checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_3719

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: exp_3719

```
Bond precision:   C-C = 0.0035 A           Wavelength=1.54184

Cell:             a=12.0996(5)     b=10.9016(5)       c=29.2496(12)
                  alpha=90         beta=96.378(4)     gamma=90
Temperature:      100 K

                 Calculated                  Reported
Volume           3834.3(3)                   3834.3(3)
Space group      P 21/n                      P 1 21/n 1
Hall group       -P 2yn                      -P 2yn
Moiety formula   C49 H40 N2, C2 H3 N         C49 H40 N2, C2 H3 N
Sum formula      C51 H43 N3                  C51 H43 N3
Mr               697.88                      697.88
Dx,g cm-3        1.209                       1.209
Z                4                           4
Mu (mm-1)        0.535                       0.535
F000             1480.0                      1480.0
F000'            1483.83
h,k,lmax         14,12,34                    14,12,34
Nref             6780                        6772
Tmin,Tmax        0.938,0.948                 0.708,1.000
Tmin'            0.852

Correction method= # Reported T Limits: Tmin=0.708 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999            Theta(max)= 66.597

R(reflections)= 0.0575( 4736)                wR2(reflections)=
                                             0.1414( 6772)
S = 1.047                  Npar= 494
```

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 ......      9.301 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595          8 Report
              -12  7  1,  -3  4  6,  -1 10 21,  -2 10 22,  -1 10 22,  -1  9 25,
                4  0 26,  -1  8 27,
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.85Ang From N2      .      -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2        .      -0.43 eA-3
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
              H2
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        62% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
               -3  4  6,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.0 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       1.61 Note
              Predicted wR2: Based on SigI**2  8.80 or SHELX Weight 14.03
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
0 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 06/01/2024; check.def file version of 05/01/2024

Datablock exp_3719 - ellipsoid plot