

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: y1

Bond precision:	C-C = 0.0113 A	Wavelength=0.71073
Cell:	a=12.0922(16)	b=5.6654(7) c=21.731(3)
	alpha=90	beta=116.040(6) gamma=90
Temperature:	296 K	
	Calculated	Reported
Volume	1337.6(3)	1337.6(3)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	C24 H16 Ag2 Br4 N6	?
Sum formula	C24 H16 Ag2 Br4 N6	C24 H16 Ag2 Br4 N6 O0
Mr	923.77	923.77
Dx,g cm-3	2.294	2.294
Z	2	2
Mu (mm-1)	7.465	7.465
F000	872.0	872.0
F000'	866.50	
h,k,lmax	15,7,28	15,7,28
Nref	3089	3071
Tmin,Tmax	0.112,0.408	0.236,1.000
Tmin'	0.069	

Correction method= # Reported T Limits: Tmin=0.236 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 27.520

R(reflections)= 0.0455(2123) wR2(reflections)= 0.1422(3071)

S = 1.032 Npar= 163

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 C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan

PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of C3 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01125 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C24 H16 Ag2 Br4 N6

● 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 2
From the CIF: _chemical_formula_sum C24 H16 Ag2 Br4 N6 O0
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	48.00	48.00	0.00
H	32.00	32.00	0.00
Ag	4.00	4.00	0.00
Br	8.00	8.00	0.00
N	12.00	12.00	0.00
O	2.00	0.00	2.00

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P21/c P21/n Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.14 Ratio
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2018 Note

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

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

