checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: p21

```
Bond precision:  C-C = 0.0200 A          Wavelength=0.71073

Cell:            a=8.4404(4)    b=9.3829(5)          c=17.692(1)
                 alpha=90       beta=115.385(4)      gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	1265.84(12)	1265.84(12)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(C8 H16 N), Cl6 Sn	C16 H32 Cl6 N2 Sn
Sum formula	C16 H32 Cl6 N2 Sn	C16 H32 Cl6 N2 Sn
Mr	583.85	583.82
Dx,g cm-3	1.532	1.532
Z	2	2
Mu (mm-1)	1.647	1.647
F000	588.0	588.0
F000’	588.57	
h,k,lmax	10,11,21	10,11,21
Nref	2222	2252
Tmin,Tmax	0.715,0.731	0.715,0.731
Tmin’	0.701	

```
Correction method= # Reported T Limits: Tmin=0.715 Tmax=0.731
AbsCorr = MULTI-SCAN

Data completeness= 1.014          Theta(max)= 25.026

R(reflections)= 0.0650( 2087)     wR2(reflections)= 0.1950( 2252)

S = 1.219                 Npar= 126
```

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

```
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full          ! Check
PLAT021_ALERT_4_C Ratio Unique / Expected Reflections too High ...      1.014
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .     0.972 Why?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.34 Report
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Sn1 Check
PLAT245_ALERT_2_C U(iso) H2        Smaller than U(eq) C2        by     0.012 Ang**2
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............      0.02 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H7A      ..CL3      .      2.87 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H4A      ..CL1      .      2.89 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1B      ..CL3      .      2.90 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H7A      ..CL3      .      2.87 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H4A      ..CL1      .      2.89 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF    Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical         ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     17.72 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  P21/c       P21/n Note
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.          2 Note
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Sn1       (IV)      .      3.95 Info
```

---

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
8 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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.

PLATON version of 06/01/2019; check.def file version of 19/12/2018

Datablock p21 - ellipsoid plot