 Fe2 Li2 N2 O Si2	C36 H58 Fe2 Li2 N2 O Si2
Mr	716.60	716.60
Dx,g cm-3	1.258	1.258
Z	2	2
Mu (mm-1)	0.859	0.859
F000	764.0	764.0
F000'	765.87	
h,k,lmax	11,12,27	11,12,27
Nref	7464	8461
Tmin,Tmax	0.940,0.962	0.952,1.000
Tmin'	0.887	

Correction method= # Reported T Limits: Tmin=0.952 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.134

Theta(max)= 25.999

R(reflections)= 0.0506( 5799)

wR2(reflections)= 0.1384( 8461)

S = 1.033

Npar= 473

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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 C

PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min)	Range	4.4	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O1	--	C35	..	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C6	--	C7	..	0.16 Ang.
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	.....			C35 Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	.....			Si2 Check

PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for .....	01	Check
PLAT341_ALERT_3_C	Low	Bond Precision on C-C Bonds .....	0.0098	Ang.
PLAT350_ALERT_3_C	Short	C-H (X0.96,N1.08A) C6 - H6 ...	0.84	Ang.
PLAT350_ALERT_3_C	Short	C-H (X0.96,N1.08A) C8 - H8 ...	0.84	Ang.
PLAT350_ALERT_3_C	Short	C-H (X0.96,N1.08A) C10 - H10 ...	0.76	Ang.
PLAT350_ALERT_3_C	Short	C-H (X0.96,N1.08A) C22 - H22 ...	0.83	Ang.
PLAT350_ALERT_3_C	Short	C-H (X0.96,N1.08A) C24 - H24 ...	0.79	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond C35 - C36 ...	1.41	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #		1	Note

C36 H58 Fe2 Li2 N2 O Si2

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### ● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1	Report
PLAT021_ALERT_4_G	Ratio Unique / Expected Reflections too High ...	1.134	
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal .....	0.00700	Degree
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C3	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C19	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	6	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
  - 14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  - 6 **ALERT level G** = General information/check it is not something unexpected
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- 1 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
  - 7 ALERT type 3 Indicator that the structure quality may be low
  - 4 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*, 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.

