checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CAN_3

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: CAN_3

Bond precision:　C-C = 0.0046 A　　　　Wavelength=0.71073

Cell:　　　　　a=9.3389(15)　　b=17.677(3)　　　c=14.735(3)
　　　　　　　alpha=90　　　　beta=93.189(5)　　gamma=90
Temperature:　173 K

	Calculated	Reported
Volume	2428.7(8)	2428.8(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H16 N2 O4 Zn, C3 H7 N O	?
Sum formula	C27 H23 N3 O5 Zn	C27 H23 N3 O5 Zn
Mr	534.87	534.85
Dx,g cm-3	1.463	1.463
Z	4	4
Mu (mm-1)	1.055	1.055
F000	1104.0	1104.0
F000'	1105.57	
h,k,lmax	12,23,19	12,22,19
Nref	5607	5584
Tmin,Tmax	0.963,0.969	0.909,0.969
Tmin'	0.909	

Correction method= # Reported T Limits: Tmin=0.909 Tmax=0.969
AbsCorr = MULTI-SCAN

Data completeness= 0.996　　　　　Theta(max)= 27.579

R(reflections)= 0.0468(3713)　　wR2(reflections)= 0.1107(5584)

S = 1.006　　　　　　　Npar= 327

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        3.5 Ratio
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      C6A Check
PLAT241_ALERT_2_C High    'MainMol' Ueq as Compared to Neighbors of      C7B Check
PLAT244_ALERT_4_C Low     'Solvent' Ueq as Compared to Neighbors of       N2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.3 Note
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⚪ Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         3 Info
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical         ? Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Zn01       --O1B_b   .      5.2 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        1 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.14 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Zn01      (II)      .      1.90 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       23 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        1 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
   9 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 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
   4 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 03/05/2019; check.def file version of 29/04/2019

Datablock CAN_3 - ellipsoid plot