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: 4

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Bond precision:  C-C = 0.0038 A          Wavelength=0.71073

Cell:            a=7.1661(3)    b=15.0840(6)        c=19.1836(9)
                 alpha=90       beta=103.732(4)     gamma=90
Temperature:     103 K

                 Calculated                Reported
Volume           2014.35(15)               2014.35(15)
Space group      P 2/c                     P2/c
Hall group       -P 2yc                    ?
                 4(C7 H7 N2 O), 4(C7 H9 N2
Moiety formula   O), 4(Cl4 Zn), H4 O, 6(H2 ?
                 O), O
Sum formula      C56 H80 Cl16 N16 O16 Zn4  C56 H80 Cl16 N16 O16 Zn4
Mr               2062.12                   2062.04
Dx,g cm-3        1.700                     1.700
Z                1                         1
Mu (mm-1)        1.778                     1.778
F000             1048.0                    1048.0
F000'            1051.80
h,k,lmax         10,21,27                  8,18,27
Nref             6419                      6299
Tmin,Tmax                                  0.751,1.000
Tmin'

Correction method= # Reported T Limits: Tmin=0.751 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.981          Theta(max)= 30.980

R(reflections)= 0.1021( 4184)     wR2(reflections)= 0.2102( 5027)

S = 1.052                 Npar= 220
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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 A

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PLAT417_ALERT_2_A Short Inter D-H..H-D       H4A      ..H5D      .       1.68 Ang.
                                          -1+x,1-y,-1/2+z  =      4_465 Check
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Alert level B

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PLAT417_ALERT_2_B Short Inter D-H..H-D       H6WA     ..H1B      .       1.85 Ang.
                                            -1-x,-y,-1-z  =      3_454 Check
PLAT417_ALERT_2_B Short Inter D-H..H-D       H6WA     ..H1B      .       2.06 Ang.
                                            1+x,-y,1/2+z  =      4_656 Check
PLAT420_ALERT_2_B D-H Without Acceptor       O6'      --H6WA     .     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O7       --H7B      .     Please Check
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Alert level C

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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       2.45 eA-3
PLAT112_ALERT_2_C ADDSYM Detects New (Pseudo) Symm. Elem         I        83 %Fit
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O7'        .         2 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O7         .         2 Check
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N1       --C1       .       5.3 s.u.
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       O6'      0.107 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O7      0.107 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O5      0.107 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        O6      0.107 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #         1 Note
             C7 H7 N2 O
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        14 Note
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        12 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  P2/c          P2/n Note
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1'        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2'        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7'        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O6'        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O7         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O7'        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O6         Constrained at       0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        30% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note
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PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  5          2.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  8          0.25 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....        O7' Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....         O6 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          1 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        27 Check
             C7   -C4   -C7'     1.555   1.555   1.555             0.00 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             C7 H9 N2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
             Cl4 Zn
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
             Cl4 Zn
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          5 Note
             H4 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          6 Note
             H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7 Note
             H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8 Note
             O
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       2.01 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2       (II)      .       2.01 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          9 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2018 Note
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ           2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           3 Units
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  1 ALERT level A = Most likely a serious problem - resolve or explain
  4 ALERT level B = A potentially serious problem, consider carefully
 15 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 38 ALERT level G = General information/check it is not something unexpected

  6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 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
 27 ALERT type 4 Improvement, methodology, query or suggestion
  6 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 03/05/2019; check.def file version of 29/04/2019

Datablock 4 - ellipsoid plot