

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) jb240121_1_1

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: jb240121_1_1

Bond precision:	C-C = 0.0084 A	Wavelength=1.54184
Cell:	a=18.2357(4)	b=7.2075(2) c=8.4490(2)
	alpha=90	beta=90.372(2) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	1110.46(5)	1110.46(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C10 H5 B Cl F3 K N O	C10 H5 B Cl F3 K N O
Sum formula	C10 H5 B Cl F3 K N O	C10 H5 B Cl F3 K N O
Mr	297.51	297.51
Dx,g cm-3	1.780	1.780
Z	4	4
Mu (mm-1)	6.684	6.684
F000	592.0	592.0
F000'	596.94	
h,k,lmax	23,9,10	23,9,10
Nref	2426	2406
Tmin,Tmax	0.405,0.765	0.463,1.000
Tmin'	0.307	

Correction method= # Reported T Limits: Tmin=0.463 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.992 Theta(max)= 79.900

R(reflections)= 0.0831(2287) wR2(reflections)= 0.2575(2406)

S = 1.198 Npar= 164

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

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.26 Report
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds	0.0084 Ang.



Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	2 Info
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.16 Report
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .	1.15 Ratio
PLAT774_ALERT_1_G Check X-Y Bond in CIF: K1 --K1 ..	4.23 Ang.
PLAT774_ALERT_1_G Check X-Y Bond in CIF: K1 --K1 ..	4.23 Ang.
PLAT774_ALERT_1_G Check X-Y Bond in CIF: K1 --K1 ..	4.38 Ang.
PLAT774_ALERT_1_G Check X-Y Bond in CIF: K1 --K1 ..	4.38 Ang.
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON	1 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..	! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	19 Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law [1 0 0] Est.d BASF	0.19 Check

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 11 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 1 ALERT type 2 Indicator that the structure model may be wrong or deficient
 2 ALERT type 3 Indicator that the structure quality may be low
 3 ALERT type 4 Improvement, methodology, query or suggestion
 3 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 05/12/2020; check.def file version of 05/12/2020

Datablock jb240121_1_1 - ellipsoid plot

