

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 = 0.0034 Å

Wavelength=0.71073

Cell: a=10.3442(12) b=12.2318(13) c=13.2856(14)
 alpha=97.470(5) beta=95.354(6) gamma=97.459(5)
Temperature: 298 K

	Calculated	Reported
Volume	1642.2(3)	1642.2(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C28 H21 Cl2 N3 Zn, 2(C2 H6 O S)	C32 H33 Cl2 N3 O2 S2 Zn
Sum formula	C32 H33 Cl2 N3 O2 S2 Zn	C32 H33 Cl2 N3 O2 S2 Zn
Mr	692.02	692.02
Dx, g cm ⁻³	1.400	1.399
Z	2	2
Mu (mm ⁻¹)	1.071	1.071
F000	716.0	716.0
F000'	717.84	
h,k,lmax	13,16,17	13,16,17
Nref	7861	7674
Tmin,Tmax	0.705,0.765	0.616,0.746
Tmin'	0.625	

Correction method= # Reported T Limits: Tmin=0.616 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 0.976

Theta(max)= 27.916

R(reflections)= 0.0406(6458)

wR2(reflections)= 0.1220(7674)

S = 1.027

Npar= 389

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ...	2.28	Report
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	01	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C30	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C31	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	S2	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	46	Report



Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)..	25	% Note
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C28	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	C2 H6 O S		
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	139	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	6	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
8 **ALERT level G** = General information/check it is not something unexpected

1 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
2 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
0 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

