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: compound_1

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Bond precision:  C-C = 0.0243 A          Wavelength=0.71073

Cell:              a=18.977(4)      b=14.282(3)      c=19.809(5)
                   alpha=90         beta=90          gamma=90
Temperature:       120 K
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	Calculated	Reported
Volume	5369(2)	5369(2)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C18 H14 Br4 Cu N6 O4 Re, C2 H3 N	C18 H14 Br4 Cu N6 O4 Re, C2 H3 N
Sum formula	C20 H17 Br4 Cu N7 O4 Re	C20 H17 Br4 Cu N7 O4 Re
Mr	988.77	988.79
Dx,g cm-3	2.447	2.447
Z	8	8
Mu (mm-1)	11.293	11.293
F000	3696.0	3696.0
F000’	3684.11	
h,k,lmax	24,18,25	24,18,25
Nref	6261	6228
Tmin,Tmax	0.100,0.184	0.165,0.498
Tmin’	0.008	

```
Correction method= # Reported T Limits: Tmin=0.165 Tmax=0.498
AbsCorr = MULTI-SCAN

Data completeness= 0.995          Theta(max)= 27.658

R(reflections)= 0.0831( 6003)     wR2(reflections)= 0.1966( 6228)

S = 1.415                 Npar= 334
```

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

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02429 Ang.
PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set Please Do !

Alert level C

PLAT213_ALERT_2_C Atom N1 has ADP max/min Ratio ..... 3.1 oblate
PLAT213_ALERT_2_C Atom C13 has ADP max/min Ratio ..... 3.7 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N2 --C10 . 0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C10 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C6 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C19 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N7 0.087 Check
PLAT368_ALERT_2_C Short C(sp2)-C(sp2) Bond C4 - C5 . 1.21 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N3 --H3A . Please Check

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 372.83 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT344_ALERT_2_G Unusual sp? Angle Range in Solvent/Ion for C19 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 25 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
12 **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
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/12/2018; check.def file version of 11/12/2018

Datablock compound_1 - ellipsoid plot