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: RUKGIO

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Bond precision:   C-C = 0.0032 A          Wavelength=0.71073

Cell:             a=9.3207(12)     b=16.841(2)          c=10.0908(13)
                  alpha=90         beta=116.678(1)      gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           1415.3(3)                 1415
Space group      P 21/n                    P 21/n
Hall group       -P 2yn                    ?
Moiety formula   C14 H15 Br N2 O4          C14 H15 Br1 N2 O4
Sum formula      C14 H15 Br N2 O4          C14 H15 Br1 N2 O4
Mr               355.18                    0.00
Dx,g cm-3        1.667                     1.667
Z                4                         4
Mu (mm-1)        2.922                     0.000
F000             720.0                     0.0
F000'            719.19
h,k,lmax
Nref
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness=                  Theta(max)=

                                                    wR2(reflections)=
R(reflections)= 0.0318( 0)                          wR= 0.0318( 0)
S = ******                 Npar= *****
```

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 A

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.
ATOM007_ALERT_1_A _atom_site_aniso_label is missing
Unique label identifying the atom site.
GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
Label identifying the atom site 1.
GEOM002_ALERT_1_A _geom_bond_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM003_ALERT_1_A _geom_bond_distance is missing
Distance between atom sites 1 and 2.
GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

PLAT029_ALERT_3_A	_diffrn_measured_fraction_theta_full value Low .	0.000 Why?
PLAT043_ALERT_1_A	Calculated and Reported Mol. Weight Differ by ..	355.18 Check
PLAT046_ALERT_1_A	Reported Z, MW and D(calc) are Inconsistent	0.000 Check
PLAT183_ALERT_1_A	Missing _cell_measurement_reflns_used Value	Please Do !
PLAT184_ALERT_1_A	Missing _cell_measurement_theta_min Value	Please Do !
PLAT185_ALERT_1_A	Missing _cell_measurement_theta_max Value	Please Do !
PLAT197_ALERT_1_A	Missing _cell_measurement_temperature Datum	Please Add
PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	21 Report
	Br1 O1 O2 O3 O4	etc.
PLAT880_ALERT_1_A	No datum for _diffrn_reflns_number supplied	Please Do !
PLAT881_ALERT_1_A	No Datum for _diffrn_reflns_av_R_equivalents ...	Please Do !

Alert level C

PLAT151_ALERT_1_C	No s.u. (esd) Given on Volume	Please Do !

Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	3 Report
PLAT793_ALERT_4_G	Model has Chirality at C2 (Centro SPGR)	S Verify
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT882_ALERT_1_G	No Datum for _diffrn_reflns_av_unetI/netI	Please Do !
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT981_ALERT_1_G	No non-zero f" Anomalous Scattering Values Found	Please Check
PLAT986_ALERT_1_G	No non-zero f' Anomalous Scattering Values Found	Please Check

17 **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
8 **ALERT level G** = General information/check it is not something unexpected

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

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  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
  3 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 20/01/2022; check.def file version of 19/01/2022

Datablock RUKGIO - ellipsoid plot