

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_b1036_0m

Bond precision: C-C = 0.0033 A

Wavelength=0.71073

Cell: a=8.996(2) b=17.382(4) c=20.982(6)
 alpha=112.633(6) beta=93.252(9) gamma=93.891(14)
Temperature: 100 K

	Calculated	Reported
Volume	3009.0(13)	3009.2(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H54 Li2 O4 Si2	C24 H54 Li2 O4 Si2
Sum formula	C24 H54 Li2 O4 Si2	C24 H54 Li2 O4 Si2
Mr	476.73	476.73
Dx,g cm-3	1.052	1.052
Z	4	4
Mu (mm-1)	0.141	0.141
F000	1056.0	1056.0
F000'	1057.02	
h,k,lmax	11,21,25	11,21,25
Nref	11815	11800
Tmin,Tmax	0.828,0.871	0.687,0.740
Tmin'	0.828	

Correction method= # Reported T Limits: Tmin=0.687 Tmax=0.740
AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 25.999

R(reflections)= 0.0482(9793)

wR2(reflections)= 0.1173(11800)

S = 1.028

Npar= 650

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

CRYSS02_ALERT_3_B The value of _exptl_crystal_size_min is > 0.6
Minimum crystal size given = 0.980
CRYSS02_ALERT_3_B The value of _exptl_crystal_size_mid is > 0.8
Mid crystal size given = 1.200
CRYSS02_ALERT_3_B The value of _exptl_crystal_size_max is > 1.0
Maximum crystal size given = 1.340

🟡 Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C22 Check
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) 05 Check
PLAT411_ALERT_2_C Short Inter H...H Contact H24A ..H42C . 2.08 Ang.

🟢 Alert level G

PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF Please Check
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size 1.34 mm
PLAT300_ALERT_4_G Atom Site Occupancy of H41A Constrained at 0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41B Constrained at 0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43A Constrained at 0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43B Constrained at 0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41C Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H41D Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43C Constrained at 0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H43D Constrained at 0.25 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 9% Note
PLAT303_ALERT_2_G Full Occupancy Atom H25B with # Connections 2.00 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C29 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C1 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C5 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 32 Check
C36A -O5 -C36B 1.555 1.555 1.555 24.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 249 Check
H41A -C41 -H41C 1.555 1.555 1.555 20.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 252 Check
H41B -C41 -H41D 1.555 1.555 1.555 19.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 262 Check
C42B -C41 -C42A 1.555 1.555 1.555 20.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 276 Check
H34C -C34 -H34B 1.555 1.555 1.555 26.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 277 Check
H34D -C34 -H34A 1.555 1.555 1.555 27.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 289 Check
C35A -C34 -C35B 1.555 1.555 1.555 27.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 333 Check
C35B -C36A -C35A 1.555 1.555 1.555 29.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 392 Check
C36A -C35B -C36B 1.555 1.555 1.555 24.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 413 Check
H43A -C43 -H43D 1.555 1.555 1.555 17.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 414 Check
H43B -C43 -H43C 1.555 1.555 1.555 20.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 418 Check
C42B -C43 -C42A 1.555 1.555 1.555 20.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 495 Check
C36B -C35A -C36A 1.555 1.555 1.555 24.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 509 Check
C35A -C36B -C35B 1.555 1.555 1.555 29.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 518 Check

C42A -C42B -H42D 1.555 1.555 1.555 42.20 Deg.
 PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 15 Check
 PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 5 Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 9 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
 25 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 09/11/2017; check.def file version of 08/11/2017

