# 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: 1r

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Bond precision:  C-C = 0.0175 A          Wavelength=0.71073

Cell:           a=24.3244(9)    b=12.2780(5)        c=17.7756(6)
                alpha=90        beta=112.772(2)     gamma=90
Temperature:    100 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 4895.0(3) | 4895.0(3) |
| Space group | C 2/c | C 1 2/c 1 |
| Hall group | -C 2yc | -C 2yc |
| Moiety formula | 4(C22 H17 Cu I N3 O), C4 Br, 4(C H2 Br) | C22 H17 Cu I N3 O, C2 H2 Br1.25 |
| Sum formula | C96 H76 Br5 Cu4 I4 N12 O4 | C24 H19 Br1.25 Cu I N3 O |
| Mr | 2622.99 | 655.75 |
| Dx,g cm-3 | 1.780 | 1.780 |
| Z | 2 | 8 |
| Mu (mm-1) | 4.215 | 4.215 |
| F000 | 2542.0 | 2542.0 |
| F000’ | 2538.75 | |
| h,k,lmax | 29,14,21 | 29,14,21 |
| Nref | 4543 | 4524 |
| Tmin,Tmax | 0.294,0.430 | 0.415,0.745 |
| Tmin’ | 0.220 | |

```
Correction method= # Reported T Limits: Tmin=0.415 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 25.448

R(reflections)= 0.1034( 3197)     wR2(reflections)= 0.2998( 4524)

S = 1.035                 Npar= 276
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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 B

PLAT366_ALERT_2_B Short? C(sp?)-C(sp?) Bond C1AA - C1AA_e . 0.71 Ang.

**Author Response: The dibromoethen molecule were present around a symmetry element due to symmerty it is growing to the other side and this alert is due to growing in the structure followed by symmetry.**

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## Alert level C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.30 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 2 Check
C1AA C0AA
PLAT213_ALERT_2_C Atom C22 has ADP max/min Ratio ..... 3.2 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Br2 0.117 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Br1 0.296 Check
PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for ..... C0AA Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01745 Ang.

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## Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.25 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 281.27 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I001 --Cu02 . 13.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I001 --Cu02_a . 8.2 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Br2 Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 33% Note
PLAT344_ALERT_2_G Unusual sp? Angle Range in Solvent/Ion for C0AA Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C0AA ..C1AA 1.98 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C0AA ..C1AA 2.62 Ang.
-x,y,1/2-z = 2_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 10 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C0AA --C1AA 1.98 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 89 Check
C1AA -BR2 -C1AA 2.000 1.555 1.555 18.90 Deg.
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 7 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
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
18 **ALERT level G** = General information/check it is not something unexpected

3 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
  3 ALERT type 3 Indicator that the structure quality may be low
  6 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check
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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.

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**PLATON version of 03/05/2019; check.def file version of 29/04/2019**

**Datablock 1r** - ellipsoid plot