

checkCIF/PLATON report

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

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: 3

Bond precision:	C-C = 0.0072 Å	Wavelength=0.71073
Cell:	a=14.9711(9)	b=22.2205(13) c=14.3508(14)
	alpha=90	beta=105.012(1) gamma=90
Temperature:	296 K	
	Calculated	Reported
Volume	4611.1(6)	4611.1(6)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C20 H13 N3 O5 Zn, C2 N	C20 H13 N3 O5 Zn, C2 N
Sum formula	C22 H13 N4 O5 Zn	C22 H13 N4 O5 Zn
Mr	478.75	478.73
Dx,g cm-3	1.379	1.379
Z	8	8
Mu (mm-1)	1.104	1.104
F000	1944.0	1944.0
F000'	1947.05	
h,k,lmax	18,27,17	18,27,17
Nref	4727	4714
Tmin,Tmax	0.767,0.802	0.635,0.746
Tmin'	0.759	

Correction method= # Reported T Limits: Tmin=0.635 Tmax=0.746
AbsCorr = NONE

Data completeness= 0.997 Theta(max)= 26.372

R(reflections)= 0.0534(3665) wR2(reflections)= 0.1721(4714)

S = 1.085 Npar= 318

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

PLAT601_ALERT_2_B Unit Cell Contains Solvent Accessible VOIDS of . 113 Ang**3

Author Response: The crystal has voids filled with severely disordered dimethylamine mo



Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 3.33 Report
PLAT221_ALERT_2_C Solv./Anion Resd 3 C Ueq(max)/Ueq(min) Range 5.3 Ratio
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N4 0.181 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N4A 0.162 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00721 Ang.



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 11.27 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Zn1 --N1 . 8.5 s.u.
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing). C21 Check
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing). C22 Check
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing). C21A Check
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing). C22A Check
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 1.95 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 42 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 13 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.1 Low

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
21 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
6 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.

