checkCIF/PLATON report

Structure factors have been supplied for datablock(s) viz3

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: viz3

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Bond precision:   C-C = 0.0054 A          Wavelength=0.71073

Cell:             a=13.6044(8)     b=17.0033(9)         c=15.2324(8)
                  alpha=90         beta=104.203(2)      gamma=90
Temperature:      150 K
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	Calculated	Reported
Volume	3415.9(3)	3415.8(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C20 H13 I N2 O4 Zn [+ solvent]	C20 H13 I N2 O4 Zn, 3[C3H7NO]
Sum formula	C20 H13 I N2 O4 Zn [+ solvent]	C29 H34 I N5 O7 Zn
Mr	537.61	756.88
Dx,g cm-3	1.045	1.472
Z	4	4
Mu (mm-1)	1.639	1.671
F000	1048.0	1528.0
F000'	1047.63	
h,k,lmax	17,21,19	17,21,19
Nref	7580	7552
Tmin,Tmax	0.942,0.951	0.610,0.746
Tmin'	0.791	

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Correction method= # Reported T Limits: Tmin=0.610 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.996           Theta(max)= 27.160
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R(reflections)= 0.0387(4875)

wR2(reflections)= 0.0937(7552)

S = 0.948 Npar= 257

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 B

PLAT230_ALERT_2_B Hirshfeld Test Diff for O3 --C19 . 8.5 s.u.

Alert level C

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -1.456 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 9 Report
3 0 0, 0 4 0, -4 1 1, -3 1 1, 1 1 1, 2 4 1,
0 0 2, -1 2 2, 0 2 2,

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C29 H34 I1 N5 O7 Zn1
Atom count from the _atom_site data: C20 H13 I1 N2 O4 Zn1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C29 H34 I N5 O7 Zn
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	116.00	80.00	36.00
H	136.00	52.00	84.00
I	4.00	4.00	0.00
N	20.00	8.00	12.00
O	28.00	16.00	12.00
Zn	4.00	4.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
Calc: C20 H13 I N2 O4 Zn
Rep.: C29 H34 I N5 O7 Zn
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C20 H13 I N2 O4 Zn
Rep.: C20 H13 I N2 O4 Zn, 3[C3H7NO]
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 1.91 %
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Zn1 --O3_e . 6.8 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 4% Note
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ..... ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 1.92 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1 Note

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PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
                  1  0  0,   0  1  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         17 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
                  1  0  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          9 Note
                 -4  1  1,  -3  1  1,  -1  2  2,   0  0  2,   0  1  1,   0  2  2,
                  0  4  0,   1  1  1,   2  4  1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       1.73 Note
                Predicted wR2: Based on SigI**2  5.41 or SHELX Weight 10.06
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          2 Info
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
2 **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

5 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
7 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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 06/01/2024; check.def file version of 05/01/2024

Datablock viz3 - ellipsoid plot