checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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 = 0.0051 A            Wavelength=0.71073

Cell:         a=6.9675(10)       b=7.6046(12)      c=20.706(3)
              alpha=83.020(12)   beta=80.403(12)  gamma=83.126(12)
Temperature:  293 K

                Calculated                  Reported
Volume          1068.2(3)                   1068.2(3)
Space group     P -1                        P -1
Hall group      -P 1                        -P 1
Moiety formula  C28 H20 Cl N O              C28 H20 Cl N O
Sum formula     C28 H20 Cl N O              C28 H20 Cl N O
Mr              421.90                      421.90
Dx,g cm-3       1.312                       1.312
Z               2                           2
Mu (mm-1)       0.199                       0.199
F000            440.0                       440.0
F000'           440.46
h,k,lmax        8,9,25                      8,9,25
Nref            4376                        7343
Tmin,Tmax       0.907,0.965                 0.743,1.000
Tmin'           0.907

Correction method= # Reported T Limits: Tmin=0.743 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.678         Theta(max)= 26.372

R(reflections)= 0.0704( 3485)     wR2(reflections)= 0.2068( 7343)

S = 0.949                  Npar= 391
```

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

```
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..      47% Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.00511 Ang.
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Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       25 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       25 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large     0.11 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)    0.012 Degree
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       30 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records        1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)      293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )      39% Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....        ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      384 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..        ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
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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
  2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 13 ALERT level G = General information/check it is not something unexpected

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  3 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
  3 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
```

Datablock: 12CHCl3

```
Bond precision:   C-C = 0.0071 A          Wavelength=0.71073

Cell:          a=10.1961(16)     b=10.8540(16)     c=14.091(2)
               alpha=84.387(12)  beta=87.485(12)   gamma=84.125(12)
Temperature:   293 K
```

```
                  Calculated              Reported
Volume            1542.9(4)               1543.0(4)
Space group       P -1                    P -1
Hall group        -P 1                    -P 1
Moiety formula    C28 H20 Cl N O, 2(C H Cl3) C28 H20 Cl N O, 2(C H Cl3)
Sum formula       C30 H22 Cl7 N O         C30 H22 Cl7 N O
Mr                660.64                  660.63
Dx,g cm-3         1.422                   1.422
Z                 2                       2
Mu (mm-1)         0.668                   0.668
F000              672.0                   672.0
F000'             674.26
h,k,lmax          12,13,16                12,13,16
Nref              5655                    5636
Tmin,Tmax         0.743,0.771             0.975,1.000
Tmin'             0.728


Correction method= # Reported T Limits: Tmin=0.975 Tmax=1.000
AbsCorr = MULTI-SCAN


Data completeness= 0.997          Theta(max)= 25.349


R(reflections)= 0.0841( 3405)     wR2(reflections)= 0.2609( 5636)


S = 1.067                    Npar= 352
```

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**
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ....   0.26 Report
PLAT244_ALERT_4_C Low   Solvent Ueq as Compared to Neighbors of   C29 Check
PLAT244_ALERT_4_C Low   Solvent Ueq as Compared to Neighbors of   C30 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   Cl2   0.147 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   Cl5   0.150 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.00707 Ang.

⚪ **Alert level G**
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large   0.11 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.012 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)   293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)   293 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #   3 Note
             C H Cl3

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```
3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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2 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 22/12/2019; check.def file version of 13/12/2019