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: Bi- O = 0.0243 A Wavelength=0.71073

Cell: a=5.537(2) b=7.153(3) c=19.372(7)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	767.3(5)	767.2(5)
Space group	P 21 2 21	P 21 2 21
Hall group	P 2ac 2ac	P 2xac;2y;2
Moiety formula	As6 Bi7.33 Cd6 O32	?
Sum formula	As6 Bi7.33 Cd6 O32	As3 Bi3.667 Cd3 O16
Mr	3168.51	1584.30
Dx,g cm-3	6.857	6.858
Z	1	2
Mu (mm-1)	52.475	52.485
F000	1350.7	1351.0
F000’	1319.28	
h,k,lmax	9,12,34	9,12,34
Nref	4609[2650]	2209
Tmin,Tmax	0.001,0.207	0.250,0.700
Tmin’	0.000	

Correction method= # Reported T Limits: Tmin=0.250 Tmax=0.700
AbsCorr = MULTI-SCAN

Data completeness= 0.83/0.48 Theta(max)= 39.480

R(reflections)= 0.0322(1858) wR2(reflections)= wR= 0.0535(2209)

S = 2.850 Npar= 81

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 A

WEIGH01_ALERT_1_A Unit weights are not acceptable for submissions to Acta Crystallographica Section C.
n.b. unit is however a legal CIF keyword.

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 2.850
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.480
From the CIF: _refine_ls_abs_structure_Flack_su 0.050

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 2xac;2y;2zac
PLAT220_ALERT_2_C	Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range	5.1 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	O4 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	O8 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Cd2 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	As1 Check

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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 !
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .	0.480 Note
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group P21221	P21212 Note
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >BiT is Constrained at	0.6667 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *Bi3 is Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *Cd3 is Constrained at	0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder ..... Percentage =	9 Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1 Note
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4 Note

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

7 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
2 ALERT type 3 Indicator that the structure quality may be low
8 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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.

PLATON version of 11/08/2016; check.def file version of 04/08/2016

Datablock I - ellipsoid plot