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: mo_b0747_0m_4

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Bond precision:   C-C = 0.0075 A            Wavelength=0.71073

Cell:          a=10.740(3)         b=11.012(3)        c=14.879(4)
               alpha=86.695(9)   beta=78.411(9)   gamma=68.404(9)
Temperature:   100 K

                   Calculated                Reported
Volume             1602.6(8)                 1602.5(7)
Space group        P -1                      P -1
Hall group         -P 1                      -P 1
                   C38 H94 K2 Li6 N6 O10 Si2
Moiety formula     [+ solvent]               C19 H47 K Li3 N3 O5 Si

                   C38 H94 K2 Li6 N6 O10 Si2
Sum formula        [+ solvent]               C19 H47 K Li3 N3 O5 Si
Mr                 971.21                    485.60
Dx,g cm-3          1.006                     1.006
Z                  1                         2
Mu (mm-1)          0.229                     0.229
F000               528.0                     528.0
F000'              528.75
h,k,lmax           13,13,18                  13,13,18
Nref               6301                      6289
Tmin,Tmax          0.944,0.960               0.473,0.746
Tmin'              0.882

Correction method= # Reported T Limits: Tmin=0.473 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998        Theta(max)= 25.999

R(reflections)= 0.0645( 4580)     wR2(reflections)= 0.1728( 6289)

S = 1.057                  Npar= 328
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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
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of   C18 Check

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⬤ Alert level C
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range   4.4 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range   4.4 Ratio
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   K1 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   Si1 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C16 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C19 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0075 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn   H3C   .. H10H   ..   1.89 Ang.

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⬤ Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   2 Note
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF   Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.50 Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.009 Degree
PLAT230_ALERT_2_G Hirshfeld Test Diff for   N2   -- C10A   ..   9.3 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   N2   -- C9B   ..   8.2 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   N3   -- C0AA   ..   5.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for   N3   -- C10   ..   9.7 s.u.
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)..   19 % Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure   158 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   23 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .   1.49 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #   327 Check
               O1   -SI1 -K1   1.555   1.555   2.666   43.11 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   1 Note
PLAT868_ALERT_4_G ALERTS Due to the use of _smtbx_masks Suppressed   ! Info
PLAT881_ALERT_1_G Missing datum for _diffrn_reflns_av_R_equivalents   Please Check

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

   4 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
   4 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 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.

PLATON version of 27/03/2017; check.def file version of 24/03/2017