# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 19gtu356_ca_13_0m_a

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: 19gtu356_ca_13_0m_a

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```
Bond precision:  C-C = 0.0043 A          Wavelength=0.71073

Cell:             a=8.393(3)     b=20.906(7)         c=11.854(4)
                  alpha=90       beta=97.963(6)      gamma=90
Temperature:      296 K

                 Calculated                Reported
Volume           2059.9(12)                2059.9(11)
Space group      P 21/c                    P 1 21/c 1
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C24 H16 Cl2 N2 O2         C24 H16 Cl2 N2 O2
Sum formula      C24 H16 Cl2 N2 O2         C24 H16 Cl2 N2 O2
Mr               435.29                    435.29
Dx,g cm-3        1.404                     1.404
Z                4                         4
Mu (mm-1)        0.339                     0.339
F000             896.0                     896.0
F000'            897.51
h,k,lmax         9,24,14                   9,24,14
Nref             3620                      3593
Tmin,Tmax        0.941,0.960               0.624,0.746
Tmin'            0.941

Correction method= # Reported T Limits: Tmin=0.624 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.993          Theta(max)= 25.026

R(reflections)= 0.0441( 2211)     wR2(reflections)= 0.1159( 3593)

S = 1.001                 Npar= 273
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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**

```
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00432 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.130 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595         27 Report
```

**Alert level G**

```
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1             107.0 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          1 Note
PLAT793_ALERT_4_G Model has Chirality at C9          (Centro SPGR)         R Verify
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         2 Info
```

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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
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   4 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   2 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 07/08/2019; check.def file version of 30/07/2019**

**Datablock 19gtu356_ca_13_0m_a** - ellipsoid plot