

# checkCIF/PLATON report

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

No syntax errors found.    CIF dictionary    Interpreting this report

## Datablock: I

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Bond precision:    C-C = 0.0050 A                      Wavelength=1.54056

Cell:              a=4.01653(10)            b=13.9440(2)            c=12.3686(2)  
                    alpha=90                      beta=90.526(1)            gamma=90

Temperature:      298 K

	Calculated	Reported
Volume	692.69(2)	692.69(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C10 H8 Br4 Cu N2	C10 H8 Br4 Cu N2
Sum formula	C10 H8 Br4 Cu N2	C10 H8 Br4 Cu N2
Mr	539.33	539.33
Dx,g cm-3	2.586	2.586
Z	2	2
Mu (mm-1)	15.568	15.568
F000	502.0	502.0
F000'	493.16	
h,k,lmax		
Nref		
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness=                      Theta(max)=


R(reflections)=                      wR2(reflections)=

S =                      Npar=


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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 C**  
PLAT241\_ALERT\_2\_C Check High                      Ueq as Compared to Neighbors for                      Cu1

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 **Alert level G**

PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	4
PLAT794_ALERT_5_G	Note: Tentative Bond Valency for Cu1 (I)	1.31
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	!
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....	47
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value	C
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value	Br
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value	Cu
PLAT982_ALERT_1_G	The reported f' Value Deviates from the IT-value	N
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value	C
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value	Br
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value	Cu
PLAT983_ALERT_1_G	The Reported f" Value Deviates from the IT-value	N

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

8 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
1 **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  
1 **ALERT type 4** Improvement, methodology, query or suggestion  
2 **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.

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### Alert level G

PUBL013\_ALERT\_1\_G The `_publ_section_comment` (discussion of study) is missing. This is required for a full paper submission (but is optional for an electronic paper).  
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  
2 **ALERT level G** = General alerts. Data that may be required is missing

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## Publication of your CIF

**You should always 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 the submission requirements of the journal and these should be commented upon in the discussion or experimental section of a paper - after all, they might represent an interesting feature.**

**If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.**

**If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.**

```
# 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 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 16/02/2011; check.def file version of 16/02/2011

Datablock I - ellipsoid plot

