checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:    C-C = 0.0012 A              Wavelength=1/2

Cell:              a=17.4631(2)      b=17.4631(2)      c=10.1640(2)
                   alpha=90          beta=90           gamma=120
Temperature:       100 K

                   Calculated                 Reported
Volume             2684.34(8)                 2684.34(8)
Space group        P 63/m                     P 63/m
Hall group         -P 6c                      -P 6c
Moiety formula     C27 H3 F6 K2 O19 Zn3 [+
                   solvent]                    (C27 H3 F6 K2 O18 Zn3), (O)

Sum formula        C27 H3 F6 K2 O19 Zn3 [+
                   solvent]                    C27 H3 F6 K2 O19 Zn3
Mr                 1019.66                    1019.60
Dx,g cm-3          1.262                      1.261
Z                  2                          2
Mu (mm-1)          0.595                      0.595
F000               998.0                      998.0
F000'              1000.46
h,k,lmax           36,36,21                   34,34,13
Nref               8863                       6922
Tmin,Tmax          0.779,0.942                0.661,1.000
Tmin'              0.700

Correction method= # Reported T Limits: Tmin=0.661 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.781             Theta(max)= 31.488
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R(reflections)= 0.0376(5449)

wR2(reflections)= 0.1261(6923)

S = 1.058   Npar= 100

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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PLAT230_ALERT_2_C Hirshfeld Test Diff for    F3      --C3      .        6.6 s.u.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        27 Report
                 0  3  0,  -4  8  0, -13 14  0,  -1 14  0, -11 15  0,  -4 15  0,
                 0  2  1,   0  3  1,  -4  5  1,   0  0  2,   0  1  2,  -1  3  2,
                 0  0  4,  -1  3  4,   0  0  6,   0  0  8,   0  0 10,   0  1 10,
                 0  1 11,  -1  2 11,   0  0 12,   0  1 12,  -1  2 12,   0  2 12,
                -2  3 12,  -1  3 12,   0  3 12,
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..        1 Check
                -8  9  1,
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.81Ang From O1       .       0.42 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.40Ang From O1       .      -0.40 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1         .      -0.34 eA-3
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⚪ Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension        3 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
            Calc: C27 H3 F6 K2 O19 Zn3
            Rep.: (C27 H3 F6 K2 O18 Zn3), (O)
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............      0.5 Check
            K1A     K1B
PLAT300_ALERT_4_G Atom Site Occupancy of O1         Constrained at    0.3333 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)      12% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....       O1 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........        ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .     1.94 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE   Suppressed       ! Info
PLAT899_ALERT_4_G SHELXL2018 is Outdated   and Succeeded by SHELXL   2019/3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        3 Note
             0  1  0,  -1  2  0,   0  1  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      289 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....        3 Note
             0  1  0,   0  0  4,   0  0  8,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File       14 Note
           -1 23 13, -18 25 13,   0  2  1,   0  3  1, -19 25 13, -19 26 13,
          -17 25 13,  -1  2  0,  -1  3  2, -18 24 13,   0  3  0,  -1  3  4,
           -4  8  0,  -4  5  1,
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ        2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ        2 Units
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ.       8 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ.       8 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........    6.640 Note
            Predicted wR2: Based on SigI**2  1.90 or SHELX Weight 11.95
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PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   3 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
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  21 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   6 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 22/08/2024; check.def file version of 21/08/2024