checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 2020_06_30_dt_btma-au-hcl_n

Bond precision: C-C = 0.0036 A Wavelength=0.71073

Cell: a=16.7055(3) b=14.3876(2) c=13.9779(2)
alpha=90 beta=114.613(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3054.37(10)	3054.37(9)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C10 H16 N, Au Cl4	C10 H16 N, Au Cl4
Sum formula	C10 H16 Au Cl4 N	C10 H16 Au Cl4 N
Mr	489.01	489.00
Dx,g cm-3	2.127	2.127
Z	8	8
Mu (mm-1)	10.308	10.308
F000	1840.0	1840.0
F000'	1830.08	
h,k,lmax	20,17,17	20,17,17
Nref	3127	3126
Tmin,Tmax	0.342,0.662	0.304,0.704
Tmin'	0.150	

Correction method= # Reported T Limits: Tmin=0.304 Tmax=0.704
AbsCorr = ANALYTICAL

Data completeness= 1.000 Theta(max)= 26.372

R(reflections)= 0.0120(2894) wR2(reflections)= 0.0257(3126)

S = 1.069 Npar= 150

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 G

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl14 ..Cl16 . 3.35 Ang.
-1/2+x,-1/2+y,z = 3_445 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Au12 (III) . 3.00 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Au15 (III) . 2.98 Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
1 1 0,

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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
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
2 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

Datablock 2020_06_30_dt_btma-au-hcl_n - ellipsoid plot

