

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: dq0052a

Bond precision: C-C = 0.0063 Å Wavelength=0.71073

Cell: a=14.9546(12) b=17.323(2) c=8.1940(7)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2122.7(3)	2122.7(4)
Space group	F m m 2	F mm2
Hall group	F 2 -2	?
Moiety formula	C20 H30 Br2 U	?
Sum formula	C20 H30 Br2 U	C20 H30 Br2 U
Mr	668.27	668.29
Dx,g cm-3	2.091	2.091
Z	4	4
Mu (mm-1)	11.410	11.410
F000	1248.0	1248.0
F000'	1208.40	
h,k,lmax	24,28,13	23,27,13
Nref	2549[1349]	2388
Tmin,Tmax	0.128,0.504	0.209,0.548
Tmin'	0.082	

Correction method= # Reported T Limits: Tmin=0.209 Tmax=0.548
AbsCorr = MULTI-SCAN

Data completeness= 1.77/0.94 Theta(max)= 35.350

R(reflections)= 0.0180(2385) wR2(reflections)= 0.0660(2388)

S = 1.270 Npar= 62

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

PLAT213_ALERT_2_C	Atom C5	has ADP max/min Ratio	3.9	prolat
PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ...		2.4	Note



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		1	Report
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF			Please Do !
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) U1 -- Br1 ..		8.0	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of *H6A is Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H6B is Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H6C is Constrained at		0.5	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		7	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL		2014	Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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*, 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.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock dq0052a - ellipsoid plot

