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: P- O = 0.0307 A Wavelength=0.71073

Cell: a=5.6344(2) b=6.9617(2) c=19.4034(6)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	761.10(4)	761.10(4)
Space group	P 21 2 21	P 21 2 21
Hall group	P 2ac 2ac	P 2xac;2y;2
Moiety formula	Bi11.37 Cd2 O32 P6	?
Sum formula	Bi11.37 Cd2 O32 P6	Bi2.843 Cd0.5 O8 P1.5
Mr	3298.74	824.80
Dx,g cm-3	7.197	7.198
Z	1	4
Mu (mm-1)	67.253	67.265
F000	1385.7	1374.0
F000'	1343.16	
h,k,lmax	10,12,35	9,11,32
Nref	4688[2697]	2183
Tmin,Tmax	0.025,0.068	0.216,0.745
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.216 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.81/0.47 Theta(max)= 39.890

R(reflections)= 0.0445(1904) wR2(reflections)= wR= 0.0705(2183)

S = 3.600 Npar= 86

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

GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
Label identifying the atom site 1.
GEOM003_ALERT_1_A _geom_bond_distance is missing
Distance between atom sites 1 and 2.
GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.
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 B

PLAT220_ALERT_2_B Non-Solvent Resd 1 Bi Ueq(max)/Ueq(min) Range 9.5 Ratio
PLAT220_ALERT_2_B Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 10.0 Ratio
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of P1 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of O7 Check

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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 = 3.600
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 0.080
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... 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
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of P2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O2B Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.3 Note

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Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 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 ... 0.25 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
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 15 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 2 Note
PLAT791_ALERT_4_G The Model has Chirality at P1 (Chiral SPGR) R Verify
PLAT791_ALERT_4_G The Model has Chirality at P2 (Chiral SPGR) R Verify
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON 8 Info
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found Please Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 11 Note
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ 3 Units

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5 **ALERT level A** = Most likely a serious problem - resolve or explain

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  4 ALERT level B = A potentially serious problem, consider carefully
  9 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

 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  8 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
  7 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.

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

Datablock I - ellipsoid plot