checkCIF/PLATON report

Structure factors have been supplied for datablock(s) zn2l2etoh2

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: zn2l2etoh2

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Bond precision:  C-C = 0.0039 A          Wavelength=0.71073

Cell:          a=9.9945(3)       b=12.8141(3)      c=13.8744(4)
               alpha=98.971(2)   beta=105.037(3)   gamma=110.495(2)
Temperature:   150 K
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	Calculated	Reported
Volume	1546.47(9)	1546.47(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C66 H56 O10 Zn2 [+ solvent]	C66 H56 O10 Zn2
Sum formula	C66 H56 O10 Zn2 [+ solvent]	C66 H56 O10 Zn2
Mr	1139.89	1139.84
Dx,g cm-3	1.224	1.224
Z	1	1
Mu (mm-1)	0.830	0.830
F000	592.0	592.0
F000’	592.81	
h,k,lmax	13,17,19	13,17,18
Nref	8416	7268
Tmin,Tmax	0.755,0.813	0.844,1.000
Tmin’	0.740	

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Correction method= # Reported T Limits: Tmin=0.844 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.864          Theta(max)= 29.251

R(reflections)= 0.0483( 5664)     wR2(reflections)= 0.1424( 7268)

S = 1.037                 Npar= 408
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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 C

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PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        4.2 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        4.7 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O5       --C32      .        6.5 s.u.
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.9 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         16 Report
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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 ...          2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          2 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        15% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H24      ..H27A     .       2.09 Ang.
                                                      x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H24      ..H27B     .       2.09 Ang.
                                                      x,y,z  =      1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H5       ..H32C             2.00 Ang.
                                                      x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C32      ..C33B             2.55 Ang.
                                        -1-x,2-y,1-z  =      2_476 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        223 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          2 Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          7 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         18 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       1124 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         15 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         16 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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  23 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 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
  11 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 07/08/2019; check.def file version of 30/07/2019

Datablock zn2l2etoh2 - ellipsoid plot