

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB1

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: MAB1

Bond precision: C-C = 0.0020 Å

Wavelength=0.71075

Cell: a=9.5275(2) b=15.1317(3) c=15.7826(3)
 alpha=90 beta=96.294(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2261.62(8)	2261.62(8)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C6 H22 B6 Cu N2 O13, 5(H2 O)	C6 H22 B6 Cu N2 O13, 5(H2 O)
Sum formula	C6 H32 B6 Cu N2 O18	C6 H32 B6 Cu N2 O18
Mr	548.75	548.73
Dx, g cm ⁻³	1.612	1.612
Z	4	4
Mu (mm ⁻¹)	1.049	1.049
F000	1140.0	1140.0
F000'	1142.01	
h, k, lmax	12, 19, 20	12, 19, 20
Nref	5192	5181
Tmin, Tmax	0.951, 0.974	0.658, 1.000
Tmin'	0.745	

Correction method= # Reported T Limits: Tmin=0.658 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 27.484

R(reflections)= 0.0250(4796)

wR2(reflections)= 0.0704(5181)

S = 1.080

Npar= 327

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report

 Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	10	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	15	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	6	Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II) .	2.08	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	9	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	4	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

