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:  V- O = 0.0063 A         Wavelength=1.54056

Cell:           a=4.88563(9)    b=11.2128(2)        c=5.69642(11)
                alpha=90        beta=96.3704(8)     gamma=90
Temperature:    298 K

                Calculated                  Reported
Volume          310.132(10)                 310.132(13)
Space group     P 21/c                      P 1 21/c 1
Hall group      -P 2ybc                     -P 2ybc
Moiety formula  Mn O14 V4, 0.75(Ca4)        Mn0.5 O7 V2, 1.5(Ca)
Sum formula     Ca3 Mn O14 V4               Ca1.50 Mn0.50 O7 V2
Mr              602.94                      301.47
Dx,g cm-3       3.228                       3.228
Z               1                           2
Mu (mm-1)       43.776                      0.000
F000            289.0                       0.0
F000'           290.87
h,k,lmax        5,12,6                      5,12,6
Nref            467                         467
Tmin,Tmax                                   1.000,1.000
Tmin'

Correction method= # Reported T Limits: Tmin=1.000 Tmax=1.000
AbsCorr = ?

Data completeness= 1.000          Theta(max)= 59.990

R(reflections)=                   wR2(reflections)=

S =                       Npar=
```

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 G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
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
PLAT092_ALERT_4_G Check: Wavelength given is not Cu,Ga,Mo,Ag,In Ka    1.54056 Ang.
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         -3 Units
PLAT300_ALERT_4_G Atom Site Occupancy of Mn      is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca      is Constrained at       0.75 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..         5% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2)..       100% Note
PLAT981_ALERT_1_G No non-zero f" Anomalous Scattering Values Found     Please Check
PLAT986_ALERT_1_G No non-zero f’ Anomalous Scattering Values Found     Please Check
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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
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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 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 13/08/2017; check.def file version of 27/07/2017

Datablock I - ellipsoid plot