checkCIF/PLATON report

Structure factors have been supplied for datablock(s) znbcatdmap_a

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: znbcatdmap_a

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Bond precision:   C-C = 0.0043 A          Wavelength=1.54178

Cell:             a=12.6072(4)     b=19.2243(8)        c=16.2759(6)
                  alpha=90         beta=94.982(3)      gamma=90
Temperature:      100 K

                 Calculated                  Reported
Volume           3929.8(3)                   3929.8(3)
Space group      P 21/c                      P 1 21/c 1
Hall group       -P 2ybc                     -P 2ybc
Moiety formula   C42 H55 B N4 O2 Zn          C42 H55 B N4 O2 Zn
Sum formula      C42 H55 B N4 O2 Zn          C42 H55 B N4 O2 Zn
Mr               724.10                      724.08
Dx,g cm-3        1.224                       1.224
Z                4                           4
Mu (mm-1)        1.165                       1.165
F000             1544.0                      1544.0
F000'            1541.48
h,k,lmax         15,23,20                    15,23,19
Nref             7785                        7541
Tmin,Tmax        0.932,0.966                 0.474,0.754
Tmin'            0.900

Correction method= # Reported T Limits: Tmin=0.474 Tmax=0.754
AbsCorr = NONE

Data completeness= 0.969           Theta(max)= 72.380

R(reflections)= 0.0524( 5546)                    wR2(reflections)=
                                                 0.1363( 7541)
S = 1.021                  Npar= 523
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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

```
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.488 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         98 Report
              -12 14  1,  11 15  1, -12 14  2,  11 15  2,  10 16  2,  12 13  3,
               11 14  3,  10 15  3,  11 15  3,   9 16  3,  11 14  4,   8 15  4,
                9 15  4,  10 15  4,   7 16  4,   8 16  4,   8 15  5,   9 15  5,
               -8  2  7,  10 10  7,  10 10  8,   9 11  8,  10 10  9,   9 14  9,
                9  9 10,   8 10 10,   9 10 10,   8 11 10,   9 11 10,   8 12 10,
                9 13 10,   8 14 10,   7 15 10,   9  8 11,   9  9 11,   8 10 11,
                9 10 11,   8 11 11,   9 11 11,   8 12 11,   7 13 11,   8 13 11,
                7 14 11,   6 15 11,   6 16 11,   9  7 12,   9  8 12,   9  9 12,
                8 10 12,   9 10 12,   8 11 12,   7 12 12,   8 12 12,   7 13 12,
                6 14 12,  -8  9 13,   8  9 13,   8 10 13,   7 12 13,  -8 13 13,
               -7 14 13,   8  8 14,  -7 13 14,  -6 12 15,   4  0 16,  -6 10 16,
               -6  8 17,  -5  8 17,  -5  9 17,  -7  0 18,  -6  0 18,  -5  0 18,
               -4  0 18,  -3  0 18,  -6  1 18,  -5  1 18,  -4  1 18,  -3  1 18,
               -5  2 18,  -4  2 18,  -5  3 18,  -4  3 18,  -5  4 18,  -4  4 18,
               -6  5 18,  -5  5 18,  -4  5 18,  -5  6 18,  -4  6 18,  -4  7 18,
               -4  1 19,  -3  1 19,  -2  1 19,  -4  2 19,  -3  2 19,  -4  3 19,
PLAT977_ALERT_2_C Check Negative Difference Density on H49A      .      -0.34 eA-3
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          12 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         12% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C13 Check
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O1       .       106.8 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O2       .       107.5 Degree
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H37      ..H34A     .        2.09 Ang.
                                                    x,y,z  =      1_555 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         108 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         137 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........         2.9 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       1.500 Note
              Predicted wR2: Based on SigI**2  9.09 or SHELX Weight 13.35
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.           1 Info
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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
14 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  7 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
  4 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 22/08/2024; check.def file version of 21/08/2024

Datablock znbcatdmap_a - ellipsoid plot