checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Zn2L2MeOH2

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: Zn2L2MeOH2

Bond precision: C-C = 0.0042 A   Wavelength=0.71073

Cell: a=9.9444(5)   b=12.9319(6)   c=13.6843(7)
               alpha=99.295(4)   beta=104.338(4)   gamma=111.088(5)
Temperature: 143 K

	Calculated	Reported
Volume	1528.44(16)	1528.45(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C64 H52 O10 Zn2 [+ solvent]	C64 H52 O10 Zn2
Sum formula	C64 H52 O10 Zn2 [+ solvent]	C64 H52 O10 Zn2
Mr	1111.84	1111.79
Dx,g cm-3	1.208	1.208
Z	1	1
Mu (mm-1)	0.838	0.838
F000	576.0	576.0
F000'	576.80	
h,k,lmax	13,17,18	13,17,18
Nref	8409	7322
Tmin,Tmax	0.794,0.897	0.793,1.000
Tmin'	0.709	

Correction method= # Reported T Limits: Tmin=0.793 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.871   Theta(max)= 29.353

R(reflections)= 0.0465(5990)   wR2(reflections)= 0.1263(7322)

S = 1.031   Npar= 384

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.

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🟡 Alert level C

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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....    3.08 Report
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range     3.3 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     C26 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C3 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....     2.5 Note
PLAT332_ALERT_2_C Large Phenyl C-C Range     C8          -C31A    .    0.16 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600      26 Report
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⚪ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...      42 Report
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...       2 Units
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       1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records       1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn1       --O5        .    6.0 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )      11% Note
PLAT410_ALERT_2_G Short Intra H...H Contact  H10       ..H29A    .     2.14 Ang.
                                             x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H10       ..H29B    .     2.10 Ang.
                                             x,y,z  =      1_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure     266 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1        (II)     .     2.17 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............     339 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).       4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600    1058 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...      26 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      11 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by       1 Check
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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
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  20 ALERT level G = General information/check it is not something unexpected

   2 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
   4 ALERT type 3 Indicator that the structure quality may be low
   6 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* 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