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: 3_21srv327

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Bond precision:    C-C = 0.0235 A             Wavelength=0.71073

Cell:              a=10.1647(10)       b=21.424(2)       c=21.601(2)
                   alpha=90            beta=90           gamma=90
Temperature:       120 K

                   Calculated                Reported
Volume             4704.0(8)                 4703.8(8)
Space group        C 2 2 21                  C 2 2 21
Hall group         C 2c 2                    C 2c 2
Moiety formula     C51 H39, B Br4, 2(C H2 Cl2) C51 H39, B Br4, 2(C H2 Cl2)
Sum formula        C53 H43 B Br4 Cl4         C53 H43 B Br4 Cl4
Mr                 1152.08                   1152.12
Dx,g cm-3          1.627                     1.627
Z                  4                         4
Mu (mm-1)          3.687                     3.687
F000               2296.0                    2296.0
F000'              2294.54
h,k,lmax           12,25,25                  12,25,25
Nref               4148[ 2317]               4141
Tmin,Tmax          0.767,0.929               0.409,0.493
Tmin'              0.667

Correction method= # Reported T Limits: Tmin=0.409 Tmax=0.493
AbsCorr = MULTI-SCAN

Data completeness= 1.79/1.00        Theta(max)= 24.999
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R(reflections)= 0.0876(2553)   wR2(reflections)= 0.2639(4141)

S = 1.040   Npar= 286

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
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.02348 Ang.

🟡 Alert level C
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full   ! Check
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   B1 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   Cl1   0.108 Check
PLAT332_ALERT_2_C Large Phenyl C-C Range   C9   -C14   .   0.16 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond C1   - C5   .   1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond C2   - C9   .   1.53 Ang.

⚪ Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...   1 Report
PLAT012_ALERT_1_G No   _shelx_res_checksum Found in CIF ...... 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   12.75 Why ?
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records   1 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   2 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   7 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..   ! Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File   5 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..   50.0 Degree

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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   5 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 18/12/2021; check.def file version of 18/12/2021