# 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: i-4

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```
Bond precision:  C-C = 0.0380 A          Wavelength=0.71073

Cell:              a=9.817(1)      b=9.817(1)      c=19.541(4)
                   alpha=90        beta=90         gamma=90
Temperature:       100 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 1883.2(5) | 1883.3(5) |
| Space group | I -4 | I -4 |
| Hall group | I -4 | I -4 |
| Moiety formula | C32 H64 Li4 N4 O8 | C32 H64 Li4 N4 O8 |
| Sum formula | C32 H64 Li4 N4 O8 | C32 H64 Li4 N4 O8 |
| Mr | 660.63 | 660.63 |
| Dx,g cm-3 | 1.165 | 1.165 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.080 | 0.080 |
| F000 | 720.0 | 720.0 |
| F000’ | 720.31 | |
| h,k,lmax | 12,12,24 | 12,12,24 |
| Nref | 2100[ 1086] | 2072 |
| Tmin,Tmax | | 0.369,0.429 |
| Tmin’ | | |

```
Correction method= # Reported T Limits: Tmin=0.369 Tmax=0.429
AbsCorr = MULTI-SCAN

Data completeness= 1.91/0.99      Theta(max)= 27.113

R(reflections)= 0.3023( 1057)     wR2(reflections)= 0.6523( 2072)

S = 2.155                 Npar= 51
```

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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   0.313
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   1.991
           Additional refinement cycles may be required.
PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 .........      0.313 Report
PLAT080_ALERT_2_A Maximum Shift/Error ............................       1.99 Why ?
PLAT082_ALERT_2_A High R1 Value ..................................       0.30 Report
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) ...................       0.65 Report
PLAT097_ALERT_2_A Large Reported Max.  (Positive) Residual Density       2.53 eA-3
PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) .......         12 Report
PLAT203_ALERT_2_A Negative Isotropic ADP for O1        ...........     -0.001 Report
PLAT203_ALERT_2_A Negative Isotropic ADP for LI1       ...........     -0.001 Report
PLAT316_ALERT_2_A Too many H on C in C=N Moiety in Main Residue ..         C4 Check
PLAT410_ALERT_2_A Short Intra H...H Contact  H4A      ..H8A              1.30 Ang.
PLAT410_ALERT_2_A Short Intra H...H Contact  H4A      ..H8B              1.69 Ang.
PLAT413_ALERT_2_A Short Inter XH3 .. XHn     H3B      ..H7B              1.89 Ang.
```

## Alert level B

```
DIFMN02_ALERT_2_B  The minimum difference density is < -0.1*ZMAX*1.00
           _refine_diff_density_min given =     -1.029
           Test value =     -0.800
PLAT098_ALERT_2_B Large Reported Min.  (Negative) Residual Density      -1.03 eA-3
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ...............      0.038 Ang.
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond  C7       - C8       .       1.32 Ang.
PLAT411_ALERT_2_B Short Inter H...H Contact  H4B      ..H7A              1.93 Ang.
```

## Alert level C

```
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
           outside the range 0.80 <> 2.00
           Goodness of fit given =      2.155
STRVA01_ALERT_4_C           Flack parameter is too small
          From the CIF: _refine_ls_abs_structure_Flack   -4.100
          From the CIF: _refine_ls_abs_structure_Flack_su    1.000
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
PLAT087_ALERT_2_C Unsatisfactory S value (Too High) ..............       2.15 Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.46 Report
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C8 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C5 Check
PLAT361_ALERT_2_C Long  C(sp3)-C(sp3) Bond  C1       - C4       ..       1.67 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H7A      ..H8B              1.94 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H7B      ..H8A              1.92 Ang.
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PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         54 Ang**3
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
              C32 H64 Li4 N4 O8
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**Alert level G**

```
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      1.000 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.20 Report
PLAT303_ALERT_2_G Full Occupancy Atom H5B       with # Connections       2.00 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for         C5 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for         C8 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C5       - C6       .       1.59 Ang.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.31 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         21 Check
              O1   -C1   -LI1     1.555   1.555   2.445             44.70 Deg.
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 16 ALERT level A = Most likely a serious problem - resolve or explain
  5 ALERT level B = A potentially serious problem, consider carefully
 20 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

  8 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
  4 ALERT type 3 Indicator that the structure quality may be low
  5 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
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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 i-4** - ellipsoid plot