

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_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: 1_a

Bond precision: C-C = 0.0053 A

Wavelength=0.71073

Cell: a=10.5527(4) b=12.1312(5) c=22.4916(8)
 alpha=98.494(1) beta=98.377(1) gamma=94.520(1)
Temperature: 100 K

	Calculated	Reported
Volume	2802.49(19)	2802.49(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40.74 H44 F27.22 Li O17 Tb, 0.259(C F3)	C40.74 H44 F27.22 Li O17 Tb, 0.26(C F3)
Sum formula	C41 H44 F28 Li O17 Tb	C41 H44 F28 Li O17 Tb
Mr	1506.63	1506.62
Dx,g cm-3	1.785	1.785
Z	2	2
Mu (mm-1)	1.420	1.420
F000	1492.0	1492.0
F000'	1493.08	
h,k,lmax	14,16,30	14,16,30
Nref	14499	14368
Tmin,Tmax	0.868,0.868	0.649,0.746
Tmin'	0.868	

Correction method= # Reported T Limits: Tmin=0.649 Tmax=0.746

AbsCorr = NONE

Data completeness= 0.991

Theta(max)= 28.700

R(reflections)= 0.0431(12791)

wR2(reflections)= 0.1114(14368)

S = 1.049

Npar= 884

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

PLAT213_ALERT_2_C	Atom C37	has ADP max/min Ratio	3.1	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	4.5	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H	Uiso(max)/Uiso(min) Range	5.5	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		017	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)		015	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)		03A	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)		08A	Check
PLAT329_ALERT_4_C	Carbon Atom Hybridisation Unclear for		C36A	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600		77	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.34A From C40		2.00	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.13A From F11A		-2.22	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H36F		-0.31	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		30	Note
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		5.58	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.001	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		9	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
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		9	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for F10 --C38		5.5	s.u.
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C10	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		C30	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		22%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 1)		130.96	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)		1.04	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H37A ..H35B		1.94	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F12J ..C41		2.74	Ang.
		x,-1+y,z =	1_545	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F2 ..F6A		2.80	Ang.
		-1+x,-1+y,z =	1_445	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F6A ..F6A		2.68	Ang.
		2-x,2-y,2-z =	2_777	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F8A ..F12J		2.64	Ang.
		x,y,z =	1_555	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F9A ..F12B		2.70	Ang.
		-1+x,y,z =	1_455	Check
PLAT793_ALERT_4_G	Model has Chirality at C14 (Centro SPGR)		R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C34 (Centro SPGR)		R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C34A (Centro SPGR)		S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		225	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary		Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		52	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.9	Low
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
12 **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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
23 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
12 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 05/12/2020; check.def file version of 05/12/2020

