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

```
Bond precision:  C-C = 0.0138 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                   ?
                C30 H23 Br2 Co N4 O4, C30
Moiety formula  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)= 0.0770( 4969)     wR2(reflections)= 0.2206( 11962)

S = 0.973                 Npar= 831
```

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

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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 %
PLAT048_ALERT_1_C MoietyFormula Not Given (or Incomplete) ..... Please Check
PLAT125_ALERT_4_C No '_symmetry_space_group_name_Hall' Given ..... Please Do !
PLAT214_ALERT_2_C Atom N9 (Anion/Solvent) ADP max/min Ratio 4.4 prolat
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 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Br3 -- C41 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C41 -- C42 .. 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C42 -- C43 .. 0.24 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
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of N9 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 ..... 0.01382 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C9 - C10 .. 1.54 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H2A .. N9 .. 2.69 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H4A .. O14 .. 2.61 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H4A .. N10 .. 2.64 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 ... 5 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
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 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 .. 3.29 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 35 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
28 **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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  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
  15 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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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.
```

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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
```

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.

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

Datablock I - ellipsoid plot