

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) GM31_23_0m_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: GM31_23_0m_a

Bond precision:	C-C = 0.0078 A	Wavelength=0.71073	
Cell:	a=14.2376(12)	b=20.6038(17)	c=20.3351(16)
	alpha=90	beta=104.476(3)	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	5775.9(8)	5775.9(8)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C66 H52 Ag N2 O P2 S2, B F4 ?		
Sum formula	C66 H52 Ag B F4 N2 O P2 S2	C66 H52 Ag B F4 N2 O P2 S2	
Mr	1209.84	1209.83	
Dx, g cm-3	1.391	1.391	
Z	4	4	
Mu (mm-1)	0.535	0.535	
F000	2480.0	2480.0	
F000'	2479.18		
h,k,lmax	16,24,24	16,24,24	
Nref	10170	10152	
Tmin,Tmax	0.950,0.968	0.617,0.746	
Tmin'	0.852		

Correction method= # Reported T Limits: Tmin=0.617 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 24.998

R(reflections)= 0.0649(7846)	wR2(reflections)= 0.1143(10152)
S = 1.171	Npar= 714

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

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Agl --P1 . 10.6 s.u.

Author Response: The assignment of the atom types is correct. The alert is probably due to the size difference between Ag and P.

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Agl --P2 . 11.0 s.u.

Author Response: The assignment of the atom types is correct. The alert is probably due to the size difference between Ag and P.



Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.127

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.0 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.9 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference S1 --C21 . 0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C18 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including F1 0.112 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 20.679 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.988 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 10 Note
1 0 0, 1 1 0, 0 2 0, -1 1 1, 0 1 1, 1 1 1,
0 2 1, -1 0 2, 0 0 2, 0 1 2,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 8 Report
-2 0 2, -11 4 20, -11 5 20, 2 0 22, -8 1 23, -8 2 23,
-3 0 24, -6 1 24,



Alert level G

PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 0.127 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 10.28 Why ?
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of B1 Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 65% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 6 Note
0 2 1, -8 1 23, 0 1 2, -6 1 24, -2 0 2, -8 2 23,
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.48 Note
Predicted wR2: Based on SigI**2 3.29 or SHELX Weight 10.12

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

