

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) VV_ML83_III_0ma_a

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: VV_ML83_III_0ma_a

Bond precision:	C-C = 0.0163 A	Wavelength=0.71073
Cell:	a=13.9459(8)	b=31.1012(19) c=10.9557(7)
	alpha=90	beta=105.449(2) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	4580.2(5)	4580.2(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C39 H29 Au2 O P2, F6 Sb, 2(C5 H10)	?
Sum formula	C49 H49 Au2 F6 O P2 Sb	C49 H49 Au2 F6 O P2 Sb
Mr	1345.52	1345.50
Dx,g cm-3	1.951	1.951
Z	4	4
Mu (mm-1)	7.107	7.107
F000	2576.0	2576.0
F000'	2560.11	
h,k,lmax	16,37,13	16,37,13
Nref	8244	8204
Tmin,Tmax	0.390,0.509	0.474,0.745
Tmin'	0.072	

Correction method= # Reported T Limits: Tmin=0.474 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 25.188

R(reflections)= 0.0419(6409) wR2(reflections)= 0.1088(8204)

S = 1.083 Npar= 603

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 B

PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 1 Check

Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio
 PLAT234_ALERT_4_C Large Hirshfeld Difference C34 --C35 . 0.17 Ang.
 PLAT234_ALERT_4_C Large Hirshfeld Difference Sb1 --F1 . 0.18 Ang.
 PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C44 Check
 PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C49 Check
 PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C43 Check
 PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C45 Check
 PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C48 Check
 PLAT260_ALERT_2_C Large Average Ueq of Residue Including Sb1 0.086 Check
 PLAT260_ALERT_2_C Large Average Ueq of Residue Including Sb1' 0.093 Check
 PLAT260_ALERT_2_C Large Average Ueq of Residue Including C40 0.091 Check
 PLAT260_ALERT_2_C Large Average Ueq of Residue Including C45 0.119 Check
 PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01629 Ang.
 PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C40 - C44 . 1.43 Ang.
 PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C45 - C49 . 1.40 Ang.
 PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.553 Check
 PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.599 33 Report
 PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
 PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1 Check
 PLAT977_ALERT_2_C Check Negative Difference Density on H26 -0.42 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H39A -0.36 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H47B -0.32 eA-3
 PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 14 Note
 PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
 PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 1 Report
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
 PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 2 4.24 Check
 PLAT304_ALERT_4_G Non-Integer Number of Atoms in Resd 3 2.77 Check
 PLAT343_ALERT_2_G Unusual Angle Range in Main Residue for C37 Check
 PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O1 106.2 Degree
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 21 Note
 PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 54% Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 24 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 14 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check

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.

