checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

```
Bond precision:    C-C = 0.0063 A              Wavelength=0.71075

Cell:              a=8.058(3)      b=9.064(3)              c=34.864(12)
                   alpha=90        beta=92.718(11)         gamma=90
Temperature:       93 K

                   Calculated                   Reported
Volume             2543.5(15)                   2543.5(16)
Space group        P 21/c                       P 1 21/c 1
Hall group         -P 2ybc                      -P 2ybc
Moiety formula     C14 H12 Cl2 O2               C14 H12 Cl2 O2
Sum formula        C14 H12 Cl2 O2               C14 H12 Cl2 O2
Mr                 283.14                       283.15
Dx,g cm-3          1.479                        1.479
Z                  8                            8
Mu (mm-1)          0.500                        0.499
F000               1168.0                       1168.0
F000'              1170.82
h,k,lmax           9,10,41                      9,10,41
Nref               4660                         4618
Tmin,Tmax          0.985,0.985                  0.552,0.985
Tmin'              0.985

Correction method= # Reported T Limits: Tmin=0.552 Tmax=0.985
AbsCorr = MULTI-SCAN

Data completeness= 0.991              Theta(max)= 25.355

R(reflections)= 0.0698( 3205)                   wR2(reflections)=
                                                0.1973( 4618)

S = 1.060                     Npar= 341
```

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
```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C21      --C21'    .      6.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C31      --C31'    .      6.2 s.u.
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.00633 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......    10.420 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       31 Report
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● Alert level G
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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       8 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       1 Report
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       2 Note
              C14 H12 Cl2 O2
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       4 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      11 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........     3.1 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       0 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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 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
   6 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 18/12/2021; check.def file version of 18/12/2021