

## 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: exp\_443\_auto

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Bond precision:      C-C = 0.0042 Å      Wavelength=1.54184

Cell:                      a=10.02947 (17)      b=22.6360 (5)      c=8.09415 (14)  
                            alpha=90                      beta=99.8389 (16)      gamma=90

Temperature:      293 K

	Calculated	Reported
Volume	1810.56 (6)	1810.56 (6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C23 H18 Br N O	C23 H18 Br N O
Sum formula	C23 H18 Br N O	C23 H18 Br N O
Mr	404.28	404.29
Dx, g cm <sup>-3</sup>	1.483	1.483
Z	4	4
Mu (mm <sup>-1</sup> )	3.172	3.172
F000	824.0	824.0
F000'	823.18	
h, k, lmax	12, 28, 10	12, 27, 9
Nref	3840	3560
Tmin, Tmax	0.472, 0.621	0.568, 1.000
Tmin'	0.088	

Correction method= # Reported T Limits: Tmin=0.568 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.927      Theta (max)= 77.143

R(reflections)= 0.0376 ( 3508)	wR2(reflections)= 0.1053 ( 3560)
S = 1.178	Npar= 237

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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.

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### Alert level C

PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 3.64 Report

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### Alert level G

PLAT012_ALERT_1_G	No	_shelx_res_checksum Found in CIF .....	Please Check
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..	0.75 mm	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.77	Why ?
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	(K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .....	(K)	293 Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O10	.	104.8 Degree
PLAT793_ALERT_4_G	Model has Chirality at C7	(Centro SPGR)	S Verify

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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  
1 **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
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 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  
2 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check
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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.

