

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) gm7_23_a_sq

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: gm7_23_a_sq

Bond precision: C-C = 0.0094 Å Wavelength=0.71073

Cell: a=19.328(4) b=19.328(4) c=32.247(6)
 alpha=90 beta=90 gamma=120

Temperature: 293 K

	Calculated	Reported
Volume	10433(5)	10433(5)
Space group	P 31 2 1	P 31 2 1
Hall group	P 31 2 "	P 31 2 "
Moiety formula	C72 H66 Ag N4 O P2 [+ solvent]	?
Sum formula	C72 H66 Ag N4 O P2 [+ solvent]	C72 H66 Ag F0 N4 O P2
Mr	1173.10	1173.10
Dx, g cm ⁻³	1.120	1.120
Z	6	6
Mu (mm ⁻¹)	0.377	0.377
F000	3666.0	3666.0
F000'	3662.98	
h, k, lmax	23, 23, 38	22, 22, 38
Nref	12317[6746]	12286
Tmin, Tmax	0.798, 0.860	0.750, 0.860
Tmin'	0.798	

Correction method= # Reported T Limits: Tmin=0.750 Tmax=0.860
AbsCorr = MULTI-SCAN

Data completeness= 1.82/1.00 Theta(max)= 25.056

R(reflections)= 0.0366(11128)

wR2(reflections)=
0.0864(12286)

S = 1.079

Npar= 743

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

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 7.2 Ratio

Author Response: This alert is generated because there is a significant amount of disorder in the structure.

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ag1 --P1 . 13.2 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) Ag1 --P2 . 13.5 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.

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note

0 1 0, -1 2 0, 0 2 0, -1 1 1, 0 1 1, -1 2 1,
-1 1 2, 0 1 2, 0 0 3, -1 1 3, 0 1 3,

Author Response: These reflections are affected by the beamstop.



Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 4.3 Ratio

Author Response: This alert is generated because there is a significant amount of disorder in the structure.

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 8.1 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for N3 --C33 . 6.4 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference N4 --C21 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21 --C22 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C64 --C65 . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C69 --C70 . 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 01 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of N3 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C23 Check
 PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00936 Ang.
 PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C33 - C34 . 1.40 Ang.
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.596 8 Report
 0 2 1, -12 23 1, -11 23 1, 0 0 6, -16 22 6, -6 22 6,
 -8 21 15, -3 18 21,

Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 6

From the CIF: _chemical_formula_sum C72 H66 Ag F0 N4 O P2

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	432.00	432.00	0.00
H	396.00	396.00	0.00
Ag	6.00	6.00	0.00
F	6.00	0.00	6.00
N	24.00	24.00	0.00
O	6.00	6.00	0.00
P	12.00	12.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
 PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 9 Report
 PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF Please Check
 PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
 Calc: C72 H66 Ag N4 O P2
 Rep.: C72 H66 Ag F0 N4 O P2
 PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.07 Why ?
 PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
 PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 2 Report
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
 PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
 PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
 PLAT301_ALERT_3_G Main Residue Disorder (Resd 1) 3% Note
 PLAT410_ALERT_2_G Short Intra H...H Contact H31 ..H35D . 2.01 Ang.
 x,y,z = 1_555 Check
 PLAT410_ALERT_2_G Short Intra H...H Contact H33B ..H35B . 1.83 Ang.
 x,y,z = 1_555 Check
 PLAT412_ALERT_2_G Short Intra XH3 .. XHn H34C ..H36F . 2.13 Ang.
 x,y,z = 1_555 Check
 PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
 PLAT722_ALERT_1_G Angle Calc 98.00, Rep 99.20 Dev... 1.20 Degree
 N3 -C35 -H35A 1_555 1_555 1_555 # 143 Check
 PLAT722_ALERT_1_G Angle Calc 98.00, Rep 99.20 Dev... 1.20 Degree
 N3 -C35 -H35B 1_555 1_555 1_555 # 145 Check
 PLAT722_ALERT_1_G Angle Calc 111.00, Rep 109.50 Dev... 1.50 Degree
 H36B -C36 -H36C 1_555 1_555 1_555 # 152 Check
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 64 Note
 PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
 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 77% Note
 PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
 0 0 6,

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.93 Note
 Predicted wR2: Based on SigI**2 2.20 or SHELX Weight 8.29
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 16 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
 10 ALERT type 4 Improvement, methodology, query or suggestion
 1 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.

Datablock gm7_23_a_sq - ellipsoid plot

