

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) isn165\_130k

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: isn165\_130k

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Bond precision:    C-C = 0.0092 Å                      Wavelength=1.34143

Cell:                      a=10.9300(4)                      b=14.2927(6)                      c=19.2894(8)  
                                    alpha=70.366(3)                      beta=86.491(3)                      gamma=73.206(3)  
Temperature:    130 K

	Calculated	Reported
Volume	2715.0(2)	2715.0(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C51 H38 Br2 Cu N2 O P2, F6 P, C H2 Cl2 [+ solvent]	C51 H38 Br2 Cu N2 O P2, F6 P, C H2 Cl2, 0.9[C4H10O1]
Sum formula	C52 H40 Br2 Cl2 Cu F6 N2 O P3 [+ solvent]	C55.60 H49 Br2 Cl2 Cu F6 N2 O1.90 P3
Mr	1210.02	1276.74
Dx, g cm <sup>-3</sup>	1.480	1.562
Z	2	2
Mu (mm <sup>-1</sup> )	4.792	4.864
F000	1212.0	1288.0
F000'	1207.75	
h,k,lmax	13,17,24	13,17,24
Nref	11131	10645
Tmin,Tmax	0.506,0.482	0.002,0.794
Tmin'	0.459	

Correction method= # Reported T Limits: Tmin=0.002 Tmax=0.794  
AbsCorr = MULTI-SCAN

Data completeness= 0.956                      Theta(max)= 57.052

R(reflections)= 0.0858( 9958)                      wR2(reflections)= 0.2384( 10645)

S = 1.059                      Npar= 624

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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.

### ● Alert level C

PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C52	Check
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor ....	2.1	Note
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor ....	2.2	Note
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including C11	0.102	Check
PLAT341_ALERT_3_C	Low	Bond Precision on C-C Bonds .....	0.00915	Ang.
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance .....	2.674	Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L= 0.600	101	Report
PLAT918_ALERT_3_C	Reflection(s)	with I(obs) much Smaller I(calc) .	24	Check
PLAT977_ALERT_2_C	Check	Negative Difference Density on H52A	-0.39	eA-3
PLAT978_ALERT_2_C	Number	C-C Bonds with Positive Residual Density.	0	Info

### ● Alert level G

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
 \_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
 Atom count from \_chemical\_formula\_sum: C55.6 H49 Br2 Cl2 Cu1 F6 N2 O1.9  
 Atom count from the \_atom\_site data: C52 H40 Br2 Cl2 Cu1 F6 N2 O1 P3

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
 not performed for this radiation type.

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.

CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a  
 symmetry error - see SYMMG tests

From the CIF: \_cell\_formula\_units\_Z 2

From the CIF: \_chemical\_formula\_sum C55.60 H49 Br2 Cl2 Cu F6 N2 O1.90

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	111.20	104.00	7.20
H	98.00	80.00	18.00
Br	4.00	4.00	0.00
Cl	4.00	4.00	0.00
Cu	2.00	2.00	0.00
F	12.00	12.00	0.00
N	4.00	4.00	0.00
O	3.80	2.00	1.80
P	6.00	6.00	0.00

PLAT041_ALERT_1_G	Calc. and Reported SumFormula	Strings Differ	Please	Check
PLAT051_ALERT_1_G	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	1.47 %		
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check	
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.14	Report	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.65	Why ?	
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003	Degree	
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P3	Check	
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	363	A**3	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	6	Note	
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info	
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed	!	Info	
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	384	Note	
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....	Please	Check	
PLAT984_ALERT_1_G	The C-f'= 0.0148 Deviates from the B&C-Value	0.0137	Check	
PLAT984_ALERT_1_G	The Br-f'= -0.9501 Deviates from the B&C-Value	-0.9338	Check	
PLAT984_ALERT_1_G	The Cu-f'= -2.9183 Deviates from the B&C-Value	-2.7974	Check	
PLAT984_ALERT_1_G	The F-f'= 0.0600 Deviates from the B&C-Value	0.0583	Check	
PLAT984_ALERT_1_G	The N-f'= 0.0253 Deviates from the B&C-Value	0.0241	Check	

PLAT984_ALERT_1_G	The O-f' =	0.0412	Deviates from the B&C-Value	0.0389	Check
PLAT984_ALERT_1_G	The P-f' =	0.2596	Deviates from the B&C-Value	0.2543	Check
PLAT985_ALERT_1_G	The Br-f" =	1.0411	Deviates from the B&C-Value	1.0006	Check
PLAT985_ALERT_1_G	The Cu-f" =	3.6937	Deviates from the B&C-Value	3.6876	Check
PLAT985_ALERT_1_G	The F-f" =	0.0411	Deviates from the B&C-Value	0.0400	Check
PLAT985_ALERT_1_G	The P-f" =	0.3354	Deviates from the B&C-Value	0.3332	Check
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt		Values Differ by	1	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  
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
30 **ALERT level G** = General information/check it is not something unexpected

18 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  
5 ALERT type 3 Indicator that the structure quality may be low  
7 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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## Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT244_isn165_130k
;
PROBLEM: Low      'Solvent' Ueq as Compared to Neighbors of      C52 Check
RESPONSE: ...
;
_vrf_PLAT250_isn165_130k
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.1 Note
RESPONSE: ...
;
_vrf_PLAT260_isn165_130k
;
PROBLEM: Large Average Ueq of Residue Including      C11      0.102 Check
RESPONSE: ...
;
_vrf_PLAT341_isn165_130k
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.00915 Ang.
RESPONSE: ...
;
_vrf_PLAT906_isn165_130k
;
PROBLEM: Large K Value in the Analysis of Variance .....      2.674 Check
RESPONSE: ...
;
_vrf_PLAT911_isn165_130k
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      101 Report
RESPONSE: ...
;
_vrf_PLAT918_isn165_130k
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .      24 Check
RESPONSE: ...
;
```

```
_vrf_PLAT977_isn165_130k
;
PROBLEM: Check Negative Difference Density on H52A          -0.39 eA-3
RESPONSE: ...
;
_vrf_PLAT978_isn165_130k
;
PROBLEM: Number C-C Bonds with Positive Residual Density.    0 Info
RESPONSE: ...
;
# end Validation Reply Form
```

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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**

