

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SD421012621\_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: SD421012621\_0m

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Bond precision:      C-C = 0.0040 Å      Wavelength=0.71073

Cell:                      a=17.127(10)              b=19.946(11)              c=23.841(14)  
                            alpha=90              beta=105.715(7)              gamma=90

Temperature:              150 K

	Calculated	Reported
Volume	7840(8)	7840(8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C72 H94 Cu4 P6, 2(C4 H8 O)	C72 H94 Cu4 P6, 2(C4 H8 O)
Sum formula	C80 H110 Cu4 O2 P6	C80 H110 Cu4 O2 P6
Mr	1543.71	1543.65
Dx, g cm <sup>-3</sup>	1.308	1.308
Z	4	4
Mu (mm <sup>-1</sup> )	1.236	1.236
F000	3248.0	3248.0
F000'	3256.27	
h, k, lmax	22, 25, 30	22, 25, 30
Nref	18017	17898
Tmin, Tmax	0.716, 0.871	0.600, 0.870
Tmin'	0.557	

Correction method= # Reported T Limits: Tmin=0.600 Tmax=0.870  
AbsCorr = MULTI-SCAN

Data completeness= 0.993                      Theta(max)= 27.504

R(reflections)= 0.0332( 13043)	wR2(reflections)=
S = 0.951	0.0839( 17898)
Npar= 847	



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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

PLAT243_ALERT_4_C	High	'Solvent' Ueq as Compared to Neighbors of	C3_2	Check
PLAT243_ALERT_4_C	High	'Solvent' Ueq as Compared to Neighbors of	O1_3	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C4_2	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C4_3	Check
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including	O1_3	0.120 Check
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond C1_3 - C2_3	.	1.41 Ang.
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...			-0.025 Report

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#### Alert level G

PLAT398_ALERT_2_G	Deviating	C-O-C	Angle From 120 for O1_2	107.8 Degree
PLAT398_ALERT_2_G	Deviating	C-O-C	Angle From 120 for O1_3	108.7 Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	.....		26 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1	(I)	.	0.73 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu2	(I)	.	0.59 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu3	(I)	.	0.73 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu4	(I)	.	0.59 Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).			3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		118 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			3 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			2 Info

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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  
7 **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  
6 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  
6 ALERT type 4 Improvement, methodology, query or suggestion  
4 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.



