

## 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: mo\_Garagan\_B105\_0m

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Bond precision:	C-C = 0.0057 A	Wavelength=0.71073
Cell:	a=22.4881(18)	b=9.9283(10)      c=16.9928(16)
	alpha=90	beta=118.907(3)      gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	3321.3(5)	3321.3(5)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C16 H22 Br N O2 S	?
Sum formula	C16 H22 Br N O2 S	C16 H22 Br N O2 S
Mr	372.31	372.31
Dx, g cm <sup>-3</sup>	1.489	1.493
Z	8	8
Mu (mm <sup>-1</sup> )	2.605	2.605
F000	1536.0	1544.0
F000'	1535.24	
h, k, lmax	31, 14, 23	31, 13, 23
Nref	4871	4862
Tmin, Tmax	0.322, 0.372	0.417, 0.746
Tmin'	0.298	

Correction method= # Reported T Limits: Tmin=0.417 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.998      Theta(max)= 30.078

R(reflections)= 0.0543( 3308)	wR2(reflections)=
S = 1.038	0.1542( 4862)
Npar= 196	

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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

ABSTY02\_ALERT\_1\_C An \_exptl\_absorpt\_correction\_type has been given without  
a literature citation. This should be contained in the  
\_exptl\_absorpt\_process\_details field.

Absorption correction given as multi-scan

PLAT068\_ALERT\_1\_C Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C14 Check

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### Alert level G

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 9.02 Why ?

PLAT128\_ALERT\_4\_G Alternate Setting for Input Space Group C2/c I2/a Note

PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check

PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check

PLAT793\_ALERT\_4\_G Model has Chirality at C3 (Centro SPGR) S Verify

PLAT793\_ALERT\_4\_G Model has Chirality at C4 (Centro SPGR) R Verify

PLAT793\_ALERT\_4\_G Model has Chirality at C13 (Centro SPGR) R 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

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

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

0 ALERT type 3 Indicator that the structure quality may be low

4 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.

