

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) furutani

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: furutani

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Bond precision:      C-C = 0.0041 Å      Wavelength=1.54187

Cell:                      a=5.7675 (2)              b=10.1491 (4)              c=14.1934 (5)  
                                    alpha=90              beta=97.177 (7)              gamma=90

Temperature:              93 K

	Calculated	Reported
Volume	824.30 (5)	824.29 (6)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C18 H20 Br N O2	C18 H20 Br N O2
Sum formula	C18 H20 Br N O2	C18 H20 Br N O2
Mr	362.25	362.27
Dx, g cm <sup>-3</sup>	1.459	1.459
Z	2	2
Mu (mm <sup>-1</sup> )	3.448	3.451
F000	372.0	372.0
F000'	371.51	
h, k, lmax	6, 12, 17	6, 12, 17
Nref	2998 [ 1590]	2892
Tmin, Tmax	0.527, 0.501	0.380, 0.501
Tmin'	0.478	

Correction method= # Reported T Limits: Tmin=0.380 Tmax=0.501  
AbsCorr = MULTI-SCAN

Data completeness= 1.82/0.96              Theta(max)= 68.230

R(reflections)= 0.0307 ( 2835)

wR2(reflections)=  
0.0749 ( 2892)

S = 1.065

Npar= 199

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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**

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18) .....	7.97	Note
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. # C18 H20 Br N O2	1	Note
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 5 0 7,	1	Check

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**Alert level G**

CHEMS02\_ALERT\_1\_G Please check that you have entered the correct  
\_publ\_requested\_category classification of your compound;  
FI or CI or EI for inorganic; FM or CM or EM for metal-organic;  
FO or CO or EO for organic.  
From the CIF: \_publ\_requested\_category CHOOSE FI FM FO CI CM CO or A  
From the CIF: \_chemical\_formula\_sum :C18 H20 Br1 N1 O2

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1 Report
	H1	
PLAT791_ALERT_4_G	Model has Chirality at C3 (Sohncke SpGr)	R Verify
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2 Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....	Please Check
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....	1.117 Note
	Predicted wR2: Based on SigI**2 6.70 or SHELX Weight	7.03
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2 Info

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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  
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

- 1 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  
2 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
4 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.

Datablock furutani - ellipsoid plot

