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) 1

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: 1

Bond precision: C-C = 0.0103 A Wavelength=1.54184
Cell: a=11.9121(2) b=13.0432(1) c=17.8371(2)
alpha=103.510(1) beta=102.825(1) gamma=95.033(1)
Temperature: 150 K

	Calculated	Reported
Volume	2598.84(6)	2598.84(6)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C43 H81 Al4 Li2 N3 O4	2(C43 H81 Al4 Li2 N3 O4)
Sum formula	C43 H81 Al4 Li2 N3 O4	C86 H162 Al8 Li4 N6 O8
Mr	825.91	1651.81
Dx,g cm-3	1.055	1.055
Z	2	1
Mu (mm-1)	1.119	1.119
F000	900.0	900.0
F000'	903.68	
h,k,lmax	15,16,22	14,16,22
Nref	22568[11284]	20140
Tmin,Tmax	0.886,0.935	0.803,0.923
Tmin'	0.836	

Correction method= # Reported T Limits: Tmin=0.803 Tmax=0.923
AbsCorr = ANALYTICAL
Data completeness= 1.78/0.89 Theta(max)= 79.283
R(reflections)= 0.0727(17878) wR2(reflections)= 0.2070(20140)
S = 1.057 Npar= 1107

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

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density .... 4.63 Report
PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 1.76 eA-3
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01034 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C61 - C62 . 1.33 Ang.

Alert level C

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
Calc: C43 H81 Al4 Li2 N3 O4
Rep.: C86 H162 Al8 Li4 N6 O8
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C43 H81 Al4 Li2 N3 O4
Rep.: 2(C43 H81 Al4 Li2 N3 O4)
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.0 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 5.1 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 9.7 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 6.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O8 --C85 . 6.9 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O2 --C61 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C59 --C60 . 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C59 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O3 Check
And 5 other PLAT242 Alerts
More ...
PLAT245_ALERT_2_C U(iso) Ha Smaller than U(eq) Li1 by 0.035 Ang**2
And 3 other PLAT245 Alerts
More ...
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C57 - C58 . 1.38 Ang.
And 2 other PLAT360 Alerts
More ...
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report
-11 -8 2, -11 -8 3, -12 -6 3, -12 -7 4, -12 -7 5, -12 -7 6,
-11 -8 12,
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.20Ang From Al5 1.82 eA-3
And 2 other PLAT971 Alerts
More ...

Alert level G

PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.120 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT303_ALERT_2_G Full Occupancy Atom Ha with # Connections 2.00 Check
And 7 other PLAT303 Alerts
More ...
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C39 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 15 Note
Ha Hb Hc Hd He Hf Hg Hh
Hi Hj Hk Hl Hm Hn Ho
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 522 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 5.261 Note
Predicted wR2: Based on SigI**2 3.93 or SHELX Weight 19.58
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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

5 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
5 ALERT type 3 Indicator that the structure quality may be low
6 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 1 - ellipsoid plot

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