

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C51H47N9O14Zn

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: C51H47N9O14Zn

Bond precision: C-C = 0.0064 Å Wavelength=0.71073

Cell: a=14.6426 (7) b=20.0946 (13) c=32.345 (2)
 alpha=90 beta=90 gamma=90

Temperature: 223 K

	Calculated	Reported
Volume	9517.1 (10)	9517.0 (10)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C36 H24 N6 Zn, C15 H13 N3 O9, 5 (H2 O)	C36 H24 N6 Zn, C15 H13 N3 O9, 5 (H2 O)
Sum formula	C51 H47 N9 O14 Zn	C51 H47 N9 O14 Zn
Mr	1075.37	1075.34
Dx, g cm ⁻³	1.501	1.501
Z	8	8
Mu (mm ⁻¹)	0.597	0.597
F000	4464.0	4464.0
F000'	4468.35	
h, k, lmax	17, 23, 38	17, 23, 38
Nref	8478	8439
Tmin, Tmax	0.812, 0.903	0.804, 0.916
Tmin'	0.764	

Correction method= # Reported T Limits: Tmin=0.804 Tmax=0.916
AbsCorr = NUMERICAL

Data completeness= 0.995 Theta (max)= 25.100

R(reflections)= 0.0536 (4396)

wR2(reflections)=
0.1162 (8439)

S = 0.908

Npar= 709

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 A

PLAT355_ALERT_3_A Long O-H (X0.82,N0.98A) O9 - H9 . 1.21 Ang.

Author Response: The carboxylate group participates in a very strong hydrogen bond which is discussed in detail in the paper.



Alert level C

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C12 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0064 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 10.662 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.508 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.597 38 Report



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 3 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT480_ALERT_4_G Long H...A H-Bond Reported H29 ..O6 . 2.64 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H40 ..N4 . 2.67 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Zn (II) . 1.79 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 4 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.3 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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- 1 **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
10 **ALERT level G** = General information/check it is not something unexpected

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
2 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: ...
;
_vrf_PLAT355_C51H47N9O14Zn
;
PROBLEM: Long O-H (X0.82,N0.98A) O9 - H9 . 1.21 Ang.
RESPONSE:
    The carboxylate group participates in a very strong hydrogen
    bond which is discussed in detail in the paper.
;
# 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.

