

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

Bond precision:	O- B = 0.0127 A	Wavelength=0.71073	
Cell:	a=10.2051(16)	b=6.3872(9)	c=12.4369(18)
	alpha=90	beta=102.597(12)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	791.2(2)	791.1(2)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ycb	
Moiety formula	B16 Bi6.66 Eu1.34 O40, 4(Ba)	?	
Sum formula	B16 Ba4 Bi6.66 Eu1.34 O40	B4 Ba1 Bi1.673 Eu0.327 O10	
Mr	2957.95	739.90	
Dx, g cm ⁻³	6.208	6.212	
Z	1	4	
Mu (mm ⁻¹)	44.548	44.651	
F000	1261.3	1262.0	
F000'	1235.19		
h,k,lmax	15,9,19	14,9,18	
Nref	3017	2601	
Tmin,Tmax	0.050,0.168	0.799,1.000	
Tmin'	0.022		

Correction method= # Reported T Limits: Tmin=0.799 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.862 Theta(max)= 33.140

R(reflections)= 0.0342(1758)	wR2(reflections)=
S = 1.120	wR= 0.0351(2601)
Npar= 156	

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

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



Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_sum B4 Ba1 Bi1.673 Eu0.327 O10

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
B	16.00	16.00	0.00
Ba	4.00	4.00	0.00
Bi	6.69	6.66	0.03
Eu	1.31	1.34	-0.03
O	40.00	40.00	0.00

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 _diffrn_ambient_temperature (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 13% Note
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)

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

- 9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
4 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.

