

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3

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: 3

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Bond precision:	C-C = 0.0192 Å	Wavelength=0.71073
Cell:	a=9.1223(4)	b=11.6466(6)      c=13.1976(6)
	alpha=90	beta=92.073(4)      gamma=90
Temperature:	170 K	
	Calculated	Reported
Volume	1401.25(11)	1401.25(11)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C12 H9 Br Hg N2 O4	?
Sum formula	C12 H9 Br Hg N2 O4	C12 H9 Br Hg N2 O4
Mr	525.70	525.71
Dx,g cm-3	2.492	2.492
Z	4	4
Mu (mm-1)	13.848	13.848
F000	968.0	968.0
F000'	958.52	
h,k,lmax	10,13,15	10,13,15
Nref	2464	4849
Tmin,Tmax		0.224,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.224 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.968      Theta(max)= 24.984

R(reflections)= 0.0575( 4066)      wR2(reflections)= 0.1896( 4849)

S = 1.105      Npar= 182

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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

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PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.0192 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.023 Check

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### Alert level G

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PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.64 Why ?
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	! Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	74% Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.0 Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check

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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  
5 **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
- 4 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  
5 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check
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## Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT053_3
;
PROBLEM: Minimum Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT054_3
;
PROBLEM: Medium Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT055_3
;
PROBLEM: Maximum Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT342_3
;
PROBLEM: Low Bond Precision on C-C Bonds .....                0.0192 Ang.
RESPONSE: ...
;
_vrf_PLAT906_3
;
```

PROBLEM: Large K Value in the Analysis of Variance ..... 2.023 Check  
RESPONSE: ...  
;  
# end Validation Reply Form

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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.

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**PLATON version of 03/06/2021; check.def file version of 02/06/2021**

