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: 1

```
Bond precision:  C-C = 0.0056 A              Wavelength=0.71073

Cell:          a=9.835(2)          b=12.723(3)        c=14.592(4)
               alpha=84.277(3)   beta=87.288(3)   gamma=76.841(3)
Temperature:   293 K

                Calculated                   Reported
Volume          1768.5(7)                    1768.5(7)
Space group     P -1                         P -1
Hall group      -P 1                         ?
                C28 H38 Cl2 N4 O4 Zn, 2(Cl C28 H38 Cl2 N4 O4 Zn, Cl
Moiety formula  O4)                          O4, Cl O4
Sum formula     C28 H38 Cl4 N4 O12 Zn        C28 H38 Cl4 N4 O12 Zn
Mr              829.81                       829.79
Dx,g cm-3       1.558                        1.558
Z               2                            2
Mu (mm-1)       1.061                        1.061
F000            856.0                        856.0
F000'           858.12
h,k,lmax        12,15,17                     11,15,17
Nref            6869                         6671
Tmin,Tmax       0.725,0.809                  0.672,0.803
Tmin'           0.648

Correction method= MULTI-SCAN

Data completeness= 0.971          Theta(max)= 25.890

R(reflections)= 0.0489( 4875)     wR2(reflections)= 0.1544( 6671)

S = 1.065                  Npar= 448
```

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

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......     0.971
PLAT220_ALERT_2_C Large Non-Solvent    C    Ueq(max)/Ueq(min) ...       3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C27    -- C28    ..      0.17 Ang.
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....      N4 Check
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF    Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .........   0.00300 Deg.
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)        293 Check
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of       Cl3 Check
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of       Cl4 Check
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  7 ALERT level G = General information/check it is not something unexpected

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  2 ALERT type 2 Indicator that the structure model may be wrong or deficient
  1 ALERT type 3 Indicator that the structure quality may be low
  3 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
```

Datablock: 2

```
Bond precision:   C-C = 0.0069 A          Wavelength=0.71073

Cell:          a=9.0372(12)      b=12.5384(16)     c=15.1211(19)
               alpha=89.705(2)   beta=86.941(2)    gamma=84.171(2)
Temperature:   293 K
```

```
                    Calculated              Reported
Volume              1702.1(4)               1702.1(4)
Space group         P -1                    P -1
Hall group          -P 1                    ?
Moiety formula      C15 H16 Cl N4 O2 S2 Zn, C15 H16 Cl N4 O2 S2 Zn,
                    C13 H20 Cl N2 O4 Zn     C13 H20 Cl N2 O4 Zn
Sum formula         C28 H36 Cl2 N6 O6 S2 Zn2 C28 H36 Cl2 N6 O6 S2 Zn2
Mr                  818.45                  818.39
Dx,g cm-3           1.597                   1.597
Z                   2                       2
Mu (mm-1)           1.739                   1.739
F000                840.0                   840.0
F000'               842.46
h,k,lmax            10,14,17                10,14,17
Nref                5709                    5592
Tmin,Tmax           0.487,0.812             0.591,0.708
Tmin'               0.477


Correction method= MULTI-SCAN


Data completeness= 0.980          Theta(max)= 24.560


R(reflections)= 0.0432( 4251)     wR2(reflections)= 0.1291( 5592)


S = 1.088                  Npar= 443
```

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

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
         Calculated sin(theta_max)/wavelength =    0.5848
PLAT220_ALERT_2_C Large Non-Solvent   C    Ueq(max)/Ueq(min) ...        3.7 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N11    -- C27      ..      5.3 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Zn1    -- N2       ..      5.5 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Zn2    -- O2W      ..      7.0 su
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       O2 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C11 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       N2 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       C15 Check
PLAT245_ALERT_2_C U(iso) H22      Smaller than U(eq) C22    by ...    0.012 AngSq
PLAT245_ALERT_2_C U(iso) H23      Smaller than U(eq) C23    by ...    0.014 AngSq
PLAT245_ALERT_2_C U(iso) H29B     Smaller than U(eq) C29    by ...    0.020 AngSq
PLAT245_ALERT_2_C U(iso) H30A     Smaller than U(eq) C30    by ...    0.017 AngSq
PLAT245_ALERT_2_C U(iso) H32A     Smaller than U(eq) C32    by ...    0.011 AngSq
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.0069 Ang.
PLAT355_ALERT_3_C Long    O-H (X0.82,N0.98A) O1W    -   H1A    ...     1.05 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF    Please Do !
```

```
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .........    0.00200 Deg.
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)      293 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       25 Do !
          N4  -ZN1 -N3  -C14   106.00 18.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       26 Do !
          N1  -ZN1 -N3  -C14   -64.00 19.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       27 Do !
          O1  -ZN1 -N3  -C14  -156.00 18.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       28 Do !
          N2  -ZN1 -N3  -C14    14.00 18.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       29 Do !
          N3  -ZN1 -N4  -C15   -24.00  4.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       30 Do !
          N1  -ZN1 -N4  -C15   147.00  4.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       31 Do !
          O1  -ZN1 -N4  -C15  -121.00  4.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       32 Do !
          N2  -ZN1 -N4  -C15    72.00  4.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       68 Do !
          ZN1 -N3  -C14 -S1     43.00 42.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #       69 Do !
          ZN1 -N4  -C15 -S2   -161.00 16.00   1.555   1.555   1.555   1.555
```

```
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  14 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  10 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: 3

