

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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

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Bond precision:	C-C = 0.0158 A	Wavelength=0.71073
Cell:	a=14.0120(11)	b=14.150(1)      c=15.147(1)
	alpha=101.189(1)	beta=103.022(1)      gamma=93.211(1)
Temperature:	298 K	
	Calculated	Reported
Volume	2854.7(4)	2854.7(4)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C58 H48 F4 N4 O10 Zn4	?
Sum formula	C58 H48 F4 N4 O10 Zn4	C58 H48 F4 N4 O10 Zn4
Mr	1298.57	1298.48
Dx,g cm-3	1.511	1.511
Z	2	2
Mu (mm-1)	1.734	1.734
F000	1320.0	1320.0
F000'	1322.83	
h,k,lmax	16,16,17	16,16,17
Nref	9350	9251
Tmin,Tmax	0.765,0.771	0.769,0.781
Tmin'	0.750	

Correction method= # Reported T Limits: Tmin=0.769 Tmax=0.781  
AbsCorr = MULTI-SCAN

Data completeness= 0.989	Theta(max)= 24.350
R(reflections)= 0.0640( 5361)	wR2(reflections)= 0.2252( 9251)
S = 1.013	Npar= 722

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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.



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### Alert level B

PLAT341\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.01575 Ang.  
PLAT420\_ALERT\_2\_B D-H Without Acceptor O9 --H9B . Please Check

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### Alert level C

THETM01\_ALERT\_3\_C The value of sine(theta\_max)/wavelength is less than 0.590  
Calculated sin(theta\_max)/wavelength = 0.5801  
PLAT023\_ALERT\_3\_C Resolution (too) Low [sin(theta)/Lambda < 0.6].. 0.58 Ang-1  
PLAT048\_ALERT\_1\_C MoietyFormula Not Given (or Incomplete) ..... Please Check  
PLAT094\_ALERT\_2\_C Ratio of Maximum / Minimum Residual Density .... 3.28 Report  
PLAT125\_ALERT\_4\_C No 'symmetry\_space\_group\_name\_Hall' Given ..... Please Do !  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C3 --C4 . 0.18 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C16 --C17 . 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C26 --C27 . 0.19 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C30 --C31 . 0.19 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C38 --C39 . 0.19 Ang.  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C38 Check  
PLAT360\_ALERT\_2\_C Short C(sp3)-C(sp3) Bond C57 - C58 . 1.41 Ang.  
PLAT601\_ALERT\_2\_C Unit Cell Contains Solvent Accessible VOIDS of . 99 Ang\*\*3

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### Alert level G

PLAT005\_ALERT\_5\_G No Embedded Refinement Details Found in the CIF Please Do !  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 3 Report  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report  
PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Zn1 (II) . 2.03 Info  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Zn2 (II) . 2.06 Info  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Zn3 (II) . 2.08 Info  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Zn4 (II) . 2.05 Info  
PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL/ 2018 Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
2 **ALERT level B** = A potentially serious problem, consider carefully  
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
9 **ALERT level G** = General information/check it is not something unexpected

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 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  
7 ALERT type 4 Improvement, methodology, query or suggestion  
6 ALERT type 5 Informative message, check
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## checkCIF publication errors

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### 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.

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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

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### 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.

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**PLATON version of 05/12/2020; check.def file version of 05/12/2020**



