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: 1_a

```
Bond precision:   C-C = 0.0057 A          Wavelength=1.54178

Cell:              a=14.7146(3)      b=8.9906(2)      c=11.0612(2)
                   alpha=90          beta=90          gamma=90
Temperature:       193 K

                 Calculated                  Reported
Volume           1463.32(5)                  1463.32(5)
Space group      P n a 21                    P n a 21
Hall group       P 2c -2n                    P 2c -2n
Moiety formula   C14 H16 N6, H2 O            H2 O, C14 H16 N6
Sum formula      C14 H18 N6 O                C14 H18 N6 O
Mr               286.34                      286.34
Dx,g cm-3        1.300                       1.300
Z                4                           4
Mu (mm-1)        0.714                       0.714
F000             608.0                       608.0
F000'            609.78
h,k,lmax         17,10,13                    17,10,13
Nref             2670[ 1409]                 2512
Tmin,Tmax        0.911,0.924
Tmin'            0.911

Correction method= Not given

Data completeness= 1.78/0.94        Theta(max)= 68.208

R(reflections)= 0.0682( 2489)                wR2(reflections)=
                                             0.1722( 2512)
S = 1.145                  Npar= 190
```

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 B

```
PLAT417_ALERT_2_B Short Inter D-H..H-D       H1A      ..H2       .       1.81 Ang.
                                                  x,-1+y,z  =      1_545 Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O1       --H1A      .     Please Check
```

Alert level C

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
              Calc: C14 H16 N6, H2 O
              Rep.: H2 O, C14 H16 N6
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00567 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H4       ..H10      .       2.03 Ang.
                                              1-x,2-y,1/2+z  =      2_675 Check
PLAT415_ALERT_2_C Short Inter D-H..H-X       H1B      ..H3       .       2.09 Ang.
                                              1/2+x,3/2-y,z  =      3_565 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
              H2    H5    H1A   H1B
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.13 Report
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
2 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
1 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 15/07/2024; check.def file version of 15/07/2024

Datablock 1_a - ellipsoid plot