

## 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: g160104c

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Bond precision:	C-C = 0.0069 A	Wavelength=0.71073
Cell:	a=16.8486(15)	b=13.7348(9)      c=19.0796(19)
	alpha=90	beta=92.053(8)      gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	4412.4(7)	4412.4(7)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C19 H28 N2 O4 Sn	C19 H28 N2 O4 Sn
Sum formula	C19 H28 N2 O4 Sn	C19 H28 N2 O4 Sn
Mr	467.14	467.12
Dx, g cm <sup>-3</sup>	1.406	1.406
Z	8	8
Mu (mm <sup>-1</sup> )	1.181	1.181
F000	1904.0	1904.0
F000'	1899.48	
h, k, lmax	20, 16, 22	20, 16, 22
Nref	3917	3912
Tmin, Tmax	0.790, 0.799	0.798, 0.807
Tmin'	0.790	

Correction method= # Reported T Limits: Tmin=0.798 Tmax=0.807  
AbsCorr = MULTI-SCAN

Data completeness= 0.999      Theta(max)= 25.100

R(reflections)= 0.0372( 2800)	wR2(reflections)=
S = 1.023	0.0954( 3912)
Npar= 239	

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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

PLAT199_ALERT_1_C	Reported _cell_measurement_temperature .....	(K)	293	Check
PLAT200_ALERT_1_C	Reported _diffn_ambient_temperature .....	(K)	293	Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range		3.8	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C18 --C19		6.0	s.u.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C10	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C14	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C17	Check
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C18 - C19		1.36	Ang.
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of		100	Ang**3

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#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		2	Note
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please	Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....		1	Report
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as		mixed	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		1	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		1	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL/		2018	Note

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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  
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **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  
1 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

