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-Zn = 0.0026 A        Wavelength=1.54186

Cell:            a=33.0011(11)     b=21.5972(9)     c=14.3006(4)
                 alpha=90          beta=90          gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	10192.5(6)	10192.5(6)
Space group	P m m n	P m m n
Hall group	-P 2ab 2a	-P 2ab 2a
Moiety formula	Bi16 Zn20, 8(K)	(C18 H38 N2 O6 K)6, Bi16 Zn20 K2
Sum formula	Bi16 K8 Zn20	C144 H288 Bi16 K8 N16 O48 Zn20
Mr	4964.28	7975.77
Dx,g cm-3	1.618	2.599
Z	2	2
Mu (mm-1)	30.411	31.009
F000	4160.0	7456.0
F000’	3987.51	
h,k,lmax	38,25,16	38,25,16
Nref	9129	9119
Tmin,Tmax	0.029,0.061	0.013,0.201
Tmin’	0.000	

```
Correction method= # Reported T Limits: Tmin=0.013 Tmax=0.201
AbsCorr = GAUSSIAN

Data completeness= 0.999          Theta(max)= 65.088

R(reflections)= 0.0732( 4410)     wR2(reflections)= 0.2170( 9119)

S = 1.113                  Npar= 117
```

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

PLAT043_ALERT_1_A Calculated and Reported Mol. Weight Differ by .. 3011.49 Check

Author Response: The ligand and solvent area was detracted by back-fourier-transform and is therefore missing in the model

PLAT044_ALERT_1_A Calculated and Reported Density Dx Differ by .. 0.9814 Check

Author Response: see above

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

Author Response: see above

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.183
PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 ..... 0.183 Report

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Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5882
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 48% Check
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 1.93 %
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.01 Report
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Bi1 0.118 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including K1 0.127 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including K2 0.130 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including K3 0.170 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including K4 0.242 Check

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Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C144 H288 Bi16 K8 N16 O48 Zn2
Atom count from _chemical_formula_moiety:C108 H228 Bi16 K8 N12 O36 Zn2
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:C144 H288 Bi16 K8 N16 O48 Zn20
Atom count from the _atom_site data: Bi16 K8 Zn20
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C144 H288 Bi16 K8 N16 O48 Zn20

```
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C        288.00      0.00  288.00
           H        576.00      0.00  576.00
           Bi        32.00     32.00    0.00
           K         16.00     16.00    0.00
           N         32.00      0.00   32.00
           O         96.00      0.00   96.00
           Zn        40.00     40.00    0.00
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  2          0.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  3          0.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  5          0.50 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       2.29 Ratio
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          2 Info
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3 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

9 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
4 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
0 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.
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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

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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 07/08/2019; check.def file version of 30/07/2019

Datablock I - ellipsoid plot