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: a_a_sq

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Bond precision:   C-C = 0.0126 A            Wavelength=0.71073

Cell:          a=10.6771(18)      b=15.343(2)        c=23.040(4)
               alpha=102.675(5)   beta=94.198(5)   gamma=99.900(5)
Temperature:   273 K

                   Calculated                   Reported
Volume             3603.3(10)                   3603.5(10)
Space group        P -1                         P -1
Hall group         -P 1                         -P 1
                   C40 H48 Ca N20 O14, 3(C6
Moiety formula     H5 N O3), Cl4 Zn [+          Cl4 Zn, C40 H48 Ca N20
                   solvent]                     O14, 3(C6 H5 N O3)
                   C58 H63 Ca Cl4 N23 O23 Zn
Sum formula        [+ solvent]                  C58 H63 Ca Cl4 N23 O23 Zn
Mr                 1697.59                      1697.56
Dx,g cm-3          1.565                        1.565
Z                  2                            2
Mu (mm-1)          0.653                        0.653
F000               1748.0                       1748.0
F000'              1750.97
h,k,lmax           12,18,27                     12,18,27
Nref               12695                        12553
Tmin,Tmax          0.901,0.925                  0.492,0.746
Tmin'              0.901

Correction method= # Reported T Limits: Tmin=0.492 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.989           Theta(max)= 24.999

R(reflections)= 0.1330( 9442)      wR2(reflections)= 0.3776( 12553)

S = 1.448                   Npar= 935
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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

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PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ...................     0.38 Report
PLAT230_ALERT_2_B Hirshfeld Test Diff for    O17      --N21      .     9.3 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for    C42      --C43      .     7.3 s.u.
PLAT415_ALERT_2_B Short Inter D-H..H-X       H19A     ..H48      .     1.98 Ang.
                                             x,y,z  =     1_555 Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O14      --H14      .     Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O18      --H18      .     Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O19      --H19B     .     Please Check
PLAT420_ALERT_2_B D-H Bond Without Acceptor  O22      --H22C     .     Please Check
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Alert level C

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DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given    0.147
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........    0.147 Report
PLAT082_ALERT_2_C High R1 Value ...............................    0.13 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....    2.26 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density    2.27 eA-3
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O15       .       6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O13       .       6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O14       .       6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for N22       .       6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O16       .       6 Check
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for O18       .       6 Check
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range    3.2 Ratio
PLAT223_ALERT_4_C Solv./Anion  Resd 4  H   Ueq(max)/Ueq(min) Range    4.5 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C48      --C49      .     5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C45      --C46      .     6.4 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C50      --C51      .     0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C53      --C58      .     0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C55      --C56      .     0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N21      --C43      .     0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C43      --C44      .     0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    N22 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C49 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of    C42 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C47 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C50 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C55 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C58 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    N21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C44 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C45 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    C46 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of    Zn1 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O11    0.107 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O12    0.126 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      O16    0.135 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C47     -C52          1.35 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.01261 Ang.
PLAT415_ALERT_2_C Short Inter D-H..H-X       H22C     ..H45      .     2.12 Ang.
                                             x,y,z  =     1_555 Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          9 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          12 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension           1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          11 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ  Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large        0.20 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.005 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records           6 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records           6 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records           1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)         273 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)          273 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure          47 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........           4 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1        (II)       .       2.05 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          78 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         113 Note
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 0 ALERT level A = Most likely a serious problem - resolve or explain
 8 ALERT level B = A potentially serious problem, consider carefully
39 ALERT level C = Check. Ensure it is not caused by an omission or oversight
19 ALERT level G = General information/check it is not something unexpected

 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
33 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
13 ALERT type 4 Improvement, methodology, query or suggestion
 3 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 03/06/2021; check.def file version of 02/06/2021

NOMOVE FORCED

Prob = 50
Temp = 273

1 Y

PLATON-Jul 1 03:31:11 2021 - (30621)

Z 2   a_a_sq   P -1   R = 0.13   RES= 0   31 X