checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ISN106_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: ISN106_123K

Bond precision: C-C = 0.0045 A   Wavelength=1.54178

Cell: a=13.8102(4)   b=18.4985(6)   c=18.0974(6)
                 alpha=90   beta=107.7455(16)   gamma=90
Temperature: 123 K

	Calculated	Reported
Volume	4403.3(2)	4403.3(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2yc
Moiety formula	C46 H43 Cu N O P2 S, F6 P	C46 H43 Cu1 F6 N1 O1 P3 S1
Sum formula	C46 H43 Cu F6 N O P3 S	C46 H43 Cu1 F6 N1 O1 P3 S1
Mr	928.33	928.37
Dx,g cm-3	1.400	1.400
Z	4	4
Mu (mm-1)	2.699	2.699
F000	1912.0	1912.0
F000'	1914.20	
h,k,lmax	16,22,22	16,22,21
Nref	8404	7939
Tmin,Tmax	0.806,0.874	0.760,0.870
Tmin'	0.806	

Correction method= # Reported T Limits: Tmin=0.760 Tmax=0.870
AbsCorr = MULTI-SCAN

Data completeness= 0.945   Theta(max)= 70.321

R(reflections)= 0.0530(6739)   wR2(reflections)= 0.1388(7893)

S = 0.991   Npar= 532

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 B**
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).   36 Note

🟡 **Alert level C**
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .   0.978 Why?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.08 Report
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit   -P 2yc
PLAT220_ALERT_2_C Non-Solvent Resd 1 C   Ueq(max)/Ueq(min) Range   3.3 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C3 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.1 Note
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .   38 Ang**3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   159 Report

⚪ **Alert level G**
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) P3   --F5   .   5.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1   --P2   .   5.5 s.u.
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of   P3 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #   2 Note
            F6 P
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found   Please Check
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......   Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   310 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....   1 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) ...   8 Check

   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   1 **ALERT level B** = A potentially serious problem, consider carefully
   8 **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

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

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_ISN106_123K
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .      0.978 Why?
RESPONSE: ...
;
_vrf_PLAT094_ISN106_123K
;
PROBLEM: Ratio of Maximum / Minimum Residual Density ....       2.08 Report
RESPONSE: ...
;
_vrf_PLAT127_ISN106_123K
;
PROBLEM: Implicit Hall Symbol  Inconsistent with Explicit     -P 2yc
```

```
RESPONSE: ...
;
_vrf_PLAT220_ISN106_123K
;
PROBLEM: Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
RESPONSE: ...
;
_vrf_PLAT241_ISN106_123K
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of       C3 Check
RESPONSE: ...
;
_vrf_PLAT250_ISN106_123K
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.1 Note
RESPONSE: ...
;
_vrf_PLAT601_ISN106_123K
;
PROBLEM: Structure Contains Solvent Accessible VOIDS of .       38 Ang**3
RESPONSE: ...
;
_vrf_PLAT911_ISN106_123K
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600       159 Report
RESPONSE: ...
;
# end Validation Reply Form
```

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.

Datablock ISN106_123K - ellipsoid plot