

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) isn167\_130k\_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: isn167\_130k\_0m

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Bond precision:    C-C = 0.0046 Å                      Wavelength=1.54178

Cell:              a=15.1949(10)              b=18.5322(12)              c=18.5423(13)  
                    alpha=107.867(2)              beta=104.444(2)              gamma=101.088(2)  
Temperature:    130 K

	Calculated	Reported
Volume	4603.2(5)	4603.2(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C48 H34 Br2 Cu N2 O P2), 2(F6 P), C4 H10 O	C48 H34 Br2 Cu N2 O P2, F6 P, 0.5(C4 H10 O)
Sum formula	C100 H78 Br4 Cu2 F12 N4 O3 P6	C50 H39 Br2 Cu F6 N2 O1.50 P3
Mr	2244.18	1122.10
Dx, g cm <sup>-3</sup>	1.619	1.619
Z	2	4
Mu (mm <sup>-1</sup> )	4.260	4.260
F000	2252.0	2252.0
F000'	2247.94	
h,k,lmax	18,22,22	18,22,22
Nref	17572	16488
Tmin,Tmax	0.458,0.682	0.547,0.753
Tmin'	0.326	

Correction method= # Reported T Limits: Tmin=0.547 Tmax=0.753  
AbsCorr = MULTI-SCAN

Data completeness= 0.938                      Theta(max)= 70.266

R(reflections)= 0.0369( 15466)              wR2(reflections)= 0.0971( 16488)

S = 1.028                                      Npar= 1182

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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**

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	value Low	0.974	Why?
PLAT220_ALERT_2_C	Non-Solvent Resd	2 C Ueq(max)/Ueq(min) Range	3.3	Ratio
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	....	2.5	Note
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C97 - C98	1.40	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C99 - C100	1.39	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	431	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H99B		-0.57	eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.		0	Info

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● **Alert level G**

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings	Differ		Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z	Differ by a Factor ...	0.50	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	6.93	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal	..(Note)	0.002	Degree
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			P5 Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			P6 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C93 ..C93	3.19	Ang.
		2-x,2-y,2-z =	2_777	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	F6 P	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	653	Note
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values	Differ by	3	Check

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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  
8 **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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
8 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  
4 ALERT type 4 Improvement, methodology, query or suggestion  
1 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 07/08/2019; check.def file version of 30/07/2019**

