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 = 0.0183 A Wavelength=0.71073

Cell: a=11.9160(17) b=11.9160(17) c=25.949(5)
alpha=90 beta=90 gamma=120
Temperature: 100 K

	Calculated	Reported
Volume	3190.9(13)	3190.9(11)
Space group	P 63/m	P 63/m
Hall group	-P 6c	-P 6c
Moiety formula	2(As9.94 Nb), 4(C18 H36 K N2 O6), C21	As9.944 Nb1, C36 H72 K2 N4 O12, C10.5
Sum formula	C93 H144 As19.89 K4 N8 Nb2 O24	C46.50 H84 As9.53 K2 N4 Nb O12
Mr	3590.39	1776.27
Dx,g cm-3	1.868	1.849
Z	1	2
Mu (mm-1)	5.492	5.279
F000	1764.3	1761.0
F000’	1762.51	
h,k,lmax	14,14,30	14,14,30
Nref	1922	1922
Tmin,Tmax	0.503,0.725	0.627,0.746
Tmin’	0.456	

Correction method= # Reported T Limits: Tmin=0.627 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 24.992

R(reflections)= 0.0526(1741) wR2(reflections)= 0.1440(1922)

S = 1.111 Npar= 138

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

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.
DIFF005_ALERT_1_A _diffrn_measurement_method is missing
Mode of intensity measurement and scan.
DIFF019_ALERT_1_A _diffrn_standards_number is missing
Number of standards used in measurement.
DIFF020_ALERT_1_A _diffrn_standards_interval_count and
_diffrn_standards_interval_time are missing. Number of measurements
between standards or time (min) between standards.
DIFF022_ALERT_1_A _diffrn_standards_decay_% is missing
Percentage decrease in standards intensity.

Alert level B

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 37.85 Check
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 4 Report
C11 C12 C13 C14
PLAT213_ALERT_2_B Atom C1 has ADP max/min Ratio ..... 4.2 prolat
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C11 Check

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Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT044_ALERT_1_C Calculated and Reported Density Dx Differ by .. 0.0195 Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 4.03 %
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
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Nb Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.6 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01829 Ang.

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: C46.5 H84 As9.53 K2 N4 Nb1 O1
Atom count from _chemical_formula_moiety:C46.5 H72 As9.943999 K2 N4 Nb
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:C46.5 H84 As9.53 K2 N4 Nb1 O12
Atom count from the _atom_site data: C46.5 H72 As9.943999 K2 N4 Nb1 O
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 C46.50 H84 As9.53 K2 N4 Nb O12
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	93.00	93.00	0.00
H	168.00	144.00	24.00
As	19.06	19.89	-0.83

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          K          4.00      4.00    0.00
          N          8.00      8.00    0.00
          Nb         2.00      2.00    0.00
          O         24.00     24.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         3 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      19.39 Why ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         2 Units
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         2 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Nb       --As5      .       5.6 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of As1        Constrained at     0.6481 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As2        Constrained at      0.648 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As3        Constrained at     0.5468 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As4        Constrained at     0.3358 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As5        Constrained at     0.1173 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As6        Constrained at     0.2347 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13        Constrained at       0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14        Constrained at       0.75 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        94% Note
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  3  )        60% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  1        10.94 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  3        10.50 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  As2      ..C13            3.28 Ang.
                                                  -y,x-y,z  =      2_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  As4      ..C13            2.59 Ang.
                                                  -y,x-y,z  =      2_555 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         77 Check
             AS5  -AS1  -AS2     2.555   1.555   3.555              8.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         80 Check
             AS5  -AS1  -AS2     3.555   1.555   1.555              8.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         81 Check
             AS5  -AS1  -AS2     1.555   1.555   2.555              8.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         88 Check
             AS5  -AS1  -AS6     3.555   1.555   1.555             16.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         89 Check
             AS5  -AS1  -AS6     2.555   1.555   3.555             16.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         96 Check
             AS5  -AS1  -AS6     1.555   1.555   2.555             16.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        103 Check
             AS6  -AS1  -AS2     2.555   1.555   2.555              9.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        104 Check
             AS6  -AS1  -AS2     3.555   1.555   3.555              9.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        106 Check
             AS6  -AS1  -AS2     1.555   1.555   1.555              9.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        113 Check
             AS1  -AS2  -AS5     1.555   1.555   1.555             17.07 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        114 Check
             AS1  -AS2  -AS5     1.555   1.555   2.555             18.15 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        127 Check
             AS5  -AS2  -AS1     3.555   1.555   1.555              4.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        130 Check
             AS5  -AS2  -AS5     3.555   1.555   1.555             13.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        131 Check
             AS5  -AS2  -AS5     3.555   1.555   2.555             19.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        132 Check
             AS5  -AS2  -AS5     2.555   1.555   1.555             24.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        145 Check
             AS6  -AS3  -AS2     1.555   1.555   1.555              7.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        146 Check
             AS6  -AS3  -AS2    10.556   1.555  10.556              7.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        153 Check
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             AS2  -AS4  -AS6     1.555   1.555   1.555              6.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        156 Check
             AS2  -AS4  -AS6    10.556   1.555  10.556              6.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        184 Check
             AS5  -AS5  -AS2     2.555   1.555   3.555             29.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        186 Check
             AS5  -AS5  -AS2     3.555   1.555   1.555             19.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        195 Check
             AS5  -AS5  -AS6     3.555   1.555   1.555             15.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        196 Check
             AS5  -AS5  -AS6     2.555   1.555   3.555             36.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        200 Check
             AS6  -AS5  -AS2     1.555   1.555   1.555              8.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        201 Check
             AS6  -AS5  -AS2     2.555   1.555   2.555             13.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        202 Check
             AS6  -AS5  -AS2     3.555   1.555   3.555              8.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        212 Check
             AS1  -AS6  -AS5     1.555   1.555   1.555             16.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        213 Check
             AS1  -AS6  -AS5     1.555   1.555   2.555             19.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        221 Check
             AS5  -AS6  -AS1     3.555   1.555   1.555              8.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        226 Check
             AS5  -AS6  -AS5     3.555   1.555   1.555             11.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        227 Check
             AS5  -AS6  -AS5     3.555   1.555   2.555             24.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        228 Check
             AS5  -AS6  -AS5     2.555   1.555   1.555             25.00 Deg.
PLAT780_ALERT_1_G Coordinates do not Form a Properly Connected Set    Please Do !
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
             C21
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          7 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
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5 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
61 **ALERT level G** = General information/check it is not something unexpected

18 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 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
44 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

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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.
```

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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.
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   7 **ALERT level A** = Data missing that is essential or data in wrong format
   0 **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).
```

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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: ...
;
_vrf_DIFF003_I
;
PROBLEM: _diffrn_measurement_device_type is missing
RESPONSE: ...
;
_vrf_DIFF005_I
;
PROBLEM: _diffrn_measurement_method is missing
RESPONSE: ...
;
_vrf_DIFF019_I
;
PROBLEM: _diffrn_standards_number is missing
RESPONSE: ...
;
_vrf_DIFF020_I
;
PROBLEM: _diffrn_standards_interval_count and
RESPONSE: ...
;
_vrf_DIFF022_I
;
PROBLEM: _diffrn_standards_decay_% 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