

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rf1126

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: rf1126

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Bond precision:	C-C = 0.0082 A	Wavelength=0.71073	
Cell:	a=14.0641(15)	b=7.3572(7)	c=24.751(3)
	alpha=90	beta=98.165(5)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2535.1(5)	2535.1(4)	
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C20 H28 Cl Cu N4 O4, Cl O4, H2 O	C20 H28 Cl N4 O4, Cl O4, H2 O	
Sum formula	C20 H30 Cl2 Cu N4 O9	C20 H30 Cl2 Cu N4 O9	
Mr	604.93	604.92	
Dx, g cm <sup>-3</sup>	1.585	1.585	
Z	4	4	
Mu (mm <sup>-1</sup> )	1.129	1.129	
F000	1252.0	1252.0	
F000'	1255.00		
h,k,lmax	17,9,30	17,9,30	
Nref	4980	4965	
Tmin,Tmax	0.794,0.883	0.763,0.890	
Tmin'	0.789		

Correction method= # Reported T Limits: Tmin=0.763 Tmax=0.890  
AbsCorr = MULTI-SCAN

Data completeness= 0.997      Theta(max)= 25.996

R(reflections)= 0.0758( 4460)      wR2(reflections)= 0.1676( 4965)

S = 1.234      Npar= 330

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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 B**

PLAT420_ALERT_2_B	D-H Without Acceptor	09	--H91	.	Please Check
PLAT420_ALERT_2_B	D-H Without Acceptor	09	--H92	.	Please Check

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**Alert level C**

PLAT213_ALERT_2_C	Atom Cl2	has ADP max/min Ratio	.....	3.1	prolat
PLAT244_ALERT_4_C	Low 'Solvent' Ueq	as Compared to Neighbors of		Cl2	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio	for Average U(i,j) Tensor	....	2.4	Note
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds	.....	0.00817	Ang.
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A)	O9	- H91	.	1.04 Ang.
PLAT415_ALERT_2_C	Short Inter D-H..H-X	H10	..H91	.	2.08 Ang.
		1/2-x,1/2+y,3/2-z =		2_556	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....		9.403	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....		2.468	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		5	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.10A	From O9	1.61	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.76A	From O7	0.49	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.58A	From O9	-0.86	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.95A	From O9	-0.75	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.97A	From O5	-0.51	eA-3

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**Alert level G**

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: C20 H30 Cl2 Cu1 N4 O9  
Atom count from \_chemical\_formula\_moiety:C20 H30 Cl2 N4 O9

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms	...		1	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	.....		2	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ				Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large			30.52	Why ?
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records			1	Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II)	.		2.22	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....		6	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	.			Please Do !
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		7	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File	...		2	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			1	Info

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

3 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
14 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
7 **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.

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**PLATON version of 03/05/2019; check.def file version of 29/04/2019**

