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: mo_b0381_0m

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Bond precision:  C-C = 0.0305 A          Wavelength=0.71073

Cell:           a=12.4905(6)    b=27.4811(12)      c=21.4644(12)
                alpha=90        beta=92.663(2)     gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          7359.8(6)                 7359.8(6)
Space group     P n                       P 1 n 1
Hall group      P -2yac                   P -2yac
Moiety formula  2(C26 H60 Br8 N4 O14 Zn9), 2(C26 H60 Br8 N4 O14 Zn9),
                4(C6 H16 N), C3 H6 O      4(C6 H16 N), C3 H6 O
Sum formula     C79 H190 Br16 N12 O29 Zn18 C79 H190 Br16 N12 O29 Zn18
Mr              4227.86                   4227.64
Dx,g cm-3       1.908                     1.908
Z               2                         2
Mu (mm-1)       7.274                     7.274
F000            4160.0                    4160.0
F000'           4163.23
h,k,lmax        15,33,26                  15,33,26
Nref            28933[ 14483]             28173
Tmin,Tmax       0.190,0.336               0.031,0.100
Tmin'           0.032

Correction method= # Reported T Limits: Tmin=0.031 Tmax=0.100
AbsCorr = MULTI-SCAN

Data completeness= 1.95/0.97      Theta(max)= 26.000

R(reflections)= 0.0479( 25238)    wR2(reflections)= 0.1380( 28173)

S = 1.083                 Npar= 1421
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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 B

PLAT213_ALERT_2_B Atom C8 has ADP max/min Ratio ..... 4.5 prolat
PLAT213_ALERT_2_B Atom C10 has ADP max/min Ratio ..... 4.4 prolat
PLAT220_ALERT_2_B Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 6.9 Ratio
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.03053 Ang.
PLAT601_ALERT_2_B Structure Contains Solvent Accessible VOIDS of . 178 Ang3
PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

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Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.500
From the CIF: _refine_ls_abs_structure_Flack_su 0.000
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 4 Check
PLAT213_ALERT_2_C Atom C2 has ADP max/min Ratio ..... 3.7 prolat
PLAT213_ALERT_2_C Atom C3 has ADP max/min Ratio ..... 3.4 prolat
PLAT213_ALERT_2_C Atom C5 has ADP max/min Ratio ..... 3.1 oblate
PLAT213_ALERT_2_C Atom C11 has ADP max/min Ratio ..... 3.9 prolat
PLAT213_ALERT_2_C Atom C12 has ADP max/min Ratio ..... 3.2 prolat
PLAT213_ALERT_2_C Atom O15 has ADP max/min Ratio ..... 3.4 oblate
PLAT214_ALERT_2_C Atom C78 (Anion/Solvent) ADP max/min Ratio 4.4 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 2 C Ueq(max)/Ueq(min) Range 4.0 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 10.0 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 2 H Uiso(max)/Uiso(min) Range 4.8 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C65 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C67 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N5 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N6 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C37 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N11 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C77 Check
PLAT245_ALERT_2_C U(iso) H1 Smaller than U(eq) O1 by ... 0.020 AngSq
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.0 Note
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C16 - C17 .. 1.43 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C37 - C38 .. 1.39 Ang.
PLAT361_ALERT_2_C Long C(sp3)-C(sp3) Bond C65 - C66 .. 1.74 Ang.
PLAT362_ALERT_2_C Short C(sp3)-C(sp2) Bond C77 - C79 .. 1.35 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H11C .. H32C .. 2.11 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 20 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 27.10 Why ?
PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry . 92 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group P21/n Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 10 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 9 Report
PLAT300_ALERT_4_G Atom Site Occupancy of >Br1B is Constrained at 0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <Br1A is Constrained at 0.25 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 1 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C65 -- C66 . 1.74 Ang.

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PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
             C6 H16 N
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        49 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  27 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  17 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  26 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
  16 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* 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 06/05/2016; check.def file version of 05/05/2016

Datablock mo_b0381_0m - ellipsoid plot