```
Bond precision:   C-C = 0.0035 A          Wavelength=0.71073

Cell:          a=16.9993(6)    b=7.5278(3)        c=13.5447(5)
               alpha=90        beta=100.037(1)    gamma=90
Temperature:   296 K
```

```
                Calculated                Reported
Volume          1706.75(11)               1706.75(11)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   ?
Moiety formula  C15 H16 Cl N5 O2 Zn       C15 H16 Cl N5 O2 Zn
Sum formula     C15 H16 Cl N5 O2 Zn       C15 H16 Cl N5 O2 Zn
Mr              399.17                    399.15
Dx,g cm-3       1.554                     1.553
Z               4                         4
Mu (mm-1)       1.613                     1.613
F000            816.0                     816.0
F000'           817.94
h,k,lmax        23,10,18                  23,10,18
Nref            4624                      4582
Tmin,Tmax       0.544,0.597               0.402,0.498
Tmin'           0.519


Correction method= MULTI-SCAN

Data completeness= 0.991          Theta(max)= 29.180

R(reflections)= 0.0347( 3541)     wR2(reflections)= 0.0944( 4582)

S = 1.024                    Npar= 217
```

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**
PLAT241_ALERT_2_C High   Ueq as Compared to Neighbors for .....   O1 Check
PLAT242_ALERT_2_C Low   Ueq as Compared to Neighbors for .....   C14 Check

⚪ **Alert level G**
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension ....   1 Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF   Please Do !
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #   68 Do !
          ZN -N3 -C14 -N5   151.50 1.70   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #   69 Do !
          C15 -N5 -C14 -N3   165.30 1.80   1.565   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #   70 Do !
          ZN -N4 -C15 -N5   165.10 1.90   1.555   1.555   1.555   1.545

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

```
      2 ALERT type 2 Indicator that the structure model may be wrong or deficient
      0 ALERT type 3 Indicator that the structure quality may be low
      3 ALERT type 4 Improvement, methodology, query or suggestion
      2 ALERT type 5 Informative message, check
```

Datablock: 4

```
Bond precision:    C-C = 0.0103 A              Wavelength=0.71073

Cell:              a=8.8137(7)     b=14.6565(11)        c=25.2937(19)
                   alpha=90        beta=96.030(3)       gamma=90
Temperature:       293 K

                   Calculated                  Reported
Volume             3249.3(4)                   3249.3(4)
Space group        P 21/n                      P 21/n
Hall group         -P 2yn                      ?
Moiety formula     C26 H34 Cl2 N10 O5 Zn2      C26 H34 Cl2 N10 O5 Zn2
Sum formula        C26 H34 Cl2 N10 O5 Zn2      C26 H34 Cl2 N10 O5 Zn2
Mr                 768.31                      768.27
Dx,g cm-3          1.571                       1.570
Z                  4                           4
Mu (mm-1)          1.693                       1.693
F000               1576.0                      1576.0
F000'              1579.88
h,k,lmax           10,17,30                    10,17,30
Nref               6209                        6142
Tmin,Tmax          0.745,0.816                 0.702,0.798
Tmin'              0.503

Correction method= MULTI-SCAN

Data completeness= 0.989          Theta(max)= 25.750

R(reflections)= 0.0623( 4194)     wR2(reflections)= 0.1599( 6142)

S = 1.092                    Npar= 412
```

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
```
PLAT241_ALERT_2_B High      Ueq as Compared to Neighbors for .....      N3 Check
PLAT242_ALERT_2_B Low       Ueq as Compared to Neighbors for .....      N4 Check
PLAT360_ALERT_2_B Short  C(sp3)-C(sp3) Bond  C9    -   C10   ...     1.32 Ang.
```

● Alert level C

```
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...        3.3 Ratio
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        O1 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        N6 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        N8 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C10 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C13 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C14 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       Zn1 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        N2 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        N7 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....       C18 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0103 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H20    .. H26B    ..       2.11 Ang.
```

● Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF    Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      8.43
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        25 Do !
        ZN1 -N3  -N4  -N5    154.00 17.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        30 Do !
        ZN1 -N6  -N7  -N8   -166.00  6.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        31 Do !
        N6  -N7  -N8  -ZN2    18.00  0.00   1.555   1.555   1.555   1.555
```

```
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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*, 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 18/09/2013; check.def file version of 12/09/2013

Datablock 1 - ellipsoid plot