

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

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Bond precision:	C-C = 0.0050 A	Wavelength=0.71073
Cell:	a=21.1006(3)      b=8.53683(13)      c=24.3975(4)	alpha=90      beta=98.4941(15)      gamma=90
Temperature:	230 K	
	Calculated	Reported
Volume	4346.57(12)	4346.57(12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C54 H110 Cl10 Cs4 N2 O26 Sb2	2(Cs), Cl5 Sb, 2(Cl2 H24 O6), C3 H7 N1 O1
Sum formula	C54 H110 Cl10 Cs4 N2 O26 Sb2	C27 H55 Cl5 Cs2 N O13 Sb
Mr	2333.10	1166.54
Dx, g cm <sup>-3</sup>	1.783	1.783
Z	2	4
Mu (mm <sup>-1</sup> )	2.646	2.646
F000	2296.0	2296.0
F000'	2294.52	
h,k,lmax	29,11,33	29,11,33
Nref	12189	12187
Tmin,Tmax	0.747,0.974	0.844,0.845
Tmin'	0.728	

Correction method= # Reported T Limits: Tmin=0.844 Tmax=0.845  
AbsCorr = MULTI-SCAN

Data completeness= 1.000      Theta(max)= 29.575

R(reflections)= 0.0376( 8574)      wR2(reflections)= 0.0587( 12187)

S = 0.995      Npar= 631

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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**

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 5.074 Check

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**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 46 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 46 Report  
PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.50 Check  
PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 4 Report  
PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records 5 Report  
PLAT177\_ALERT\_4\_G The CIF-Embedded .res File Contains DELU Records 2 Report  
PLAT187\_ALERT\_4\_G The CIF-Embedded .res File Contains RIGU Records 2 Report  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Sb1 --Cl1 . 12.8 s.u.  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Sb1 --Cl3 . 6.4 s.u.  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Sb1 --Cl4 . 14.2 s.u.  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1 ) 47% Note  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 6 Note  
PLAT780\_ALERT\_1\_G Coordinates do not Form a Properly Connected Set Please Do !  
PLAT811\_ALERT\_5\_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 616 Note  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 1 Info

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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  
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
18 **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  
4 ALERT type 3 Indicator that the structure quality may be low  
5 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.

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**PLATON version of 22/04/2020; check.def file version of 09/03/2020**

