

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 = 0.0119 Å Wavelength=0.71073

Cell: a=8.660(6) b=11.612(7) c=24.620(9)
 alpha=90 beta=98.478(9) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	2449(2)	2449(2)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C15 H17 Cl2 N5 O S2 Zn, 2(C H4 O)	(C15 H17 Cl2 N5 O1 S2 Zn), 2(Ch3Oh)
Sum formula	C17 H25 Cl2 N5 O3 S2 Zn	C17 H25 Cl2 N5 O3 S2 Zn
Mr	547.83	547.81
Dx, g cm ⁻³	1.486	1.486
Z	4	4
Mu (mm ⁻¹)	1.419	1.419
F000	1128.0	1128.0
F000'	1131.59	
h,k,lmax	10,13,28	10,13,28
Nref	4182	4099
Tmin,Tmax	0.855,0.893	0.536,0.745
Tmin'	0.855	

Correction method= # Reported T Limits: Tmin=0.536 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.980 Theta(max)= 24.745

R(reflections)= 0.0772(2399) wR2(reflections)= 0.2615(4099)

S = 1.002 Npar= 274

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 B

PLAT415_ALERT_2_B Short Inter D-H..H-X H2S .. H11B .. 2.09 Ang.

Alert level C

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25

Weighted R factor given 0.262

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590

Calculated sin(theta_max)/wavelength = 0.5889

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.26 Report

PLAT234_ALERT_4_C Large Hirshfeld Difference S2 -- C15 .. 0.17 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference N5 -- C15 .. 0.18 Ang.

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C14 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C15 Check

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0119 Ang.

PLAT906_ALERT_3_C Large K value in the Analysis of Variance 8.769 Check

PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.041 Check

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.589 85 Report

PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1 Check

PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density 0 Note

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report

PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.16 Report

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6 Note

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

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

13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

1 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

8 ALERT type 3 Indicator that the structure quality may be low

3 ALERT type 4 Improvement, methodology, query or suggestion

1 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 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.

PLATON version of 11/08/2016; check.def file version of 04/08/2016

