

checkCIF/PLATON report

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. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0039 Å Wavelength=0.71073

Cell: a=11.065(2) b=17.610(3) c=11.531(6)
 alpha=90 beta=107.31(3) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	2145.1(13)	2145.1(13)
Space group	I 2/a	I 2/a
Hall group	-I 2ya	-I 2ya
Moiety formula	C22 H15 Cl2 N3 O2 Zn, 2(H2 O)	C22 H19 Cl2 N3 O4 Zn
Sum formula	C22 H19 Cl2 N3 O4 Zn	C22 H19 Cl2 N3 O4 Zn
Mr	525.69	525.69
Dx, g cm ⁻³	1.628	1.628
Z	4	4
Mu (mm ⁻¹)	1.430	1.430
F000	1072.0	1072.0
F000'	1074.68	
h,k,lmax	15,24,16	14,22,15
Nref	3019	2558
Tmin,Tmax	0.501,0.651	0.604,1.000
Tmin'	0.491	

Correction method= # Reported T Limits: Tmin=0.604 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.847 Theta(max)= 29.586

R(reflections)= 0.0430(2265) wR2(reflections)= 0.1355(2558)

S = 1.046 Npar= 148

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

PLAT976_ALERT_2_C	Check Calcd Residual Density	0.71A From	O2	-0.91 eA-3
PLAT976_ALERT_2_C	Check Calcd Residual Density	0.55A From	O2	-0.84 eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on		H2E	-0.69 eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on		H2F	-0.47 eA-3



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		3	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ			Please Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1E is Constrained at		0.5	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	H2 O			
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL		2014	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min)		3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		416	Note
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ		2	Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ		2	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		3	Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
4 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

checkCIF publication errors



Alert level A

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.

4 **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_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 you wish to submit your CIF for publication in IUCrData 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.

Datablock I - ellipsoid plot

