

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Cj1508

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: Cj1508

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Bond precision:    C-C = 0.0033 A                      Wavelength=1.54184

Cell:                      a=10.3159(1)              b=19.3423(2)              c=28.3898(2)  
                            alpha=90                      beta=99.091(1)              gamma=90

Temperature:            123 K

	Calculated	Reported
Volume	5593.55(9)	5593.55(9)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C57 H87 Li N2 O), C6 H14, C4 H10 O	?
Sum formula	C124 H198 Li2 N4 O3	C62 H99 Li N2 O1.50
Mr	1806.74	903.37
Dx,g cm-3	1.073	1.073
Z	2	4
Mu (mm-1)	0.461	0.461
F000	2000.0	2000.0
F000'	2004.77	
h,k,lmax	12,23,34	12,23,34
Nref	10311	10265
Tmin,Tmax	0.908,0.916	0.572,1.000
Tmin'	0.908	

Correction method= # Reported T Limits: Tmin=0.572 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.996                      Theta(max)= 68.498

R(reflections)= 0.0775( 8524)              wR2(reflections)= 0.2296( 10265)

S = 1.056                      Npar= 603

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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 B

PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density	0.91 eA-3
PLAT910_ALERT_3_B	Missing # of FCF Reflection(s) Below Theta(Min).	17 Note

### Alert level C

DIFMX02_ALERT_1_C	The maximum difference density is > 0.1*ZMAX*0.75 The relevant atom site should be identified.	
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.2 Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C52 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C54 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	3.341 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	22 Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H64B	-0.47 eA-3

### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11 Note
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing .....	0.00020 Ang.
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	2 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C62 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C63 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C64 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C65 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C66 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C67 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H62A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H62B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H62C Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H63A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H63B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H64A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H64B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H65A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H65B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H66A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H66B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H67A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H67B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H67C Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C58 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C59 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C60 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C61 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H58A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H58B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59C Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H61A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H61B Constrained at	0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H61C	Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3 )		7.50	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H49B ..H64A .		1.82	Ang.
	1-x,1-y,2-z =		3_667	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H20B ..H67C .		1.69	Ang.
	-1/2+x,1/2-y,-1/2+z =		4_565	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H46A ..H67A .		1.82	Ang.
	2-x,1-y,2-z =		3_767	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		1	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		16	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		7	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		3.9	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		7	Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 10 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  
 43 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 13/07/2021; check.def file version of 13/07/2021

Datablock Cj1508 - ellipsoid plot

