

## checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: WCM3-112\_PHI\_2

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Bond precision:	C-C = 0.0078 A	Wavelength=0.71073
Cell:	a=16.4768 (17)      b=10.4768 (4)      c=17.6691 (10)	
	alpha=90      beta=107.092 (9)      gamma=90	
Temperature:	293 K	
	Calculated	Reported
Volume	2915.4 (4)	2915.4 (4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C18 H22 B2 Cu3 F8 N12 O	C18 H22 B2 Cu3 F8 N12 O
Sum formula	C18 H22 B2 Cu3 F8 N12 O	C18 H22 B2 Cu3 F8 N12 O
Mr	786.75	786.75
Dx, g cm <sup>-3</sup>	1.793	1.793
Z	4	4
Mu (mm <sup>-1</sup> )	2.257	2.257
F000	1564.0	1564.0
F000'	1568.53	
h, k, lmax	20, 12, 21	20, 12, 21
Nref	5722	5713
Tmin, Tmax	0.805, 0.854	0.804, 0.854
Tmin'	0.713	

Correction method= # Reported T Limits: Tmin=0.804 Tmax=0.854  
AbsCorr = MULTI-SCAN

Data completeness= 0.998      Theta (max)= 25.999

R(reflections)= 0.0515 ( 3654)	wR2(reflections)= 0.0930 ( 5713)
S = 1.010	Npar= 413

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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.

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● **Alert level C**

PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00775	Ang.
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of .	35	Ang**3

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	8	Note
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	4	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .....	293	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II)	2.18	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	4	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.1	Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	52.0	Degree

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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  
10 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
1 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.

