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: compound1

```
Bond precision:  C-C = 0.0045 A          Wavelength=0.71069

Cell:          a=8.659(5)        b=10.320(5)      c=10.788(5)
               alpha=69.251(5)   beta=78.746(5)   gamma=66.233(5)
Temperature:   293 K
```

	Calculated	Reported
Volume	823.5(7)	823.5(7)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	K O16 V5, C3 H10 N2	K O16 H4 V5, C3 H12 N2
Sum formula	C3 H10 K N2 O16 V5	C3 H16 K N2 O16 V5
Mr	623.93	629.93
Dx,g cm-3	2.516	2.516
Z	2	2
Mu (mm-1)	3.072	3.072
F000	608.0	608.0
F000’	611.73	
h,k,lmax	11,13,14	11,13,14
Nref	4076	4076
Tmin,Tmax	0.344,0.423	0.344,0.423
Tmin’	0.318	

```
Correction method= # Reported T Limits: Tmin=0.344 Tmax=0.423
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 28.250

R(reflections)= 0.0278( 3493)     wR2(reflections)= 0.0831( 4050)

S = 0.947                 Npar= 245
```

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

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       6.00 Check
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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:C3 H16 K1 N2 O16 V5
           Atom count from the _atom_site data:  C3 H10 K1 N2 O16 V5
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  C3 H16 K N2 O16 V5
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C          6.00      6.00    0.00
          H         32.00     20.00   12.00
          K          2.00      2.00    0.00
          N          4.00      4.00    0.00
          O         32.00     32.00    0.00
          V         10.00     10.00    0.00
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 !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.005 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.60 Ratio
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF:   K1     --  K1      ..       4.40 Ang.
PLAT793_ALERT_4_G The Model has Chirality at C2      (Centro SPGR)          S Verify
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
   2 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

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   3 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 24/11/2016; check.def file version of 23/11/2016

Datablock compound1 - ellipsoid plot