

# 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: 6559

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Bond precision:    As- O = 0.0119 A                      Wavelength=0.71073

Cell:                      a=13.2681(6)              b=6.6209(3)              c=10.8113(5)  
                            alpha=90                      beta=90                      gamma=90  
Temperature:              293 K

	Calculated	Reported
Volume	949.74(8)	949.74(7)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	As8 O40 Sn3.85 Ti4.15, 8(K)	?
Sum formula	As8 K8 O40 Sn3.85 Ti4.15	As2 K2 O10 Sn0.96 Ti1.04
Mr	2208.00	551.98
Dx,g cm-3	3.861	3.860
Z	1	4
Mu (mm-1)	11.236	11.235
F000	1019.9	1020.0
F000'	1021.04	
h,k,lmax	17,8,14	17,8,14
Nref	2348[ 1234]	2348
Tmin,Tmax	0.245,0.863	0.146,0.859
Tmin'	0.066	

Correction method= # Reported T Limits: Tmin=0.146 Tmax=0.859  
AbsCorr = GAUSSIAN

Data completeness= 1.90/1.00                      Theta(max)= 28.268

R(reflections)= 0.0502( 2235)                      wR2(reflections)= 0.1054( 2348)

S = 1.175                                      Npar= 108

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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

STRVA01_ALERT_4_C	Flack test results are ambiguous.	
	From the CIF: <code>_refine_ls_abs_structure_Flack</code>	0.460
	From the CIF: <code>_refine_ls_abs_structure_Flack_su</code>	0.040
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.47 Report
PLAT220_ALERT_2_C	Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range	3.6 Ratio

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### Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.25 Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	16.23 Why ?
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem n	85 %Fit
PLAT113_ALERT_2_G	ADDSYM Suggests Possible Pseudo/New Space Group	Pcca Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2 Report
PLAT199_ALERT_1_G	Reported <code>_cell_measurement_temperature</code> ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported <code>_diffrn_ambient_temperature</code> ..... (K)	293 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	14% Note
PLAT883_ALERT_1_G	No Info/Value for <code>_atom_sites_solution_primary</code> .	Please Do !
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2 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  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **ALERT level G** = General information/check it is not something unexpected
- 5 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  
1 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
1 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.

