

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:    O- C = 0.0050 A                      Wavelength=0.71073

Cell:                      a=10.9403(10)              b=12.7296(11)              c=10.5843(9)  
                                    alpha=90                      beta=103.353(7)              gamma=90

Temperature:              200 K

	Calculated	Reported
Volume	1434.2(2)	1434.2(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C6 H18 O8 P2 Sn	C6 H18 O8 P2 Sn
Sum formula	C6 H18 O8 P2 Sn	C6 H18 O8 P2 Sn
Mr	398.85	398.83
Dx,g cm-3	1.847	1.847
Z	4	4
Mu (mm-1)	2.028	2.028
F000	792.0	792.0
F000'	790.59	
h,k,lmax	13,15,12	13,15,12
Nref	2515	2516
Tmin,Tmax	0.647,0.922	0.779,0.923
Tmin'	0.406	

Correction method= # Reported T Limits: Tmin=0.779 Tmax=0.923  
AbsCorr = INTEGRATION

Data completeness= 1.000                      Theta(max)= 24.991

R(reflections)= 0.0227( 1793)              wR2(reflections)= 0.0534( 2516)

S = 0.918                      Npar= 160

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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 B**PLAT019\_ALERT\_1\_B \_diffn\_measured\_fraction\_theta\_full/\_max < 1.0 0.969 Report

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**Alert level C**PLAT242\_ALERT\_2\_C Low Ueq as Compared to Neighbors for ..... P1 Check  
PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 3.590 Check

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**Alert level G**PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 1 Info  
PLAT764\_ALERT\_4\_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.11 Ratio  
PLAT909\_ALERT\_3\_G Percentage of Observed Data at Theta(Max) still 51 %  
PLAT953\_ALERT\_1\_G Reported (CIF) and Actual (FCF) Hmax Differ by . 1 Units  
PLAT961\_ALERT\_5\_G Dataset Contains no Negative Intensities ..... Please Check

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
1 **ALERT level B** = A potentially serious problem, consider carefully  
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
5 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 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  
1 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*, 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 29/01/2015; check.def file version of 29/01/2015

Datablock shelx - ellipsoid plot

