# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

# Datablock: kla0343

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Bond precision: C-C = 0.0052 A Wavelength=0.71073

Cell: a=13.1310(15) b=19.404(2) c=19.771(2)
alpha=97.840(2) beta=107.809(2) gamma=97.599(2)
Temperature: 200 K

| | Calculated | Reported |
|---|---|---|
| Volume | 4669.8(9) | 4669.6(9) |
| Space group | P -1 | P-1 |
| Hall group | -P 1 | ? |
| Moiety formula | C34 H31 B Cu N9 O4, 3(C4 H8 O) | ? |
| Sum formula | C46 H55 B Cu N9 O7 | C46 H55 B Cu N9 O7 |
| Mr | 920.35 | 920.34 |
| Dx,g cm-3 | 1.309 | 1.309 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.527 | 0.527 |
| F000 | 1936.0 | 1936.0 |
| F000’ | 1937.99 | |
| h,k,lmax | 17,25,25 | 17,25,25 |
| Nref | 21680 | 21442 |
| Tmin,Tmax | 0.858,0.919 | 0.863,0.919 |
| Tmin’ | 0.858 | |

Correction method= MULTI-SCAN

Data completeness= 0.989 Theta(max)= 27.600

R(reflections)= 0.0535( 12780) wR2(reflections)= 0.1442( 21442)

S = 1.022 Npar= 1177

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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**
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for O8

**Author Response: Atom O8 is the oxygen atom of a carbonyl ligand on one of two symmetry unique compound molecules. Atom identity is consistent with synthetic methods and spectroscopic characterization.**

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**Alert level C**

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PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for         O4
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**Author Response: Atom O8 is the oxygen atom of a carbonyl ligand on one of two symmetry unique compound molecules. Atom identity is consistent with synthetic methods and spectroscopic characterization.**

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PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C30
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**Author Response: Atom O8 is the oxygen atom of a carbonyl ligand on one of two symmetry unique compound molecules. Atom identity is consistent with synthetic methods and spectroscopic characterization.**

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PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of         C69
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of         C72
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of         C76
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of         C78
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of         C82
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors of         C91
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of          O9
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         C71
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         O10
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         O11
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of         O12
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C82    -   C83    ...       1.43 Ang.
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**Alert level G**

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         12
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites ....         10
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .........    0.00200 Deg.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu1    --  C34     ..        6.3 su
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        169
            N4  -CU1 -C34 -O4    146.00  8.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        170
            N7  -CU1 -C34 -O4    -93.00  8.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        171
            N1  -CU1 -C34 -O4     23.00  8.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        256
            N13 -CU2 -C68 -O8     18.00  0.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        257
            N10 -CU2 -C68 -O8     55.00 16.00   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        258
            N16 -CU2 -C68 -O8    -65.00 16.00   1.555   1.555   1.555   1.555
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          7
              C4 H8 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8
              C4 H8 O
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         95
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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
 14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 14 ALERT level G = General information/check it is not something unexpected

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  7 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
 19 ALERT type 4 Improvement, methodology, query or suggestion
  1 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*, 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 05/11/2012; check.def file version of 05/11/2012**

**Datablock kla0343 -** ellipsoid plot