

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) qiyanyu_0m

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: qiyanyu_0m

Bond precision: C-C = 0.0156 Å Wavelength=0.71073

Cell: a=13.645(2) b=16.443(3) c=28.430(5)
 alpha=90 beta=92.423(8) gamma=90

Temperature: 153 K

	Calculated	Reported
Volume	6373.0(19)	6372.8(18)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C33 H38 B I2 N O	?
Sum formula	C33 H38 B I2 N O	C33 H38 B I2 N O
Mr	729.25	729.25
Dx,g cm-3	1.520	1.520
Z	8	8
Mu (mm-1)	1.999	1.999
F000	2896.0	2896.0
F000'	2889.30	
h,k,lmax	16,19,33	16,19,33
Nref	11227	11233
Tmin,Tmax	0.625,0.670	
Tmin'	0.544	

Correction method= Not given

Data completeness= 1.001 Theta(max)= 25.000

R(reflections)= 0.0691(10551) wR2(reflections)= 0.2023(11233)

S = 1.085 Npar= 691

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

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	6.0 Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 2 C	Ueq(max)/Ueq(min) Range	5.5 Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H	Uiso(max)/Uiso(min) Range	6.6 Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 2 H	Uiso(max)/Uiso(min) Range	6.0 Ratio
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.01561 Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C52	- C53	1.38 Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		7 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595	56 Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF		5 Note

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		76 Report
PLAT012_ALERT_1_G	N.O.K. _shelx_res_checksum Found in CIF		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		150.35 Why ?
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		3 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		3 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		2 Report
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1		110.9 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2		109.7 Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact I3	..C27	3.46 Ang.
		$3/2-x, 1/2+y, 3/2-z =$	2_656 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		1078 Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..		! Info
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		86% Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 0 1)	Est.d BASF	0.24 Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		11 Note

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

2 **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
8 **ALERT type 3** Indicator that the structure quality may be low
4 **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 19/10/2018; check.def file version of 15/10/2018

