

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:      C-C = 0.0039 A      Wavelength=1.54178

Cell:                      a=13.9543 (16)      b=9.4508 (11)      c=13.968 (2)  
                                    alpha=90      beta=111.638 (2)      gamma=90

Temperature:      100 K

	Calculated	Reported
Volume	1712.3 (4)	1712.3 (4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C17 H19 N5 O4 Zn	?
Sum formula	C17 H19 N5 O4 Zn	C17 H19 N5 O4 Zn
Mr	422.76	422.74
Dx, g cm <sup>-3</sup>	1.640	1.640
Z	4	4
Mu (mm <sup>-1</sup> )	2.315	2.315
F000	872.0	872.0
F000'	868.22	
h, k, lmax	16, 11, 16	16, 11, 16
Nref	1569	1491
Tmin, Tmax	0.692, 0.740	0.564, 0.753
Tmin'	0.586	

Correction method= # Reported T Limits: Tmin=0.564 Tmax=0.753  
AbsCorr = MULTI-SCAN

Data completeness= 0.950      Theta (max)= 68.233

R(reflections)= 0.0419 ( 1489)

wR2(reflections)=  
0.1139 ( 1491)

S = 1.175

Npar= 126

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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.

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**Alert level B**

PLAT029\_ALERT\_3\_B \_diffn\_measured\_fraction\_theta\_full value Low . 0.952 Why?

**Author Response: The data completeness for the compound is lower than usual due to geometrical constraints of the instrument and the use of copper radiation. In general typical data completeness values ranges from 85-97% for monoclinic crystal system.**

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**Alert level C**

PLAT369\_ALERT\_2\_C Long C(sp2)-C(sp2) Bond C9 - C11 . 1.53 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.014 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 74 Report

0	2	0,	0	10	0,	2	6	0,	2	10	0,	8	4	0,	8	8	0,
-6	2	1,	-6	6	1,	-3	1	1,	-2	10	1,	-1	11	1,	1	9	1,
4	10	1,	12	6	1,	-14	0	2,	-12	0	2,	-9	3	2,	-3	7	2,
-2	0	2,	-2	10	2,	-1	1	2,	0	0	2,	0	4	2,	4	0	2,
6	0	2,	12	0	2,	-4	4	3,	5	9	3,	-10	0	4,	-4	4	4,
-2	10	4,	0	4	4,	2	0	4,	3	5	4,	4	0	4,	6	0	4,
8	0	4,	8	8	4,	-11	7	5,	-3	5	5,	-1	7	5,	2	10	5,
6	2	5,	-12	0	6,	-6	4	6,	-1	5	6,	1	5	6,	2	0	6,
4	8	6,	10	0	6,	-5	3	7,	-4	10	7,	-2	6	7,	-13	5	8,
-8	4	8,	0	0	8,	2	0	8,	4	0	8,	7	5	8,	8	4	8,
10	0	8,	6	6	9,	-12	0	10,	-4	8	10,	0	0	10,	6	0	10,
-14	2	12,	-13	1	12,	-8	0	12,	0	0	12,	-12	0	14,	-6	0	14,
-4	4	14,	0	0	14,												

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**Alert level G**

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 1 Report  
H2  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 5.09 Why ?  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Zn1 (II) . 1.94 Info  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT899\_ALERT\_4\_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 4 Note  
PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 2 Note  
-6 6 1, 0 4 2,  
PLAT961\_ALERT\_5\_G Dataset Contains no Negative Intensities ..... Please Check  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 4.943 Note  
Predicted wR2: Based on SigI\*\*2 2.30 or SHELX Weight 9.69  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 3 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

3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

10 **ALERT level G** = General information/check it is not something unexpected

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  - 4 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
  - 2 ALERT type 4 Improvement, methodology, query or suggestion
  - 4 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.

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**PLATON version of 15/07/2024; check.def file version of 15/07/2024**

