

# 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 = 0.0068 A                      Wavelength=0.71073

Cell:                a=7.9533(6)                b=10.3661(8)                c=11.6080(9)  
                      alpha=110.728(7)        beta=96.109(6)        gamma=102.015(6)

Temperature:    298 K

	Calculated	Reported
Volume	858.33(13)	858.33(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C14 H15 Br N3 O5 V	C14 H15 Br N3 O5 V
Sum formula	C14 H15 Br N3 O5 V	C14 H15 Br N3 O5 V
Mr	436.13	436.14
Dx,g cm-3	1.688	1.688
Z	2	2
Mu (mm-1)	2.934	2.934
F000	436.0	436.0
F000'	436.21	
h,k,lmax	9,12,14	9,12,14
Nref	3189	3185
Tmin,Tmax	0.457,0.509	0.438,1.000
Tmin'	0.448	

Correction method= # Reported T Limits: Tmin=0.438 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.999                      Theta(max)= 25.499

R(reflections)= 0.0489( 2304)                wR2(reflections)= 0.1191( 3185)

S = 1.025                                      Npar= 222

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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

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C10	Check
PLAT341_ALERT_3_C	Low	Bond Precision on C-C Bonds .....	0.00675	Ang.
PLAT431_ALERT_2_C	Short	Inter HL..A Contact Br1 ..04 .	3.25	Ang.
		x,l+y,l+z =	1_566	Check

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### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C13	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for V1 (V) .	5.15	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	1	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.0	Low

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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  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
7 **ALERT level G** = General information/check it is not something unexpected

1 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  
3 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
1 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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7 **ALERT level A** = Data missing that is essential or data in wrong format  
0 **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 22/04/2020; check.def file version of 09/03/2020**

Datablock I - ellipsoid plot

