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: md482_mc145y

```
Bond precision:    C-C = 0.0025 A          Wavelength=0.71073

Cell:             a=15.7258(15)     b=7.9668(8)      c=16.0813(14)
                  alpha=90          beta=90          gamma=90
Temperature:      293 K

                  Calculated                Reported
Volume            2014.7(3)                 2014.7(3)
Space group       P b c n                   P b c n
Hall group        -P 2n 2ab                 -P 2n 2ab
Moiety formula    C23 H30 N2                C23 H30 N2
Sum formula       C23 H30 N2                C23 H30 N2
Mr                334.49                    334.49
Dx,g cm-3         1.103                     1.103
Z                 4                         4
Mu (mm-1)         0.064                     0.064
F000              728.0                     728.0
F000'             728.23
h,k,lmax          19,10,20                  19,10,20
Nref              2084                      2080
Tmin,Tmax         0.959,0.973               0.880,1.000
Tmin'             0.940

Correction method= # Reported T Limits: Tmin=0.880 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998        Theta(max)= 26.496

R(reflections)= 0.0552( 1527)    wR2(reflections)= 0.1570( 2080)

S = 1.018                 Npar= 124
```

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

```
PLAT012_ALERT_1_G No        _shelx_res_checksum Found in CIF ......    Please Check
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....    0.97 mm
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 C2        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2A       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3        Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2AA      Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2AB      Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2A       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2B       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3A       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3B       Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A      Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B      Constrained at      0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       8% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........       2 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #       9 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       2 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
  19 ALERT level G = General information/check it is not something unexpected

   3 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
   2 ALERT type 3 Indicator that the structure quality may be low
  14 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 09/11/2017; check.def file version of 08/11/2017