checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: compound_1

Bond precision: C-C = 0.0063 A   Wavelength=0.71073

Cell: a=8.0716(18)   b=8.1663(19)   c=9.1623(11)
               alpha=90   beta=90   gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	603.9(2)	603.9(2)
Space group	P n a 21	Pna21
Hall group	P 2c -2n	?
Moiety formula	C4 H6 O5 Zn	?
Sum formula	C4 H6 O5 Zn	C4 H6 O5 Zn
Mr	199.48	199.46
Dx,g cm-3	2.194	2.194
Z	4	4
Mu (mm-1)	4.022	4.022
F000	400.0	400.0
F000'	401.36	
h,k,lmax	11,11,13	11,11,13
Nref	1014[1920]	1782
Tmin,Tmax	0.749,0.851	
Tmin'	0.725	

Correction method= Not given

Data completeness= 1.76/0.93   Theta(max)= 30.980

R(reflections)= 0.0466(1548)   wR2(reflections)= 0.1029(1782)

S = 0.988   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
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.973
PLAT057_ALERT_3_C Correction for Absorption Required   RT(exp) ...   1.14
PLAT222_ALERT_3_C Large Non-Solvent   H   Uiso(max)/Uiso(min) ..   6.8 Ratio
PLAT245_ALERT_2_C U(iso) H1WA   Smaller than U(eq) O1W   by ...   0.018 AngSq

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PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0063 Ang
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #        1
            C4 H6 O5 Zn
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⬤ Alert level G

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REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
            correct. If it is not, please give the correct count in the
            _publ_section_exptl_refinement section of the submitted CIF.
            From the CIF: _diffrn_reflns_theta_max         30.98
            From the CIF: _reflns_number_total             1782
            Count of symmetry unique reflns         1014
            Completeness (_total/calc)          175.74%
            TEST3: Check Friedels for noncentro structure
            Estimate of Friedel pairs measured        768
            Fraction of Friedel pairs measured      0.757
            Are heavy atom types Z>Si present         yes
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        3
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .        3
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....        ?
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....        ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....        ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....        ?
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature     293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature     293 K
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        2
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .     1.38 Ratio
PLAT792_ALERT_1_G Note: The Model has Chirality at C2       (Verify)       R
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and su ..     0.03
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        4
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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
  14 ALERT level G = General information/check it is not something unexpected

   6 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
   5 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   2 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*, 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 21/12/2011; check.def file version of 16/12/2011