

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ALM007A\_123K

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: ALM007A\_123K

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Bond precision:    C-C = 0.0038 A

Wavelength=1.54178

Cell:                a=10.9132(6)                b=14.9862(9)                c=15.3881(9)  
                      alpha=83.394(3)            beta=73.300(3)            gamma=72.099(3)  
Temperature:        123 K

	Calculated	Reported
Volume	2292.9(2)	2292.9(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C53 H42 Cu N2 O P2, F6 P	C53 H42 Cu1 F6 N2 O1 P3
Sum formula	C53 H42 Cu F6 N2 O P3	C53 H42 Cu1 F6 N2 O1 P3
Mr	993.35	993.38
Dx,g cm-3	1.439	1.439
Z	2	2
Mu (mm-1)	2.228	2.228
F000	1020.0	1020.0
F000'	1020.72	
h,k,lmax	13,18,18	13,18,18
Nref	8723	8415
Tmin,Tmax	0.895,0.935	0.780,0.940
Tmin'	0.895	

Correction method= # Reported T Limits: Tmin=0.780 Tmax=0.940  
AbsCorr = MULTI-SCAN

Data completeness= 0.965

Theta(max)= 70.144

R(reflections)= 0.0471( 7317)

wR2(reflections)= 0.1180( 8406)

S = 0.994

Npar= 721

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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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .....	0.965 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600	77 Report



### Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	94 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .....	0.00300 Degree
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	42 Note
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 -- P1 ..	5.5 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 -- P2 ..	6.0 su
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of	P3 Check
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....	270 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...	2 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	234 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not checked	! Info
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ...	12 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  
 2 **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
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 3 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  
 3 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_PLAT029_ALM007A_123K
;
PROBLEM: _diffrn_measured_fraction_theta_full Low .....      0.965 Note
RESPONSE: ...
;
_vrf_PLAT911_ALM007A_123K
;
PROBLEM: Missing # FCF Refl Between THmin & STh/L= 0.600      77 Report
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*, 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.

