

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) GM16_22B_0m

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: GM16_22B_0m

Bond precision: C-C = 0.0092 A

Wavelength=0.71073

Cell: a=17.5294 (8) b=18.6280 (9) c=19.9345 (9)
 alpha=70.918 (3) beta=67.775 (2) gamma=82.362 (3)
Temperature: 296 K

	Calculated	Reported
Volume	5694.3 (5)	5694.3 (5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C66 H51 Ag N2 O3 P2, C66 H52 Ag N2 O3 P2, 2(F6 P)	?
Sum formula	C132 H103 Ag2 F12 N4 O6 P6	C132 H103 Ag2 F12 N4 O6 P6
Mr	2470.75	2470.75
Dx, g cm ⁻³	1.441	1.441
Z	2	2
Mu (mm ⁻¹)	0.508	0.508
F000	2526.0	2526.0
F000'	2524.80	
h, k, lmax	20, 22, 23	15, 22, 23
Nref	20060	17980
Tmin, Tmax	0.823, 0.867	0.650, 0.746
Tmin'	0.776	

Correction method= # Reported T Limits: Tmin=0.650 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.896

Theta(max)= 25.000

R(reflections)= 0.0535 (13600)

wR2(reflections)=
0.1463 (17980)

S = 1.081

Npar= 1462

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 A**

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.896 Why?

Author Response: This is due to diffractions with low intensity at high angles.

 **Alert level B**

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ag1 --P1 . 17.1 s.u.

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

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ag2 --P4 . 15.0 s.u.

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 14 Note
1 0 0, -1 1 0, 0 1 0, 1 1 0, 0 -1 1, 1 -1 1,
-1 0 1, 0 0 1, 1 0 1, -1 1 1, 0 1 1, 1 1 1,
1 0 2, 1 1 2,

Author Response: These reflections are affected by the beamstop.

 **Alert level C**

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C113 --C114 . 6.4 s.u.
PLAT231_ALERT_4_C Hirshfeld Test (Solvent) P5 --F6 . 6.9 s.u.
PLAT231_ALERT_4_C Hirshfeld Test (Solvent) P6 --F9 . 5.6 s.u.
PLAT231_ALERT_4_C Hirshfeld Test (Solvent) P6 --F12 . 9.0 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference P5 --F3 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P5 --F5 . 0.16 Ang.
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 4) 2.2 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including P5 0.201 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including P6 0.208 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C24 -C29 . 1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00915 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H26 ..H30A . 1.90 Ang.
x,y,z = 1_555 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.217 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 263 Report

2	0	0,	0	2	0,	15	7	0,	15	8	0,	15	9	0,	15	10	0,
15	11	0,	15	12	0,	15	13	0,	-11	17	0,	-9	18	0,	15-13	1,	
-15	-12	1,	-15	-11	1,	-15	-10	1,	-15	-9	1,	-15	-8	1,	-15	-7	1,
-1	-1	1,	2	-1	1,	4	1	1,	1	2	1,	15	7	1,	15	8	1,
15	9	1,	15	10	1,	15	11	1,	15	12	1,	15	13	1,	15	14	1,
-11	17	1,	10-17	2,	10-16	2,	12-16	2,	15-12	2,	-15-11	2,					
-15	-10	2,	-15	-9	2,	-15	-8	2,	-15	-7	2,	0	0	2,	0	1	2,
15	7	2,	15	8	2,	15	9	2,	15	10	2,	15	11	2,	15	12	2,
15	13	2,	15	14	2,	-8	18	2,	-7	19	2,	8-18	3,	9-17	3,		
10-17	3,	15-13	3,	-15-10	3,	-15	-9	3,	-15	-8	3,	15	7	3,	15	8	3,
15	8	3,	15	9	3,	15	10	3,	15	11	3,	15	12	3,	15	13	3,
15	14	3,	15	15	3,	-9	17	3,	-8	19	3,	10-17	4,	10-16	4,		
15-12	4,	-15	-9	4,	-15	-8	4,	15	7	4,	15	8	4,	15	9	4,	
15	10	4,	15	11	4,	15	12	4,	-13	13	4,	15	13	4,	15	14	4,
15	15	4,	-5	20	4,	7-18	5,	12-15	5,	-15	-8	5,	15	7	5,		
15	8	5,	15	9	5,	15	10	5,	15	11	5,	15	12	5,	15	13	5,

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.60 Why ?
 PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P5 Check
 PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P6 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 59% Note
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 9 Note
 0 0 2, 2 -1 1, 4 1 1, 1 2 1, 12-15 6, 10-17 3,
 10-17 4, 15-12 4, 13-14 6,
 PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 5 Units
 PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 5 Units
 PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
 PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged 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 5.52 Note
 Predicted wR2: Based on SigI**2 2.65 or SHELX Weight 14.12
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

- 2 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
 - 6 ALERT type 3 Indicator that the structure quality may be low
 - 9 ALERT type 4 Improvement, methodology, query or suggestion
 - 4 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.

