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: shelxl

```
Bond precision:  C-C = 0.0123 A          Wavelength=0.71073

Cell:            a=14.207(2)    b=13.9892(14)         c=16.133(3)
                 alpha=90       beta=113.877(12)      gamma=90
Temperature:     150 K
```

	Calculated	Reported
Volume	2931.9(8)	2932.1(7)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	C26 H34 Br4 Cl2 Cu N4	?
Sum formula	C26 H34 Br4 Cl2 Cu N4	C26 H34 Br4 Cl2 Cu N4
Mr	856.62	856.65
Dx,g cm-3	1.941	1.941
Z	4	4
Mu (mm-1)	6.403	6.420
F000	1684.0	1684.0
F000’	1682.56	
h,k,lmax	19,19,22	19,19,22
Nref	8543	8517
Tmin,Tmax	0.327,0.598	0.489,0.833
Tmin’	0.266	

```
Correction method= INTEGRATION

Data completeness= 0.997          Theta(max)= 30.000

R(reflections)= 0.0594( 3449)     wR2(reflections)= 0.1405( 8517)

S = 0.854                 Npar= 335
```

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 C

```
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....         40 Perc.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C3     --  C4      ..        6.6 su
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0123 Ang
PLAT410_ALERT_2_C Short Intra H...H Contact  H1A    ..  H11B    ..       1.91 Ang.
```

PLAT410_ALERT_2_C Short Intra H...H Contact H6A   .. H12A   ..   1.98 Ang.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....   ?
PLAT793_ALERT_4_G The Model has Chirality at N1   (Verify) ....   R
PLAT793_ALERT_4_G The Model has Chirality at N2   (Verify) ....   R
PLAT793_ALERT_4_G The Model has Chirality at N3   (Verify) ....   R
PLAT793_ALERT_4_G The Model has Chirality at N4   (Verify) ....   R
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Cu1   (II)   1.96

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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

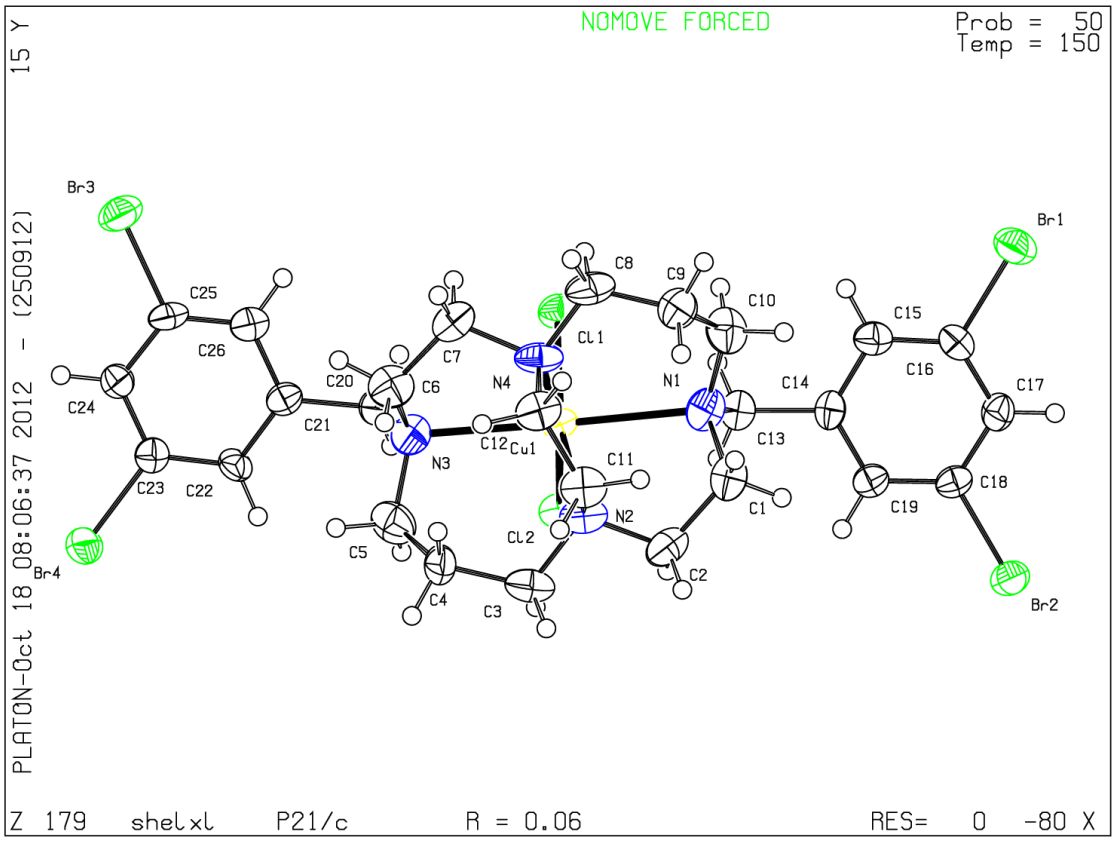
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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 25/09/2012; check.def file version of 20/09/2012

Datablock shelxl - ellipsoid plot



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

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Datablock: shelxl

```
Bond precision:  C-C = 0.0062 A          Wavelength=0.71073

Cell:         a=8.7231(15)       b=14.248(3)       c=14.316(2)
              alpha=117.139(12)  beta=100.121(13)  gamma=95.291(14)
Temperature:  150 K
```

	Calculated	Reported
Volume	1528.3(5)	1528.3(5)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C28 H42 Cu N5 O3, N O3, C H O	?
Sum formula	C29 H43 Cu N6 O7	C29 H43 Cu N6 O7
Mr	651.24	651.23
Dx,g cm-3	1.415	1.415
Z	2	2
Mu (mm-1)	0.770	0.770
F000	688.0	688.0
F000’	688.91	
h,k,lmax	12,20,20	12,20,20
Nref	8906	8901
Tmin,Tmax	0.887,0.926	0.817,0.975
Tmin’	0.812	

```
Correction method= INTEGRATION

Data completeness= 0.999          Theta(max)= 30.000

R(reflections)= 0.0510( 3806)     wR2(reflections)= 0.1406( 8901)

S = 0.802                 Npar= 390
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
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Alert level C

```
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....         43 Perc.
PLAT244_ALERT_4_C Low   ’Solvent’ Ueq as Compared to Neighbors of          N6
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0062 Ang
```

```
PLAT410_ALERT_2_C Short Intra H...H Contact  H2B    ..  H4A     ..       1.99 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H7B    ..  H9B     ..       1.98 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H7B    ..  H11A    ..       1.99 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H9B    ..  H11A    ..       1.95 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms .............         1
PLAT344_ALERT_2_G Check sp?     Angle Range in Solvent/Ion for ...        C29
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety        C28
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2
             N O3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3
             C H O
PLAT793_ALERT_4_G The Model has Chirality at N1      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at N2      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at N3      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at N4      (Verify) ....          S
PLAT794_ALERT_5_G Note: Tentative Bond Valency for Cu1     (II)          1.98
```

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