checkCIF/PLATON report

Structure factors have been supplied for datablock(s) gawco5

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: gawco5

```
Bond precision:   C-C = 0.0114 A              Wavelength=1.54184

Cell:             a=8.2266(11)     b=19.245(2)         c=12.8581(18)
                  alpha=90         beta=95.932(8)      gamma=90
Temperature:      100 K

                  Calculated                 Reported
Volume            2024.8(4)                  2024.8(5)
Space group       P 21/n                     P 1 21/n 1
Hall group        -P 2yn                     -P 2yn
Moiety formula    C14 H18 Cl Ga N2 O5 S2 W   C14 H18 Cl Ga N2 O5 S2 W
Sum formula       C14 H18 Cl Ga N2 O5 S2 W   C14 H18 Cl Ga N2 O5 S2 W
Mr                647.43                     647.44
Dx,g cm-3         2.124                      2.124
Z                 4                          4
Mu (mm-1)         15.371                     15.370
F000              1240.0                     1240.0
F000'             1219.42
h,k,lmax          9,21,14                    9,21,14
Nref              3128                       3117
Tmin,Tmax         0.832,0.858                0.045,0.156
Tmin'             0.215

Correction method= # Reported T Limits: Tmin=0.045 Tmax=0.156
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 61.262

R(reflections)= 0.0320( 2951)     wR2(reflections)= 0.0800( 3117)

S = 1.026                  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 B

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THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =     0.5687
```

Alert level C

```
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0114 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     2.496 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=     0.569         12 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     12.00 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for     O1         --C1        .     5.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  W1         --C1        .     6.0 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )        4% Note
PLAT793_ALERT_4_G Model has Chirality at N1            (Centro SPGR)        R Verify
PLAT793_ALERT_4_G Model has Chirality at N2            (Centro SPGR)        S Verify
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       85% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
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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
   9 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
   7 ALERT type 3 Indicator that the structure quality may be low
   3 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 03/05/2019; check.def file version of 29/04/2019

NOMOVE FORCED

Prob = 50
Temp = 100

70 Y

PLATON-Jul 24 19:15:09 2019 - (70316)

Z -28   gawco5   P 1 21/n 1   R = 0.03   RES=   0   101 X