

# 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 = 0.0141 A	Wavelength=0.71073
Cell:	a=13.4057(11)      b=27.443(2)      c=18.1422(18)	
	alpha=90      beta=101.147(8)      gamma=90	
Temperature:	298 K	
	Calculated	Reported
Volume	6548.5(10)	6548.5(10)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C30 H23 Br2 Co N4 O4, C30 H25 Br2 Co N4 O4, 2(N O3), H2 O	C30 H23 Br2 Co N4 O4, C30 H25 Br2 Co N4 O4, 2(N O3), H2 O
Sum formula	C60 H50 Br4 Co2 N10 O15	C60 H50 Br4 Co2 N10 O15
Mr	1588.56	1588.60
Dx, g cm-3	1.611	1.611
Z	4	4
Mu (mm-1)	3.019	3.019
F000	3176.0	3176.0
F000'	3175.54	
h,k,lmax	16,33,21	16,33,21
Nref	12181	11962
Tmin,Tmax	0.420,0.456	0.465,0.507
Tmin'	0.389	

Correction method= # Reported T Limits: Tmin=0.465 Tmax=0.507  
AbsCorr = MULTI-SCAN

Data completeness= 0.982      Theta(max)= 25.500

R(reflections)= 0.0793( 4969)      wR2(reflections)= 0.2315( 11962)

S = 0.978      Npar= 831

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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.

### Alert level B

PLAT420\_ALERT\_2\_B D-H Without Acceptor O15 -- H15A ... Please Check

### Alert level C

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12

Rint given 0.124

PLAT020_ALERT_3_C	The value of Rint is greater than 0.12 .....	0.124	Report
PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	42	%
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C1 -- C6 ..	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C11 -- C12 ..	0.21	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C14 -- C15 ..	0.23	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C16 -- C21 ..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference Br3 -- C41 ..	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C31 -- C32 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C41 -- C42 ..	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C42 -- C43 ..	0.25	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C14	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C29	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C43	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C10	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C15	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C41	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	N10	Check
PLAT334_ALERT_2_C	Small Average Benzene C-C Dist. C55 -C60	1.37	Ang.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.01413	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C9 - C10 ..	1.53	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H2A .. N9 ..	2.66	Ang.

### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	12	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	9	Report
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please	Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	8	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....	2	Note
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety ....	C7	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact Br2 .. C15 ..	3.30	Ang.
PLAT726_ALERT_2_G	H...A Calc 1.93000, Rep 1.94000 Dev...	0.01	Ang.
	H2A -O10 1.555 1.555 .....	Bond #	154 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	59	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

23 **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

14 ALERT type 2 Indicator that the structure model may be wrong or deficient

6 ALERT type 3 Indicator that the structure quality may be low

12 ALERT type 4 Improvement, methodology, query or suggestion

2 ALERT type 5 Informative message, check

# 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

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 06/05/2016; check.def file version of 05/05/2016**

