

# 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 = 0.0030 Å                      Wavelength=0.71073

Cell:                      a=15.2247(5)              b=15.5719(6)              c=37.7204(17)  
                                alpha=90                      beta=90                      gamma=90  
Temperature:              150 K

|                        | Calculated       | Reported         |
|------------------------|------------------|------------------|
| Volume                 | 8942.7(6)        | 8942.7(6)        |
| Space group            | I b c a          | I b c a          |
| Hall group             | -I 2b 2c         | -I 2b 2c         |
| Moiety formula         | C24 H20 N2 O6 Zn | C24 H20 N2 O6 Zn |
| Sum formula            | C24 H20 N2 O6 Zn | C24 H20 N2 O6 Zn |
| Mr                     | 497.81           | 497.79           |
| Dx, g cm <sup>-3</sup> | 1.479            | 1.479            |
| Z                      | 16               | 16               |
| Mu (mm <sup>-1</sup> ) | 1.142            | 1.142            |
| F000                   | 4096.0           | 4096.0           |
| F000'                  | 4102.31          |                  |
| h, k, lmax             | 21, 22, 53       | 21, 21, 52       |
| Nref                   | 6760             | 6220             |
| Tmin, Tmax             | 0.814, 0.843     | 0.770, 1.000     |
| Tmin'                  | 0.752            |                  |

Correction method= # Reported T Limits: Tmin=0.770 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.920                      Theta(max)= 30.396

R(reflections)= 0.0339( 4140)              wR2(reflections)= 0.0950( 6220)

S = 1.025                      Npar= 307

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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 C

|                   |                                                  |        |        |
|-------------------|--------------------------------------------------|--------|--------|
| PLAT905_ALERT_3_C | Negative K value in the Analysis of Variance ... | -1.409 | Report |
| PLAT910_ALERT_3_C | Missing # of FCF Reflection(s) Below Theta(Min). | 6      | Note   |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L= 0.600    | 4      | Report |
| PLAT934_ALERT_3_C | Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. | 1      | Check  |

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### ● Alert level G

|                   |                                                  |      |              |
|-------------------|--------------------------------------------------|------|--------------|
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large  | 6.47 | Why ?        |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Zn1 (II) .            | 1.90 | Info         |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Zn2 (II) .            | 1.86 | Info         |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600  | 517  | Note         |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity .....       | 4.0  | Low          |
| PLAT965_ALERT_2_G | The SHELXL WEIGHT Optimisation has not Converged |      | Please Check |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 10   | 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  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
5 ALERT type 3 Indicator that the structure quality may be low  
1 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 05/12/2020; check.def file version of 05/12/2020

Datablock shelx - ellipsoid plot

