

## checkCIF (full publication check) running

## checkCIF/PLATON (full publication check)

Structure factors have been supplied for datablock(s) I

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.  
Please wait while processing ....

[CIF dictionary](#)  
[Interpreting this report](#)

[Structure factor report](#)

## Datablock: I

Bond precision:	C-C = 0.0050 Å	Wavelength=0.71073
Cell:	a=9.537(3)      b=6.865(2)      c=17.120(5)	
	alpha=90      beta=90      gamma=90	
Temperature: 150 K		
	Calculated	Reported
Volume	1120.9(6)	1120.8(6)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C6 H8 N8 O5 Zn	C6 H8 N8 O5 Zn
Sum formula	C6 H8 N8 O5 Zn	C6 H8 N8 O5 Zn
Mr	337.59	337.57
Dx, g cm <sup>-3</sup>	2.000	2.000
Z	4	4
Mu (mm <sup>-1</sup> )	2.232	2.232
F000	680.0	680.0
F000'	681.38	
h,k,lmax	11,8,21	11,8,21
Nref	1148	1146
Tmin,Tmax	0.898,0.956	0.230,0.290
Tmin'	0.800	
Correction method=	# Reported T Limits: Tmin=0.230 Tmax=0.290	
AbsCorr =	MULTI-SCAN	
Data completeness=	0.998      Theta(max)= 26.367	
R(reflections)=	0.0393( 870)      wR2(reflections)= 0.0944( 1146)	
S =	1.190      Npar= 105	

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

PLAT906\_ALERT\_3\_C Large K value in the Analysis of Variance ..... 2.467 Check

### Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	7 Note
PLAT112_ALERT_2_G ADDSYM Detects Additional (Pseudo) Symm. Elem...	C Check
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	4 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....	4 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...	2 Report

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

1 **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

0 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
- 3 ALERT type 3 Indicator that the structure quality may be low
- 1 ALERT type 4 Improvement, methodology, query or suggestion
- 0 ALERT type 5 Informative message, check

# checkCIF publication errors

## Alert level A

- PUBL004\_ALERT\_1\_A The contact author's name and address are missing, \_publ\_contact\_author\_name and \_publ\_contact\_author\_address.
- PUBL005\_ALERT\_1\_A \_publ\_contact\_author\_email, \_publ\_contact\_author\_fax and \_publ\_contact\_author\_phone are all missing. At least one of these should be present.
- PUBL006\_ALERT\_1\_A \_publ\_requested\_journal is missing e.g. 'Acta Crystallographica Section C'
- PUBL008\_ALERT\_1\_A \_publ\_section\_title is missing. Title of paper.
- PUBL009\_ALERT\_1\_A \_publ\_author\_name is missing. List of author(s) name(s).
- PUBL010\_ALERT\_1\_A \_publ\_author\_address is missing. Author(s) address(es).
- PUBL012\_ALERT\_1\_A \_publ\_section\_abstract is missing. Abstract of paper in English.

## Alert level G

- PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or empty.

- 7 **ALERT level A** = Data missing that is essential or data in wrong format
- 1 **ALERT level G** = General alerts. Data that may be required is missing

## Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

## Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
```

RESPONSE: ...

;

\_vrf\_PUBL010\_GLOBAL

;

PROBLEM: \_publ\_author\_address is missing. Author(s) address(es).

RESPONSE: ...

;

\_vrf\_PUBL012\_GLOBAL

;

PROBLEM: \_publ\_section\_abstract is missing.

RESPONSE: ...

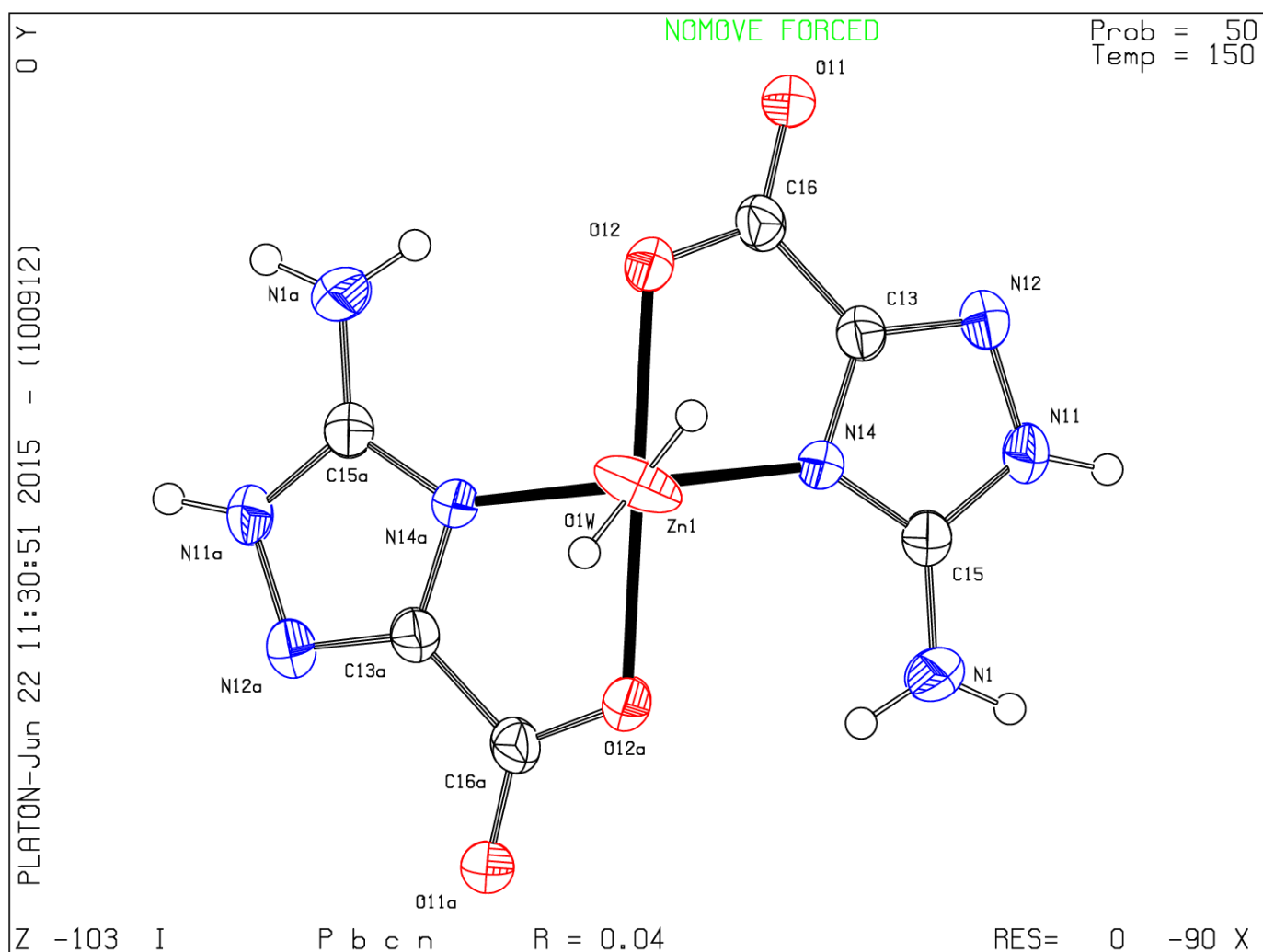
;

# end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via [the web](#). If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic [submission](#) or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 21/06/2015; check.def file version of 21/06/2015

## Datablock I - ellipsoid plot



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