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_b0378_0m

```
Bond precision:   C-C = 0.0017 A            Wavelength=0.71073

Cell:          a=9.9122(8)         b=13.2804(10)     c=14.5570(12)
               alpha=81.866(3)   beta=88.357(3)   gamma=68.748(3)
Temperature:   100 K

                 Calculated                  Reported
Volume           1767.4(2)                   1767.4(2)
Space group      P -1                        P -1
Hall group       -P 1                        -P 1
Moiety formula   C28 H62 Li4 N2 O6           0.5(C28 H62 Li4 N2 O6)
Sum formula      C28 H62 Li4 N2 O6           C14 H31 Li2 N O3
Mr               550.56                      275.28
Dx,g cm-3        1.035                       1.035
Z                2                           4
Mu (mm-1)        0.068                       0.068
F000             608.0                       608.0
F000'            608.25
h,k,lmax         13,18,19                    13,18,19
Nref             9399                        9360
Tmin,Tmax        0.925,0.982                 0.626,0.747
Tmin'            0.914

Correction method= # Reported T Limits: Tmin=0.626 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.996        Theta(max)= 29.000

R(reflections)= 0.0461( 8086)     wR2(reflections)= 0.1291( 9360)

S = 1.022                  Npar= 455
```

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

```
CRYSS02_ALERT_3_B  The value of _exptl_crystal_size_mid is > 0.8
   Mid crystal size given     =   0.960
CRYSS02_ALERT_3_B  The value of _exptl_crystal_size_max is > 1.0
   Maximum crystal size given =   1.320
PLAT351_ALERT_3_B Long    C-H (X0.96,N1.08A) C26    -   H26B   ..        1.18 Ang.
```

Alert level C

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....     2.07 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C25    -- C27     ..        5.4 s.u.
```

Alert level G

```
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
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....     1.32 mm
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)    0.003 Degree
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for     C21    Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for     C25    Check
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C21    -   C22    ..     1.53 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C21    -   C23    ..     1.53 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C21    -   C24    ..     1.53 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C25    -   C26    ..     1.52 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C25    -   C27    ..     1.52 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C25    -   C28    ..     1.52 Ang.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .     1.11 Ratio
PLAT793_ALERT_4_G The Model has Chirality at N1       (Centro SPGR)        R Verify
PLAT793_ALERT_4_G The Model has Chirality at N2       (Centro SPGR)        R Verify
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   4 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 06/05/2016; check.def file version of 05/05/2016

NOMOVE FORCED

Prob = 50
Temp = 100

1 Y

PLATON-Jun 15 14:05:41 2016 - (70316)

Z -57   mo_b0378_OP -1   R = 0.05   RES=   0   -99 X