checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB1

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: MAB1

Bond precision: C-C = 0.0030 A Wavelength=0.71075

Cell: a=26.0212(3) b=9.1562(1) c=13.6318(2)
alpha=90 beta=99.580(1) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3202.56(7)	3202.55(7)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C4 H19 B6 N3 O13 Zn), H2 O	C4 H19 B6 N3 O13 Zn, 0.5(H2 O)
Sum formula	C8 H40 B12 N6 O27 Zn2	C4 H20 B6 N3 O13.50 Zn
Mr	912.96	456.46
Dx,g cm-3	1.893	1.893
Z	4	8
Mu (mm-1)	1.613	1.613
F000	1864.0	1864.0
F000’	1867.36	
h,k,lmax	33,11,17	33,11,17
Nref	3674	3651
Tmin,Tmax	0.660,0.879	0.752,1.000
Tmin’	0.503	

Correction method= # Reported T Limits: Tmin=0.752 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 27.483

R(reflections)= 0.0240(3541) wR2(reflections)= 0.0666(3651)

S = 1.095 Npar= 287

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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PLAT220_ALERT_2_C Non-Solvent  Resd 1  O   Ueq(max)/Ueq(min) Range        3.7 Ratio
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) ........         O1 Check
PLAT417_ALERT_2_C Short Inter D-H..H-D       H9       ..H12      .       2.10 Ang.
                                          1-x,1-y,1-z  =      5_666 Check
PLAT420_ALERT_2_C D-H Without Acceptor       N3       --H3AB     .     Please Check
PLAT420_ALERT_2_C D-H Without Acceptor       N3       --H3BC     .     Please Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         17 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         13 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.54 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          6 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          3 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    N3       --C4       .        8.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C3       --C4B      .        6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn1      --N3       .        6.1 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O10         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O10B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4          Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4B         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3AA        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3AB        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3BC        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3BD        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4A         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4B         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3BE        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3BF        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3AC        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3AD        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4BA        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4BB        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O21         Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21B        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )          7% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  2           1.50 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O21      ..B6               2.90 Ang.
                                                  x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         10 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         12 Note
PLAT883_ALERT_1_G No Info for _atom_sites_solution_primary .......     Please Do !
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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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  39 ALERT level G = General information/check it is not something unexpected
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  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 11 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
 27 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 18/02/2019; check.def file version of 18/02/2019

Datablock MAB1 - ellipsoid plot