checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_1242

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_1242

```
Bond precision:    C-C = 0.0095 A              Wavelength=1.54184

Cell:            a=19.2386(5)      b=14.0313(3)          c=15.2313(4)
                 alpha=90          beta=95.628(2)        gamma=90
Temperature:     100 K

                 Calculated                   Reported
Volume           4091.76(18)                  4091.76(18)
Space group      C c                          C 1 c 1
Hall group       C -2yc                       C -2yc
Moiety formula   C49 H43 N3 O, C H Cl3        C H Cl3, C49 H43 N3 O
Sum formula      C50 H44 Cl3 N3 O             C50 H44 Cl3 N3 O
Mr               809.23                       809.23
Dx,g cm-3        1.314                        1.314
Z                4                            4
Mu (mm-1)        2.353                        2.353
F000             1696.0                       1696.0
F000'            1704.36
h,k,lmax         22,16,18                     22,16,18
Nref             7222[ 3615]                  4376
Tmin,Tmax        0.790,0.889                  0.758,1.000
Tmin'            0.790

Correction method= # Reported T Limits: Tmin=0.758 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.21/0.61      Theta(max)= 66.595

R(reflections)= 0.0734( 4142)      wR2(reflections)= 0.1978( 4376)

S = 1.021                    Npar= 520
```

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

```
PLAT220_ALERT_2_B NonSolvent    Resd 1  C   Ueq(max)/Ueq(min) Range       7.6 Ratio
PLAT416_ALERT_2_B Short Intra D-H..H-D        H2      ..H3      .       1.80 Ang.
                                              x,y,z =       1_555 Check
```

Alert level C

```
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........      6.95 Note
PLAT222_ALERT_3_C NonSolvent Resd 1   H   Uiso(max)/Uiso(min) Range      8.6 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C2 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.00955 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn      H1B     ..H9A     .       2.10 Ang.
                                          x,2-y,1/2+z  =    2_575 Check
PLAT416_ALERT_2_C Short Intra D-H..H-D        H1      ..H2      .       1.92 Ang.
                                              x,y,z =       1_555 Check
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...      16 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............       3 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large    0.15 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    6.08 Why ?
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records       3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records       4 Report
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #       2 Note
            C H Cl3
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............     131 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still     92% Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage     21 %
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........     2.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       2 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
   7 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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   1 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 18/09/2020; check.def file version of 20/08/2020

Datablock exp_1242 - ellipsoid plot

NOMOVE FORCED
Prob = 50
Temp = 100

46 Y

PLATON-Oct 26 00:03:57 2020 - (180920)

Z 66   exp_1242   C 1 c 1   R = 0.07   RES= 0   20 X