checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:    N- C = 0.0174 A          Wavelength=0.71073

Cell:             a=7.539(3)      b=12.059(4)          c=11.144(3)
                  alpha=90        beta=129.48(2)       gamma=90
Temperature:      173 K

                  Calculated                 Reported
Volume            782.0(5)                   782.0(5)
Space group       P c                        P c
Hall group        P -2yc                     P -2yc
Moiety formula    2(C2 H6 N5), Br4 Zn        2(C2 H6 N5), Br4 Zn
Sum formula       C4 H12 Br4 N10 Zn          C4 H12 Br4 N10 Zn
Mr                585.23                     585.25
Dx,g cm-3         2.485                      2.486
Z                 2                          2
Mu (mm-1)         11.793                     11.793
F000              552.0                      552.0
F000'             550.66
h,k,lmax          9,15,14                    9,15,14
Nref              3591[ 1803]                3082
Tmin,Tmax         0.074,0.171                0.112,0.259
Tmin'             0.013

Correction method= # Reported T Limits: Tmin=0.112 Tmax=0.259
AbsCorr = MULTI-SCAN

Data completeness= 1.71/0.86        Theta(max)= 27.514

                                              wR2(reflections)=
R(reflections)= 0.0437( 2918)                 0.1190( 3082)

S = 1.064                 Npar= 168
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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

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PLAT420_ALERT_2_C D-H Bond Without Acceptor  N9      --H9A    .       Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N9      --H9B    .       Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600      12 Report
PLAT977_ALERT_2_C Check Negative Difference Density on H5A    .     -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H9B    .     -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H10B   .     -0.51 eA-3
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⚪ Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............       10 Report
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  Pc         Pn Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records      1 Report
PLAT480_ALERT_4_G Long H...A H-Bond Reported H5A     ..BR1    .     3.05 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H9A     ..BR3    .     3.03 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H9B     ..BR2    .     3.02 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H9B     ..BR4    .     2.94 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H6      ..BR3    .     3.08 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      2 Note
            C2 H6 N5
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1      (II)    .     2.03 Info
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      6 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage    73 %
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........    2.6 Low
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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
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 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
   9 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 06/07/2023; check.def file version of 30/06/2023

Datablock shelx - ellipsoid plot