

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: 1

Bond precision:	C-C = 0.0099 Å	Wavelength=0.71073	
Cell:	a=15.0279(13)	b=7.1943(6)	c=11.7348(9)
	alpha=90	beta=101.273(3)	gamma=90
Temperature:	273 K		
	Calculated	Reported	
Volume	1244.23(18)	1244.23(18)	
Space group	P 21/c	P21/c	
Hall group	-P 2ybc	?	
Moiety formula	C22 H32 N6 O6 Zn	?	
Sum formula	C22 H32 N6 O6 Zn	C22 H32 N6 O6 Zn	
Mr	541.93	541.91	
Dx, g cm-3	1.446	1.446	
Z	2	2	
Mu (mm-1)	1.036	1.036	
F000	568.0	568.0	
F000'	568.78		
h, k, lmax	17, 8, 14	17, 8, 14	
Nref	2215	2215	
Tmin, Tmax	0.830, 0.902		
Tmin'	0.813		

Correction method= Not given

Data completeness= 1.000 Theta(max)= 25.110

R(reflections)= 0.0689(1270) wR2(reflections)= 0.2371(2215)

S = 1.116 Npar= 158

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.131
PLAT031_ALERT_4_C Refined Extinction Parameter within Range 3.200 Sigma
PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT165_ALERT_3_C Nr. of Status R Flagged Non-Hydrogen Atoms 1 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00986 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H5B .. H8 .. 1.99 Ang.

● Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT020_ALERT_3_G The value of Rint is greater than 0.12 0.131 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 273 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 273 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 4 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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

4 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
5 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

