

# 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: BiI3-hs3112034

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Bond precision:    Bi- I = 0.0165 A                      Wavelength=0.41312

Cell:                      a=3.961(1)              b=12.550(6)              c=9.310(4)  
                                alpha=90              beta=90              gamma=90  
Temperature:              295 K

	Calculated	Reported
Volume	462.8(3)	462.9(5)
Space group	C m c m	C m c m
Hall group	-C 2c 2	?
Moiety formula	Bi I3	?
Sum formula	Bi I3	BiI3
Mr	589.68	589.67
Dx,g cm-3	8.463	8.460
Z	4	4
Mu (mm-1)	13.935	15.830
F000	968.0	968.0
F000'	943.02	
h,k,lmax	3,12,9	
Nref	156	
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.000                      Theta(max)=

R(reflections)=                      wR2(reflections)=

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 B

POWD002\_ALERT\_1\_B `_refine_ls_goodness_of_fit_all` is missing (this is chi, i.e. the square root of 'chi squared'). This should be present for a powder diffraction study.

POWD004\_ALERT\_1\_B No 'Bragg' R factor has been given. Please supply a value for `_refine_ls_R_factor_all` [R(F)], `_refine_ls_R_Fsqd_factor` [R(F<sup>2</sup>)] or `_refine_ls_R_I_factor` [R(I)].

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## 🟢 Alert level C

REFI015\_ALERT\_1\_C `_refine_ls_shift/su_max` is missing  
Maximum shift/s.u. ratio after final refinement cycle.  
The following tests will not be performed  
SHFSU\_01

CRYSC01\_ALERT\_1\_C No recognised colour has been given for crystal colour.

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT702\_ALERT\_1\_C Angle Calc 78.9(3), Rep 79.23(3), Dev.. 1.10 Sigma

I2	-BI	-I2	11.564	1.555	11.464	#	20	Check
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PLAT702\_ALERT\_1\_C Angle Calc 78.9(3), Rep 79.23(3), Dev.. 1.10 Sigma

I2	-BI	-I2	13.566	1.555	13.466	#	35	Check
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## 🟠 Alert level G

ABSMU01\_ALERT\_1\_G Calculation of `_exptl_absorpt_correction_mu` not performed for this radiation type.

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT092\_ALERT\_4\_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.41312 Ang.

PLAT152\_ALERT\_1\_G The Supplied and Calc. Volume s.u. Differ by ... -2 Units

PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact I1 ..I2 3.55 Ang.

-1/2-x,1/2-y,-1/2+z = 12\_454 Check

PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact I1 ..I2 3.55 Ang.

1/2-x,1/2-y,-1/2+z = 12\_554 Check

PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact I1 ..I2 3.55 Ang.

-1/2+x,1/2-y,1-z = 14\_456 Check

PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact I1 ..I2 3.55 Ang.

1/2+x,1/2-y,1-z = 14\_556 Check

PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact I2 ..I2 3.49 Ang.

x,1-y,1-z = 6\_566 Check

PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact I2 ..I2 3.52 Ang.

-x,y,3/2-z = 7\_556 Check

PLAT794\_ALERT\_5\_G Tentative Bond Valency for Bi (III) 3.73 Info

PLAT984\_ALERT\_1\_G The I-f' = -1.9060 Deviates from the B&C-Value -1.9047 Check

PLAT985\_ALERT\_1\_G The Bi-f" = 4.4290 Deviates from the B&C-Value 4.4264 Check

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
- 2 **ALERT level B** = A potentially serious problem, consider carefully
- 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 13 **ALERT level G** = General information/check it is not something unexpected

- 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 6 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
- 1 ALERT type 4 Improvement, methodology, query or suggestion
- 2 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.

