

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 11

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: 11

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Bond precision:	C-C = 0.0042 Å	Wavelength=0.71073	
Cell:	a=13.2505(11)	b=6.2444(5)	c=17.704(2)
	alpha=90	beta=103.454(10)	gamma=90
Temperature:	298 K		
	Calculated	Reported	
Volume	1424.7(2)	1424.6(2)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C16 H11 Br F3 N	C16 H11 Br F3 N	
Sum formula	C16 H11 Br F3 N	C16 H11 Br F3 N O0	
Mr	354.16	354.17	
Dx, g cm <sup>-3</sup>	1.651	1.651	
Z	4	4	
Mu (mm <sup>-1</sup> )	2.910	2.910	
F000	704.0	704.0	
F000'	703.24		
h, k, lmax	18, 8, 24	18, 8, 23	
Nref	3926	3301	
Tmin, Tmax	0.502, 0.559	0.840, 0.860	
Tmin'	0.492		

Correction method= # Reported T Limits: Tmin=0.840 Tmax=0.860  
AbsCorr = MULTI-SCAN

Data completeness= 0.841      Theta(max)= 29.364

R(reflections)= 0.0429( 2016)	wR2(reflections)= 0.0891( 3301)
S = 0.999	Npar= 191

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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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....	5.702	Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).	6	Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	11	Report

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### 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 4

From the CIF: \_chemical\_formula\_sum C16 H11 Br F3 N O0

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	64.00	64.00	0.00
H	44.00	44.00	0.00
Br	4.00	4.00	0.00
F	12.00	12.00	0.00
N	4.00	4.00	0.00
O	4.00	0.00	4.00

PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of	C10	Check
PLAT793_ALERT_4_G Model has Chirality at C9 (Centro SPGR)	R	Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	597	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....	1.9	Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	3	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  
7 **ALERT level G** = General information/check it is not something unexpected

- 2 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  
4 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.

