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_b0525_0m

```
Bond precision:  C-C = 0.0232 A          Wavelength=0.71073

Cell:            a=11.323(7)    b=31.44(2)          c=21.554(13)
                 alpha=90       beta=93.006(10)     gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          7663(8)                   7662(9)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C49 H108 Li8 N4 O11       C49 H108 Li8 N4 O11
Sum formula     C49 H108 Li8 N4 O11       C50.57 H108 Li8 N4 O11
Mr              984.91                    1003.73
Dx,g cm-3       0.854                     0.870
Z               4                         4
Mu (mm-1)       0.057                     0.058
F000            2168.0                    2206.0
F000'           2168.89
h,k,lmax        12,33,23                  12,33,23
Nref            10012                     9932
Tmin,Tmax                                 0.324,0.430
Tmin'

Correction method= # Reported T Limits: Tmin=0.324 Tmax=0.430
AbsCorr = MULTI-SCAN

Data completeness= 0.992          Theta(max)= 22.499

R(reflections)= 0.2321( 3876)     wR2(reflections)= 0.5829( 9932)

S = 1.606                 Npar= 307
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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 A

```
EXPT005_ALERT_1_A  _exptl_crystal_description is missing
           Crystal habit description.
           The following tests will not be performed.
           CRYSR_01
ATOM007_ALERT_1_A  _atom_site_aniso_label is missing
           Unique label identifying the atom site.
RINTA01_ALERT_3_A  The value of Rint is greater than 0.25
           Rint given   0.299
SHFSU01_ALERT_2_A  The absolute value of parameter shift to su ratio > 0.20
           Absolute value of the parameter shift to su ratio given   3.459
           Additional refinement cycles may be required.
THETM01_ALERT_3_A  The value of sine(theta_max)/wavelength is less than 0.550
           Calculated sin(theta_max)/wavelength =    0.5384
PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 .........      0.299 Report
PLAT080_ALERT_2_A Maximum Shift/Error ............................       3.46 Why ?
PLAT082_ALERT_2_A High R1 Value ..................................       0.23 Report
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ...................       0.58 Report
PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) .......         72 Report
PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
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Alert level B

```
PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low ..        39% Check
PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by ..      18.82 Check
PLAT049_ALERT_1_B Calculated Density Less Than 1.0 gcm-3 .........     0.8537 Check
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       1.27 eA-3
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ...............    0.02318 Ang.
```

Alert level C

```
CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
           calculated from the _atom_site* data lies outside
           the range 0.99 <> 1.01
          From the CIF: _cell_formula_units_Z                   4
          From the CIF: _chemical_formula_weight          1003.73
          TEST: Calculate formula weight from _atom_site_*
          atom     mass    num     sum
          C        12.01   49.00  588.54
          H         1.01  108.00  108.86
          Li        6.94    8.00   55.53
          N        14.01    4.00   56.03
          O        16.00   11.00  175.99
          Calculated formula weight             984.95
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT074_ALERT_1_C Occupancy Parameter = 0.0 for ..................       CNT2 Check
PLAT074_ALERT_1_C Occupancy Parameter = 0.0 for ..................        C1A Check
PLAT074_ALERT_1_C Occupancy Parameter = 0.0 for ..................        C1B Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.20 Report
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .       CNT2 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C1A Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .        C1B Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .       CNT2 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C1A Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .        C1B Check
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PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .       CNT2 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C1A Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .        C1B Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C29 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C47 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        Li2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C32 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C39 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C46 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C48 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C31      - C32      .       1.43 Ang.
PLAT361_ALERT_2_C Long  C(sp3)-C(sp3) Bond  C7       - C8       ..      1.73 Ang.
PLAT361_ALERT_2_C Long  C(sp3)-C(sp3) Bond  C47      - C48      ..      1.70 Ang.
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C50.57 H108 Li8 N4 O11
           Atom count from _chemical_formula_moiety:C49 H108 Li8 N4 O11
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C50.57 H108 Li8 N4 O11
           Atom count from the _atom_site data:  C49 H108 Li8 N4 O11
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C50.57 H108 Li8 N4 O11
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        202.28    196.00    6.28
          H        432.00    432.00    0.00
          Li        32.00     32.00    0.00
          N         16.00     16.00    0.00
          O         44.00     44.00    0.00
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT300_ALERT_4_G Atom Site Occupancy of CnT2       Constrained at        0.0 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1A        Constrained at        0.0 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1B        Constrained at        0.0 Check
PLAT303_ALERT_2_G Full Occupancy Atom H42B      with # Connections       2.00 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C38 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C42 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C46 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C38      - C39      .       1.54 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C42      - C43      .       1.51 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          1 Note
PLAT721_ALERT_1_G Bond    Calc     0.98000, Rep     1.02230 Dev...       0.04 Ang.
             C33      -H33A            1.555   1.555 ........     #  207 Check
PLAT721_ALERT_1_G Bond    Calc     0.98000, Rep     1.02360 Dev...       0.04 Ang.
             C33      -H33B            1.555   1.555 ........     #  208 Check
PLAT721_ALERT_1_G Bond    Calc     0.98000, Rep     1.01960 Dev...       0.04 Ang.
             C33      -H33C            1.555   1.555 ........     #  209 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      113.60 Dev...       4.60 Degree
             O10     -C33     -H33A       1.555  1.555  1.555     #  535 Check
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PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      113.90 Dev...       3.90 Degree
             O10     -C33     -H33B       1.555  1.555  1.555     #  536 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      112.80 Dev...       2.80 Degree
             O10     -C33     -H33C       1.555  1.555  1.555     #  537 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      105.10 Dev...       3.90 Degree
             H33A    -C33     -H33B       1.555  1.555  1.555     #  538 Check
PLAT722_ALERT_1_G Angle   Calc      109.00, Rep      105.20 Dev...       3.80 Degree
             H33A    -C33     -H33C       1.555  1.555  1.555     #  539 Check
PLAT722_ALERT_1_G Angle   Calc      110.00, Rep      105.40 Dev...       4.60 Degree
             H33B    -C33     -H33C       1.555  1.555  1.555     #  540 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C8       --C7              1.73 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C38      --CnT2            1.85 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C42      --C1A             1.80 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C46      --C1B             1.85 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        113 Check
             O6   -C18  -LI4     1.555   1.555   1.555             43.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        232 Check
             O11  -C35  -LI8     1.555   1.555   1.555             43.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        278 Check
             O3   -C8   -LI3     1.555   1.555   1.555             40.00 Deg.
PLAT793_ALERT_4_G Model has Chirality at N2          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at N4          (Centro SPGR)          R Verify
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11 **ALERT level A** = Most likely a serious problem - resolve or explain
5 **ALERT level B** = A potentially serious problem, consider carefully
33 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
34 **ALERT level G** = General information/check it is not something unexpected

26 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
33 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
18 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 23/04/2018; check.def file version of 23/04/2018

Datablock mo_b0525_0m - ellipsoid plot