

## 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: IRIWUC

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Bond precision:    C-C = 0.0041 A                      Wavelength=0.71073

Cell:                      a=16.845 (3)              b=11.374 (2)              c=14.680 (3)  
                                    alpha=90              beta=103.822 (2)              gamma=90

Temperature:              295 K

	Calculated	Reported
Volume	2731.2 (9)	2731
Space group	C 2/c	C 2/c
Hall group	-C 2yc	?
Moiety formula	C13 H13 Br N2 O2 S	C13 H13 Br1 N2 O2 S1
Sum formula	C13 H13 Br N2 O2 S	C13 H13 Br1 N2 O2 S1
Mr	341.21	0.00
Dx, g cm <sup>-3</sup>	1.660	1.660
Z	8	8
Mu (mm <sup>-1</sup> )	3.162	0.000
F000	1376.0	0.0
F000'	1375.21	
h, k, lmax		
Nref		
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness=                      Theta (max)=

R(reflections)= 0.0355 ( 0)

wR2(reflections)=  
wR= 0.0355 ( 0)

S = \*\*\*\*\*

Npar= \*\*\*\*\*

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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 A**

DIFF003\_ALERT\_1\_A \_diffrn\_measurement\_device\_type is missing  
Diffractometer make and type. Replaces \_diffrn\_measurement\_type.  
ATOM007\_ALERT\_1\_A \_atom\_site\_aniso\_label is missing  
Unique label identifying the atom site.  
GEOM001\_ALERT\_1\_A \_geom\_bond\_atom\_site\_label\_1 is missing  
Label identifying the atom site 1.  
GEOM002\_ALERT\_1\_A \_geom\_bond\_atom\_site\_label\_2 is missing  
Label identifying the atom site 2.  
GEOM003\_ALERT\_1\_A \_geom\_bond\_distance is missing  
Distance between atom sites 1 and 2.  
GEOM006\_ALERT\_1\_A \_geom\_angle\_atom\_site\_label\_2 is missing  
Label identifying the atom site 2.  
GEOM007\_ALERT\_1\_A \_geom\_angle\_atom\_site\_label\_3 is missing  
Label identifying the atom site 3.  
PLAT029\_ALERT\_3\_A \_diffrn\_measured\_fraction\_theta\_full value Low . 0.000 Why?  
PLAT043\_ALERT\_1\_A Calculated and Reported Mol. Weight Differ by .. 341.21 Check  
PLAT046\_ALERT\_1\_A Reported Z, MW and D(calc) are Inconsistent .... 0.000 Check  
PLAT183\_ALERT\_1\_A Missing \_cell\_measurement\_reflns\_used Value .... Please Do !  
PLAT184\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_min Value ..... Please Do !  
PLAT185\_ALERT\_1\_A Missing \_cell\_measurement\_theta\_max Value ..... Please Do !  
PLAT197\_ALERT\_1\_A Missing \_cell\_measurement\_temperature Datum .... Please Add  
PLAT201\_ALERT\_2\_A Isotropic non-H Atoms in Main Residue(s) ..... 19 Report  
Br1 S1 O1 O2 N1 etc.  
PLAT880\_ALERT\_1\_A No datum for \_diffrn\_reflns\_number supplied .... Please Do !  
PLAT881\_ALERT\_1\_A No Datum for \_diffrn\_reflns\_av\_R\_equivalents ... Please Do !

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**Alert level C**

PLAT151\_ALERT\_1\_C No s.u. (esd) Given on Volume ..... Please Do !

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**Alert level G**

PLAT005\_ALERT\_5\_G No Embedded Refinement Details Found in the CIF Please Do !  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 2 Report  
PLAT793\_ALERT\_4\_G Model has Chirality at C1 (Centro SPGR) R Verify  
PLAT793\_ALERT\_4\_G Model has Chirality at C8 (Centro SPGR) R Verify  
PLAT793\_ALERT\_4\_G Model has Chirality at C10 (Centro SPGR) S Verify  
PLAT808\_ALERT\_5\_G No Parseable SHELXL Style Weighting Scheme Found Please Check  
PLAT882\_ALERT\_1\_G No Datum for \_diffrn\_reflns\_av\_unetI/netI ..... Please Do !  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT981\_ALERT\_1\_G No non-zero f" Anomalous Scattering Values Found Please Check  
PLAT986\_ALERT\_1\_G No non-zero f' Anomalous Scattering Values Found Please Check

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- 17 **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  
10 **ALERT level G** = General information/check it is not something unexpected  
  
20 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  
1 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

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**PLATON version of 20/01/2022; check.def file version of 19/01/2022**

