

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: 11

Bond precision: C-C = 0.0022 A

Wavelength=1.54184

Cell: a=9.2658(2) b=14.8807(3) c=17.1665(5)
 alpha=101.324(2) beta=99.732(2) gamma=90.224(2)
Temperature: 150 K

	Calculated	Reported
Volume	2285.78(10)	2285.78(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H12 Cl Cu N2 O4, C5 H12 N	C20 H12 Cl Cu N2 O4, C5 H12 N
Sum formula	C25 H24 Cl Cu N3 O4	C25 H24 Cl Cu N3 O4
Mr	529.47	529.46
Dx, g cm-3	1.539	1.539
Z	4	4
Mu (mm-1)	2.749	2.749
F000	1092.0	1092.0
F000'	1088.38	
h,k,lmax	11,18,21	11,18,21
Nref	9394	9361
Tmin,Tmax	0.755,0.872	0.256,1.000
Tmin'	0.631	

Correction method= # Reported T Limits: Tmin=0.256 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996

Theta(max)= 74.836

R(reflections)= 0.0297(8533)

wR2(reflections)= 0.0799(9361)

S = 1.029

Npar= 629

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**

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for  O32      --C310    .           5.9 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for  O41      --C410    .           5.5 s.u.
PLAT411_ALERT_2_C Short Inter H...H Contact H12      ..H12    .           2.11 Ang.
                                     -x,1-y,2-z =      2_567 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #           1 Note
                   C20 H12 C1 Cu N2 O4
```

● **Alert level G**

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)           0.002 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1      --C11    .           6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu2      --C12    .           6.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu2      --N3     .           6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu2      --N4     .           6.8 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact C16      ..C49    .           3.18 Ang.
                                     1+x,y,z =      1_655 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #           2 Note
                   C20 H12 C1 Cu N2 O4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #           3 Note
                   C5 H12 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #           4 Note
                   C5 H12 N
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1      (II)    .           2.17 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2      (II)    .           2.16 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .      Please Do !
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
12 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 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 22/12/2019; check.def file version of 13/12/2019

