checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait **. . . . .**

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) xstr1591_autored2

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
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: xstr1591_autored2

```
Bond precision:       C-C = 0.0085 A                Wavelength=1.54184
Cell:       a=7.7848(2)       b=10.9557(3)      c=15.1427(3)
            alpha=90          beta=90           gamma=90
Temperature: 150 K
                    Calculated                        Reported
Volume              1291.49(5)                        1291.49(5)
Space group         P 21 21 21                        P 21 21 21
Hall group          P 2ac 2ab                         P 2ac 2ab
Moiety formula      C8 H20 Al2 Li N O                 C8 H20 Al2 Li N O
Sum formula         C8 H20 Al2 Li N O                 C8 H20 Al2 Li N O
Mr                  207.15                            207.15
Dx,g cm-3           1.065                             1.065
Z                   4                                 4
Mu (mm-1)           1.751                             1.751
F000                448.0                             448.0
F000'               450.51
h,k,lmax            9,13,19                           9,13,19
Nref                2774[ 1608]                       2705
Tmin,Tmax           0.863,0.900                       0.828,1.000
Tmin'               0.756
Correction method= # Reported T Limits: Tmin=0.828 Tmax=1.000
AbsCorr = GAUSSIAN
Data completeness= 1.68/0.98       Theta(max)= 78.945
R(reflections)= 0.0646( 2505)                  wR2(reflections)= 0.1768(
                                               2705)
S = 1.138               Npar= 140
```

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 C

```
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.350
          From the CIF: _refine_ls_abs_structure_Flack_su    0.110
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       3.57 Report
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0085 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.155 Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         4 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         1 Info
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .     0.350 Note
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.10 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         2 Report
PLAT303_ALERT_2_G Full Occupancy Atom Hb        with # Connections      2.00 Check
And 2 other PLAT303 Alerts
More ...
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         4 Note
          Ha      Hb      Hc      Hd
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.46 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         9 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        17 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     6.998 Note
            Predicted wR2: Based on SigI**2  2.53 or SHELX Weight 15.53
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         2 Info
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  4 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

  0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  7 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
  7 ALERT type 4 Improvement, methodology, query or suggestion
  2 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 11/11/2024; check.def file version of 11/11/2024

Datablock xstr1591_autored2 - ellipsoid plot

Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry