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_b0542_0ma

```
Bond precision:  C-C = 0.0034 A          Wavelength=0.71073

Cell:           a=20.6642(12)    b=19.9484(14)     c=19.8692(11)
                alpha=90         beta=91.024(2)    gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          8189.1(9)                 8189.1(9)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C31.55 H69.64 Li4 N4 O8,  C32 H72 Li4 N4 O8, C32 H71
                C32 H72 Li4 N4 O8, 0.455(C Li4 N4 O8
                H3)
Sum formula     C64 H143 Li8 N8 O16       C64 H143 Li8 N8 O16
Mr              1336.38                   1336.38
Dx,g cm-3       1.084                     1.084
Z               4                         4
Mu (mm-1)       0.074                     0.074
F000            2940.0                    2940.0
F000'           2941.25
h,k,lmax        26,25,25                  26,25,25
Nref            17881                     17852
Tmin,Tmax       0.984,0.991               0.381,0.431
Tmin'           0.954

Correction method= # Reported T Limits: Tmin=0.381 Tmax=0.431
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 27.000

R(reflections)= 0.0681( 12171)    wR2(reflections)= 0.1814( 17852)

S = 1.026                 Npar= 917
```

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

PLAT213_ALERT_2_B Atom C47 has ADP max/min Ratio ..... 4.3 prolat
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C47 Check

---

Alert level C

PLAT213_ALERT_2_C Atom C45 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C46 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom C51 has ADP max/min Ratio ..... 3.5 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.7 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 4.0 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 2 O Ueq(max)/Ueq(min) Range 4.2 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 4.8 Ratio

---

Alert level G

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size .... 0.64 mm
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.03 Why ?
PLAT230_ALERT_2_G Hirshfeld Test Diff for O12B -- C47 .. 17.8 s.u.
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 2 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage = 100 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (117.18) in Resd. # 1 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (1.82) in Resd. # 3 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C47 .. C48A .. 2.26 Ang.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.12 Ratio
PLAT793_ALERT_4_G The Model has Chirality at N1 (Centro SPGR) S Verify
PLAT793_ALERT_4_G The Model has Chirality at N2 (Centro SPGR) R Verify
PLAT793_ALERT_4_G The Model has Chirality at N3 (Centro SPGR) R Verify
PLAT793_ALERT_4_G The Model has Chirality at N4 (Centro SPGR) S Verify
PLAT793_ALERT_4_G The Model has Chirality at N5 (Centro SPGR) R Verify
PLAT793_ALERT_4_G The Model has Chirality at N6 (Centro SPGR) R Verify
PLAT793_ALERT_4_G The Model has Chirality at N7 (Centro SPGR) S Verify
PLAT793_ALERT_4_G The Model has Chirality at N8 (Centro SPGR) R Verify

---

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
13 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

Datablock mo_b0542_0ma - ellipsoid plot