

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound-3c

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: Compound-3c

Bond precision:	C-C = 0.0039 Å	Wavelength=1.54184	
Cell:	a=8.9277(3)	b=17.2011(5)	c=7.9491(3)
	alpha=90	beta=107.712(4)	gamma=90
Temperature:	295 K		

	Calculated	Reported
Volume	1162.85 (7)	1162.84 (7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H14 B N O2	?
Sum formula	C13 H14 B N O2	C13 H14 B N O2
Mr	227.06	227.06
Dx, g cm ⁻³	1.297	1.297
Z	4	4
Mu (mm ⁻¹)	0.688	0.688
F000	480.0	480.0
F000'	481.42	
h, k, l _{max}	11, 21, 10	11, 21, 9
Nref	2468	2299
Tmin, Tmax	0.976, 0.986	0.941, 0.986
Tmin'	0.940	

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Correction method= # Reported T Limits: Tmin=0.941 Tmax=0.986
AbsCorr = MULTI-SCAN
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Data completeness= 0.932 Theta (max)= 77.570

R(reflections)= 0.0633(1822)	wR2(reflections)= 0.2096(2299)
S = 1.107	Npar= 159

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

PLAT410_ALERT_2_B Short Intra H...H Contact H1 ..H8A . 1.87 Ang.
x,y,z = 1_555 Check

Author Response: The crystal diffracted weakly and so the quality of data is not very good. For that, The hydrogen atoms were included in geometrically calculated position and were refined according to the riding model.

Alert level C

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C9 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C12 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.950 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
9 8 1, -4 19 2, 4 5 7,

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
H1A
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT899_ALERT_4_G SHELXL-97 is Outdated and Succeeded by SHELXL 2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 160 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 5.693 Note
Predicted wR2: Based on SigI**2 3.68 or SHELX Weight 18.93
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
2 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.

