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: C-C = 0.0048 A Wavelength=0.71073

Cell: a=9.4841(15) b=15.777(2) c=12.832(2)
alpha=90 beta=104.738(4) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	1856.9(5)	1856.9(5)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	C12 H14 N2, 0.5(Bi2 Cl10), H2 O	C24 H36 Bi2 Cl10 N4 O2
Sum formula	C12 H16 Bi Cl5 N2 O	C24 H36 Bi2 Cl10 N4 O2
Mr	590.50	1185.03
Dx,g cm-3	2.112	2.119
Z	4	2
Mu (mm-1)	10.213	10.213
F000	1112.0	1120.0
F000’	1099.42	
h,k,lmax	12,20,16	12,20,16
Nref	4257	4187
Tmin,Tmax	0.239,0.360	0.239,0.360
Tmin’	0.169	

Correction method= # Reported T Limits: Tmin=0.239 Tmax=0.360
AbsCorr = MULTI-SCAN

Data completeness= 0.984 Theta(max)= 27.490

R(reflections)= 0.0179(3586) wR2(reflections)= 0.0392(4187)

S = 1.007 Npar= 198

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
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 2.02 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... Please Do !
PLAT193_ALERT_1_C Cell and Diffraction Temperatures Differ by .... 3 Degree
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Bi1 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C12 H14 N2

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C24 H36 Bi2 Cl10 N4 O2
Atom count from the _atom_site data: C24 H32 Bi2 Cl10 N4 O2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C24 H36 Bi2 Cl10 N4 O2
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	48.00	48.00	0.00
H	72.00	64.00	8.00
Bi	4.00	4.00	0.00
Cl	20.00	20.00	0.00
N	8.00	8.00	0.00
O	4.00	4.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2.00 Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Bi1 -- Cl2 .. 10.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Bi1 -- Cl3 .. 13.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Bi1 -- Cl4 .. 19.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Bi1 -- Cl5 .. 11.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Bi1 -- Cl4_a .. 17.0 s.u.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C1 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C12 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 2 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3 Note
H2 O
PLAT794_ALERT_5_G Tentative Bond Valency for Bi1 (III) ..... 3.26 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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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
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
21 **ALERT level G** = General information/check it is not something unexpected

10 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
   1 ALERT type 3 Indicator that the structure quality may be low
   7 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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checkCIF publication errors

Alert level A

```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
            _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
            _publ_contact_author_phone are all missing.
            At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   1 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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

Datablock I - ellipsoid plot