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: epidotexf-0.90s-10m

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Bond precision:    Si- O = 0.0020 A           Wavelength=0.71073

Cell:              a=8.9094(3)      b=5.65071(15)         c=10.1717(4)
                   alpha=90         beta=115.404(4)       gamma=90
Temperature:       293 K

                   Calculated                  Reported
Volume             462.57(3)                   462.57(3)
Space group        P 21/m                      P 1 21/m 1
Hall group         -P 2yb                      -P 2yb
Moiety formula     Al4.09 Fe1.88 H2 O26 Si6,   Al2.047 Ca2 Fe0.942 H O13
                   4(Ca)                       Si3
Sum formula        Al4.09 Ca4 Fe1.88 H2 O26    Al2.05 H Ca2 Fe0.94 O13 Si3
                   Si6
Mr                 962.55                      481.11
Dx,g cm-3          3.455                       3.454
Z                  1                           2
Mu (mm-1)          3.325                       3.321
F000               476.2                       476.0
F000'              478.73
h,k,lmax           13,8,15                     13,8,14
Nref               1984                        1729
Tmin,Tmax          0.520,0.515                 0.793,1.000
Tmin'              0.510

Correction method= # Reported T Limits: Tmin=0.793 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.871             Theta(max)= 33.627
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R(reflections)= 0.0224(1644)   wR2(reflections)=
                                       0.0660(1729)

S = 1.106   Npar= 123

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
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check

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⚪ **Alert level G**
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   2 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT012_ALERT_1_G No   _shelx_res_checksum Found in CIF ...... Please Check
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.50 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records   3 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   3 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)   293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe3   Constrained at   0.87 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Al3   Constrained at   0.119 Check
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   22% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   1 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

   7 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
   2 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 13/07/2021; check.def file version of 13/07/2021