

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: ov_1124-yf-jm-ii06

Bond precision:	C-C = 0.0112 Å	Wavelength=0.71073
Cell:	a=9.607(5)	b=10.533(6) c=11.070(7)
	alpha=79.41(5)	beta=64.70(6) gamma=87.98(4)
Temperature:	296 K	
	Calculated	Reported
Volume	994.3(11)	994.3(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H15 Cl2 N3 O Zn	C21 H15 Cl2 N3 O Zn
Sum formula	C21 H15 Cl2 N3 O Zn	C21 H15 Cl2 N3 O Zn
Mr	461.65	461.63
Dx, g cm ⁻³	1.542	1.542
Z	2	2
Mu (mm ⁻¹)	1.520	1.520
F000	468.0	468.0
F000'	469.28	
h, k, lmax	11, 12, 13	11, 12, 13
Nref	3512	3451
Tmin, Tmax	0.723, 0.761	0.731, 0.771
Tmin'	0.709	

Correction method= # Reported T Limits: Tmin=0.731 Tmax=0.771
AbsCorr = ?

Data completeness= 0.983 Theta(max)= 25.020

R(reflections)= 0.0751(2072)	wR2(reflections)= 0.2492(3451)
S = 1.009	Npar= 253

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

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.

dull

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT193_ALERT_1_C	Cell and Diffraction Temperatures Differ by		3 Degree
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Zn1	--N .	5.3 s.u.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0112 Ang.



Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.13 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II) .	1.89 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 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.

