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: 140624-1

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Bond precision:   C-C = 0.0056 A            Wavelength=0.71075

Cell:             a=13.9697(7)    b=15.0061(7)          c=14.9113(6)
                  alpha=90        beta=107.8430(13)     gamma=90
Temperature:      108 K

                  Calculated                 Reported
Volume            2975.5(2)                  2975.5(2)
Space group       P 21/n                     P 1 21/n 1
Hall group        -P 2yn                     -P 2yn
                  C42 H40 B4 Cl2 Gd2 N24 O4, C42 H40 B4 Cl2 Gd2 N24 O4,
Moiety formula
                  2(C H2 Cl2)                2(C H2 Cl2)
Sum formula       C44 H44 B4 Cl6 Gd2 N24 O4  C44 H44 B4 Cl6 Gd2 N24 O4
Mr                1543.47                    1543.45
Dx,g cm-3         1.723                      1.723
Z                 2                          2
Mu (mm-1)         2.543                      2.548
F000              1516.0                     1516.0
F000'             1517.43
h,k,lmax          18,19,19                   18,19,19
Nref              6829                       6789
Tmin,Tmax         0.744,0.775                0.602,0.775
Tmin'             0.277

Correction method= # Reported T Limits: Tmin=0.602 Tmax=0.775
AbsCorr = MULTI-SCAN

Data completeness= 0.994          Theta(max)= 27.478

R(reflections)= 0.0331( 5620)     wR2(reflections)= 0.0671( 6789)

S = 1.085                  Npar= 379
```

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
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond C1   -   C2   ..   1.54 Ang.

⚪ Alert level G
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   7.48 Why ?
PLAT333_ALERT_2_G Check Large Av C6-Ring C-C Dist. C1   -C3_a   1.45 Ang.
PLAT882_ALERT_1_G Missing datum for _diffrn_reflns_av_unetI/netI .   Please Check

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

   1 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
   0 ALERT type 3 Indicator that the structure quality may be low
   0 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 13/08/2017; check.def file version of 27/07/2017