

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

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 ⁻³	1.783	1.783
Z	2	4
Mu (mm ⁻¹)	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

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.074 Check



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.

