

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2_a

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: 2_a

Bond precision: C-C = 0.0048 A

Wavelength=0.71073

Cell: a=10.6905(6) b=14.5385(8) c=22.0395(12)
 alpha=102.861(2) beta=98.191(2) gamma=105.287(2)
Temperature: 100 K

	Calculated	Reported
Volume	3146.8(3)	3146.8(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C45 H44 F36 Li O17 Tb	C45 H44 F36 Li O17 Tb
Sum formula	C45 H44 F36 Li O17 Tb	C45 H44 F36 Li O17 Tb
Mr	1706.67	1706.66
Dx,g cm-3	1.801	1.801
Z	2	2
Mu (mm-1)	1.294	1.294
F000	1684.0	1684.0
F000'	1685.36	
h,k,lmax	14,19,29	14,19,29
Nref	15632	15503
Tmin,Tmax	0.856,0.974	0.572,0.746
Tmin'	0.824	

Correction method= # Reported T Limits: Tmin=0.572 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.992

Theta(max)= 28.282

R(reflections)= 0.0368(14046)

wR2(reflections)= 0.0936(15503)

S = 1.052

Npar= 969

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**

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	F24	--C32	.	6.3 s.u.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			114 Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.10A	From F27		1.97 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.26A	From F26		1.85 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.01A	From O4		1.61 eA-3

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				4 Note
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large			5.96 Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)				0.002 Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records				1 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records				1 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records				2 Report
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of				C11 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of				C20 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of				C22 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of				C33 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of				C44 Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)			6% Note
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F9	..F19			2.80 Ang.
		1+x,1+y,z =			1_665 Check
PLAT793_ALERT_4_G	Model has Chirality at C4	(Centro SPGR)			R Verify
PLAT793_ALERT_4_G	Model has Chirality at C37B	(Centro SPGR)			R Verify
PLAT793_ALERT_4_G	Model has Chirality at C37A	(Centro SPGR)			S Verify
PLAT794_ALERT_5_G	Tentative Bond Valency for Tb1	(III)			3.35 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				3 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			12 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...				2 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				0 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 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
7 ALERT type 4 Improvement, methodology, query or suggestion
1 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 22/03/2021; check.def file version of 19/03/2021

