checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0314_0m

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_b0314_0m

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Bond precision:   C-C = 0.0022 A              Wavelength=0.71073

Cell:            a=13.137(6)      b=17.220(8)            c=19.039(9)
                 alpha=90         beta=96.585(12)        gamma=90
Temperature:     100 K

                 Calculated                 Reported
Volume           4279(3)                    4279(4)
Space group      P 21/c                     P 1 21/c 1
Hall group       -P 2ybc                    -P 2ybc
Moiety formula   C34 H76 Li5 N3 O8          C34 H76 Li5 N3 O8
Sum formula      C34 H76 Li5 N3 O8          C34 H76 Li5 N3 O8
Mr               689.68                     689.67
Dx,g cm-3        1.071                      1.071
Z                4                          4
Mu (mm-1)        0.072                      0.072
F000             1520.0                     1520.0
F000'            1520.64
h,k,lmax         16,21,23                   16,21,23
Nref             8413                       8397
Tmin,Tmax        0.981,0.990
Tmin'            0.971

Correction method= Not given

Data completeness= 0.998          Theta(max)= 25.999

R(reflections)= 0.0449( 6555)     wR2(reflections)= 0.1212( 8397)

S = 1.031                  Npar= 521
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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

PLAT413_ALERT_2_B Short Inter XH3 .. XHn   H14A   .. H23D   ..   1.99 Ang.

🟡 Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given   Please Do !
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range   3.8 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range   4.1 Ratio
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min)   7 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600   10 Report

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⚪ Alert level G

PLAT230_ALERT_2_G Hirshfeld Test Diff for   C23   -- C24   ..   5.2 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .... Percentage =   4 Note
PLAT343_ALERT_2_G Unusual sp?   Angle Range in Main Residue for   C11   Check
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond C11   -   C12   ..   1.53 Ang.
PLAT793_ALERT_4_G The Model has Chirality at N1   (Centro SPGR)   R Verify
PLAT793_ALERT_4_G The Model has Chirality at N3   (Centro SPGR)   R Verify
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density   5 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
   5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
   7 **ALERT level G** = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 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
   2 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 30/03/2016; check.def file version of 30/03/2016