

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3216_twin1_hklf4

Bond precision: C-C = 0.0116 Å

Wavelength=0.71073

Cell: a=9.510(6) b=10.509(4) c=11.173(6)
 alpha=81.19(4) beta=71.92(5) gamma=72.75(5)
Temperature: 173 K

	Calculated	Reported
Volume	1011.5(10)	1011.4(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H60 Fe2 Li2 N2 O4 Si2	C19 H30 Fe Li N O2 Si
Sum formula	C38 H60 Fe2 Li2 N2 O4 Si2	C19 H30 Fe Li N O2 Si
Mr	790.64	395.32
Dx,g cm-3	1.298	1.298
Z	1	2
Mu (mm-1)	0.815	0.816
F000	420.0	420.0
F000'	420.97	
h,k,lmax	11,12,13	11,12,13
Nref	3972	13640
Tmin,Tmax	0.943,0.952	0.953,1.000
Tmin'	0.863	

Correction method= # Reported T Limits: Tmin=0.953 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 3.434

Theta(max)= 25.999

R(reflections)= 0.0661(5731)

wR2(reflections)= 0.1723(13640)

S = 0.846

Npar= 234

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

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections too Low	42 %
PLAT213_ALERT_2_C	Atom C19 has ADP max/min Ratio	3.5 prolat
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) Range	5.4 Ratio
PLAT222_ALERT_3_C	Large Non-Solvent H Uiso(max)/Uiso(min) ...	5.0 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C3 -- C7 ..	6.1 su

PLAT241_ALERT_2_C High	Ueq as Compared to Neighbors for	C12 Check
PLAT241_ALERT_2_C High	Ueq as Compared to Neighbors for	C18 Check
PLAT242_ALERT_2_C Low	Ueq as Compared to Neighbors for	C3 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor		2.3 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds		0.0116 Ang.



Alert level G

PLAT021_ALERT_4_G Ratio Unique / Expected Reflections too High ...	3.434	
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by	0.50 Ratio	
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for	C15	Check
PLAT793_ALERT_4_G The Model has Chirality at Sil (Centro SPGR)		S Verify

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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
 - 10 **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
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- 2 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
 - 3 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*, 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.

Datablock 3216_twin1_hklf4 - ellipsoid plot

