No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: 2x4H2O

```
Bond precision:      C-C = 0.0027 A          Wavelength=0.71073
Cell:        a=7.4411(15)    b=10.581(2)    c=11.235(2)
             alpha=108.96(3) beta=96.14(3)  gamma=107.41(3)
Temperature   293 K
:
                 Calculated                  Reported
Volume           777.6(4)                    777.6(3)
Space group      P -1                        P -1
Hall group       -P 1                        -P 1
Moiety formula   C13 H14 N2 O2, 4(H2 O)      C13 H22 N2 O6
Sum formula      C13 H22 N2 O6               C13 H22 N2 O6
Mr               302.33                      302.32
Dx,g cm-3        1.291                       1.291
Z                2                           2
Mu (mm-1)        0.102                       0.102
F000             324.0                       324.0
F000'            324.19
h,k,lmax         8,12,13                     8,12,13
Nref             2849                        2847
Tmin,Tmax        0.966,0.981                 0.959,0.983
Tmin'            0.930
Correction method= # Reported T Limits: Tmin=0.959
Tmax=0.983 AbsCorr = ANALYTICAL
Data completeness= 0.999       Theta(max)= 25.341
R(reflections)= 0.0443( 2225)      wR2(reflections)= 0.1196( 2847)
S = 1.042             Npar= 214
```

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.
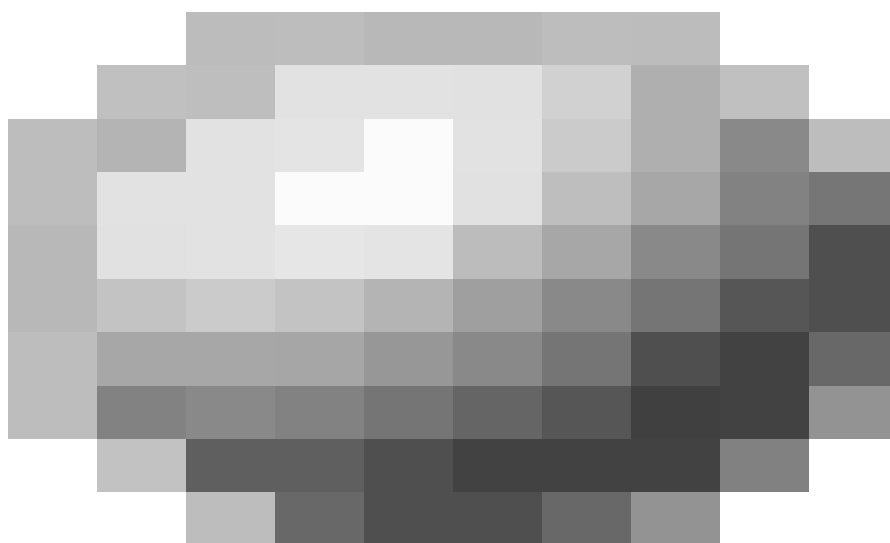
Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   12 Note
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF   Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ   Please Check
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..   0.71 mm
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)   0.03 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)   293 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #   2 Note
              H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #   5 Note
              H2 O
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   8 Note

---

```
   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
  12 ALERT level G = General information/check it is not something unexpected

   5 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
   1 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 05/12/2020; check.def file version of 05/12/2020

Datablock 2x4H2O - ellipsoid plot

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