checkCIF/PLATON report

Structure factors have been supplied for datablock(s) fs257_0m

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: fs257_0m

```
Bond precision:  = 0.0000 A              Wavelength=0.71073

Cell:            a=16.235(1)    b=7.0750(4)         c=13.4759(8)
                 alpha=90       beta=113.848(4)     gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          1415.72(15)               1415.72(15)
Space group     C c                       C c
Hall group      C -2yc                    C -2yc
Moiety formula  C17 H16 N4                C17 H16 N4
Sum formula     C17 H16 N4                C17 H16 N4
Mr              276.34                    276.34
Dx,g cm-3       1.296                     1.296
Z               4                         4
Mu (mm-1)       0.080                     0.080
F000            584.0                     584.0
F000'           584.18
h,k,lmax        19,8,16                   19,8,16
Nref            2652[ 1328]               1327
Tmin,Tmax       0.977,0.991               0.977,0.991
Tmin'           0.977

Correction method= MULTI-SCAN

Data completeness= 1.00/0.50      Theta(max)= 25.530

R(reflections)= 0.0620( 889)      wR2(reflections)= 0.1297( 1327)

S = 1.071                  Npar= 273
```

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

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PLAT089_ALERT_3_B Poor Data / Parameter Ratio (Zmax  <   18) .....       4.86
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Alert level C

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PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.4
PLAT332_ALERT_2_C Large Phenyl C-C Range           C1     -C6            0.16 Ang.
PLAT332_ALERT_2_C Large Phenyl C-C Range           C1X    -C6X           0.20 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.045
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         42
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         42
PLAT007_ALERT_5_G Note: Number of Unrefined Donor-H Atoms ........          2
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................        100 %
PLAT335_ALERT_2_G Check Large C6 Ring    C-C Range C9     -C14           0.21 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring    C-C Range C9X    -C14X          0.21 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          6
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        517
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          2
```

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

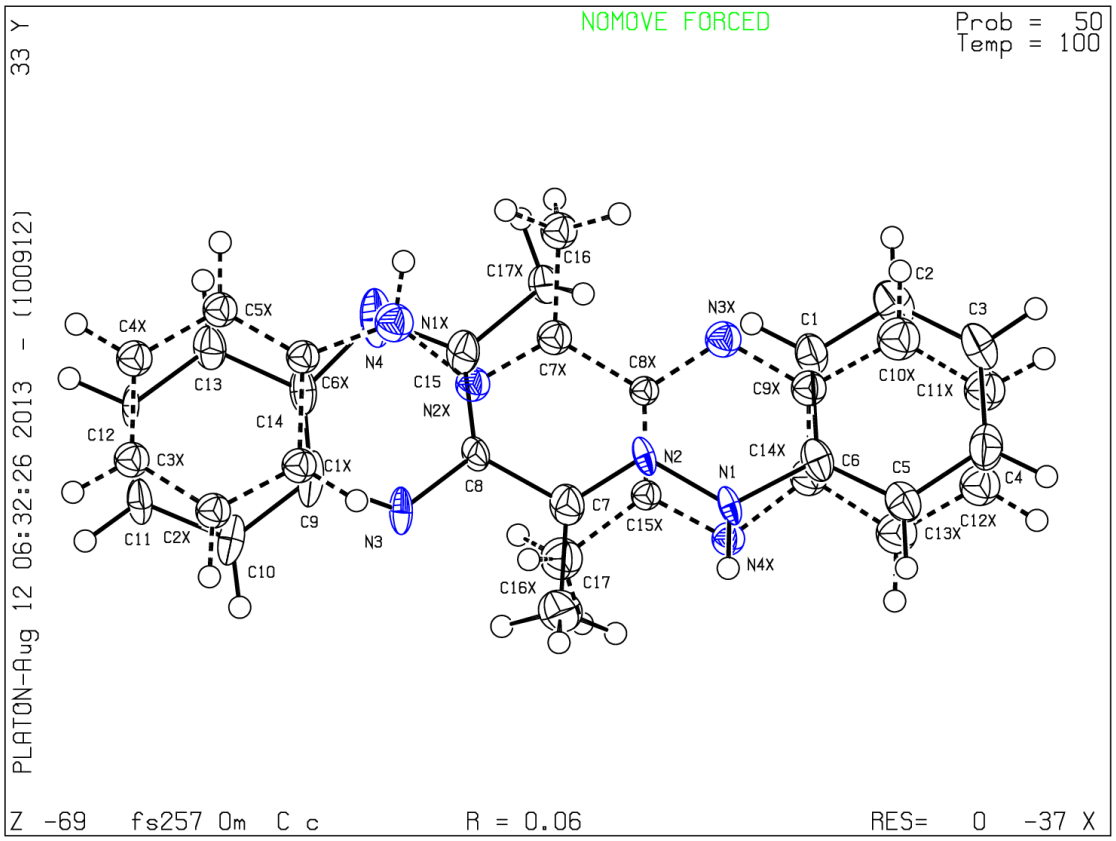
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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*, 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 01/06/2013; check.def file version of 24/05/2013

Datablock fs257_0m - ellipsoid plot