

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_b0280\_0m\_4

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\_b0280\_0m\_4

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Bond precision:	C-C = 0.0144 Å	Wavelength=0.71073
Cell:	a=15.9023(13)	b=10.8845(9)      c=22.8822(19)
	alpha=90	beta=91.977(3)      gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	3958.3(6)	3958.3(6)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C30 H44 Br2 Fe2 N2 O2 Si2 Zn2, C3 H6 O	C30 H44 Br2 Fe2 N2 O2 Si2 Zn2, C3 H6 O
Sum formula	C33 H50 Br2 Fe2 N2 O3 Si2 Zn2	C33 H50 Br2 Fe2 N2 O3 Si2 Zn2
Mr	981.21	981.19
Dx, g cm <sup>-3</sup>	1.646	1.646
Z	4	4
Mu (mm <sup>-1</sup> )	4.029	4.029
F000	1984.0	1984.0
F000'	1987.93	
h,k,lmax	21,14,30	21,14,30
Nref	19107[ 10051]	24737
Tmin,Tmax	0.774,0.814	0.010,0.032
Tmin'	0.578	

Correction method= # Reported T Limits: Tmin=0.010 Tmax=0.032  
AbsCorr = MULTI-SCAN

Data completeness= 2.46/1.29      Theta(max)= 27.998

R(reflections)= 0.0433( 21342)      wR2(reflections)= 0.1062( 24737)

S = 1.078      Npar= 850

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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.



#### **Alert level C**

PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.01438	Ang.
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	92	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1	Check



#### **Alert level G**

PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	157	Note
PLAT931_ALERT_5_G	Found Twin Law ( 0 0 1)[ ] Estimated BASF	0.21	Check
PLAT933_ALERT_2_G	Number of OMIT records in Embedded RES .....	4	Note
PLAT996_ALERT_1_G	Non-Standard SHELXL LIST 4 Style FCF Supplied ..	!	Check

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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  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
5 **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  
4 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
1 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.

