

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_b0273\_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\_b0273\_0m\_4

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Bond precision:    C-C = 0.0095 A

Wavelength=0.71073

Cell:                a=9.606(3)                b=14.581(6)                c=15.922(6)  
                      alpha=88.661(11)        beta=86.404(8)        gamma=77.905(11)  
Temperature:        100 K

	Calculated	Reported
Volume	2176.2(14)	2176.1(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H60 Br2 Fe2 N2 O2 Si4 Zn2	2(C18 H30 Br Fe N O Si2 Zn)
Sum formula	C36 H60 Br2 Fe2 N2 O2 Si4 Zn2	C36 H60 Br2 Fe2 N2 O2 Si4 Zn2
Mr	1067.50	1067.48
Dx, g cm <sup>-3</sup>	1.629	1.629
Z	2	2
Mu (mm <sup>-1</sup> )	3.722	3.722
F000	1088.0	1088.0
F000'	1090.27	
h,k,lmax	11,17,19	11,17,19
Nref	8552	11416
Tmin,Tmax	0.563,0.742	0.061,0.098
Tmin'	0.552	

Correction method= # Reported T Limits: Tmin=0.061 Tmax=0.098  
AbsCorr = MULTI-SCAN

Data completeness= 1.335

Theta(max)= 25.998

R(reflections)= 0.0482( 10054)

wR2(reflections)= 0.1001( 11416)

S = 1.171

Npar= 467

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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

PLAT213_ALERT_2_C	Atom C3	has ADP max/min Ratio .....	3.5	oblate
PLAT213_ALERT_2_C	Atom C25	has ADP max/min Ratio .....	3.2	prolat
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....		0.00945	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance .....		2.262	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600	29	Report



#### Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		14.03	Why ?
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C36 H60 Br2 Fe2 N2 O2 Si4 Zn2			
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..		!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min)		4	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	39	Note
PLAT931_ALERT_5_G	Found Twin Law ( 0 0 1)[		0.23	Check
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  
5 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 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  
3 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.

