checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ds27transform

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: ds27transform

```
Bond precision:   C-C = 0.0054 A            Wavelength=0.71073

Cell:          a=10.1896(4)        b=11.5565(5)       c=11.5966(5)
               alpha=65.090(3)   beta=83.184(3)   gamma=84.962(4)
Temperature:   173 K

                  Calculated                 Reported
Volume          1228.69(9)                   1228.69(9)
Space group     P -1                         P -1
Hall group      -P 1                         -P 1
Moiety formula  C44 H82 Ga2 Ho2 N2           ?
Sum formula     C44 H82 Ga2 Ho2 N2           C44 H82 Ga2 Ho2 N2
Mr              1108.42                      1108.41
Dx,g cm-3       1.498                        1.498
Z               1                            1
Mu (mm-1)       4.297                        4.297
F000            556.0                        556.0
F000'           556.16
h,k,lmax        13,14,14                     13,14,14
Nref            5392                         5384
Tmin,Tmax       0.440,0.651                  0.598,0.913
Tmin'           0.407

Correction method= # Reported T Limits: Tmin=0.598 Tmax=0.913
AbsCorr = NUMERICAL

Data completeness= 0.999          Theta(max)= 27.100

R(reflections)= 0.0296( 5025)     wR2(reflections)= 0.0661( 5384)

S = 1.082                    Npar= 239
```

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

```
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......    2.895 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Th(Min) ...        8 Report
```

Alert level G

```
PLAT303_ALERT_2_G Full Occupancy H-Atom  H19B   with # Connections     2.00 Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range  in Main Residue for      C19    Check
PLAT343_ALERT_2_G Unusual sp?     Angle Range  in Main Residue for      C20    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
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   3 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 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
   0 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*, 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 21/06/2015; check.def file version of 21/06/2015