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: cu_b0490_0m

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Bond precision:    C-C = 0.0043 A            Wavelength=1.54178

Cell:            a=18.2841(8)     b=9.1092(4)         c=24.3776(10)
                 alpha=90         beta=111.387(2)     gamma=90
Temperature:     100 K

                 Calculated                 Reported
Volume           3780.6(3)                  3780.6(3)
Space group      P 21/c                     P 1 21/c 1
Hall group       -P 2ybc                    -P 2ybc
Moiety formula   C28 H64 Li5 N3 O8          C27 H61 Li5 N3 O8, C H3
Sum formula      C28 H64 Li5 N3 O8          C28 H64 Li5 N3 O8
Mr               605.52                     605.52
Dx,g cm-3        1.064                      1.064
Z                4                          4
Mu (mm-1)        0.586                      0.586
F000             1328.0                     1328.0
F000'            1331.80
h,k,lmax         21,10,29                   21,10,29
Nref             6881                       6869
Tmin,Tmax        0.869,0.895                0.351,0.473
Tmin'            0.815

Correction method= # Reported T Limits: Tmin=0.351 Tmax=0.473
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 67.992

R(reflections)= 0.0792( 5124)      wR2(reflections)= 0.2261( 6869)

S = 1.032                 Npar= 431
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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.

Alert level B

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PLAT230_ALERT_2_B Hirshfeld Test Diff for    O6     -- C21    ..        9.0 s.u.
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Alert level C

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DIFMX01_ALERT_2_C  The maximum difference density is > 0.1*ZMAX*0.75
           _refine_diff_density_max given =      0.742
           Test value =       0.600
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.132
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 .........      0.132 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.07 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       0.74 eA-3
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00433 Ang.
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        8 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.11 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         2 Report
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for    C11    Check
PLAT343_ALERT_2_G Unusual         Angle Range in Main Residue for    C18    Check
PLAT793_ALERT_4_G The Model has Chirality at N1      (Centro SPGR)        S Verify
PLAT793_ALERT_4_G The Model has Chirality at N3      (Centro SPGR)        S Verify
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
   1 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   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
   4 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
```

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 11/08/2016; check.def file version of 04/08/2016