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: exp_2b

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Bond precision:   C-C = 0.0070 A            Wavelength=0.71073

Cell:          a=10.6008(5)        b=11.0655(6)      c=11.8075(6)
               alpha=103.848(4)  beta=101.399(4)  gamma=93.204(4)
Temperature:   150 K

                Calculated                 Reported
Volume          1310.50(12)                1310.50(12)
Space group     P -1                       P -1
Hall group      -P 1                       ?
                C42 H34 Br4 N2 O2 Zn2, 4(C C42 H34 Br4 N2 O2 Zn2, 4(C
Moiety formula
                H2 Cl2)                    H2 Cl2)
Sum formula     C46 H42 Br4 Cl8 N2 O2 Zn2  C46 H42 Br4 Cl8 N2 O2 Zn2
Mr              1388.80                    1388.80
Dx,g cm-3       1.760                      1.760
Z               1                          1
Mu (mm-1)       4.411                      4.411
F000            684.0                      684.0
F000'           684.82
h,k,lmax        12,13,14                   12,13,14
Nref            5022                       4913
Tmin,Tmax       0.477,0.516                0.509,1.000
Tmin'           0.468

Correction method= MULTI-SCAN

Data completeness= 0.978          Theta(max)= 25.760

R(reflections)= 0.0516( 4597)     wR2(reflections)= 0.1407( 4913)

S = 0.956                   Npar= Npar = 292
```

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

```
DIFMX01_ALERT_2_C  The maximum difference density is > 0.1*ZMAX*0.75
            _refine_diff_density_max given =      2.685
            Test value =      2.625
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......    0.977 Note
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density     2.68 eA-3
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of       C23 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.0070 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C1    -  C2     ...      1.54 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H5     .. H19B    ..      2.12 Ang.
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Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      6.14 Why ?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .     mixed
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........  0.00400 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Br1    --  Zn1     ..      15.3 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Br2    --  Zn1     ..      16.8 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Br2    --  Zn1_a   ..      19.5 su
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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
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   7 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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*, 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 05/02/2014; check.def file version of 05/02/2014