

## 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: I

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Bond precision:	O- B = 0.0109 A	Wavelength=0.71073
Cell:	a=10.1862(16)      b=6.3819(9)      c=12.4466(18)	
	alpha=90      beta=102.701(12)      gamma=90	
Temperature:	293 K	
	Calculated	Reported
Volume	789.3(2)	789.3(2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ycb
Moiety formula	B16 Bi7.76 Eu0.24 O40, 4(Ba)	?
Sum formula	B16 Ba4 Bi7.76 Eu0.24 O40	B4 Ba1 Bi1.942 Eu0.058 O10
Mr	3020.44	755.20
Dx, g cm <sup>-3</sup>	6.354	6.355
Z	1	4
Mu (mm <sup>-1</sup> )	48.599	48.626
F000	1283.2	1283.0
F000'	1253.22	
h,k,lmax	15,9,19	14,9,19
Nref	3090	2701
Tmin,Tmax	0.068,0.143	0.543,1.000
Tmin'	0.006	
Correction method=	# Reported T Limits: Tmin=0.543 Tmax=1.000	
AbsCorr =	MULTI-SCAN	
Data completeness=	0.874	Theta(max)= 33.480
R(reflections)=	0.0317( 1954)	wR2(reflections)=
		wR= 0.0329( 2701)
S =	1.130	Npar= 150

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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

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check
PLAT127_ALERT_1_C	Implicit Hall Symbol	Inconsistent with Explicit	-P 2ycb Check
PLAT213_ALERT_2_C	Atom O3	has ADP max/min Ratio .....	3.2 oblate
PLAT213_ALERT_2_C	Atom O7	has ADP max/min Ratio .....	3.1 oblate

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#### Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	(K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature .....	(K)	293 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	6% Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi2	(III)	2.81 Info
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0	Sig(I)

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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  
11 **ALERT level G** = General information/check it is not something unexpected

- 7 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  
1 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
5 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.

