

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu\_20200610\_0ma\_a

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: cu\_20200610\_0ma\_a

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Bond precision:    C-C = 0.0048 A                      Wavelength=1.54178

Cell:                      a=8.4390(4)              b=19.938(1)              c=6.4295(4)  
                                    alpha=90                      beta=90                      gamma=90

Temperature:              296 K

	Calculated	Reported
Volume	1081.81(10)	1081.81(10)
Space group	P 21 21 2	P 21 21 2
Hall group	P 2 2ab	P 2 2ab
Moiety formula	C12 H12 O5	C12 H12 O5
Sum formula	C12 H12 O5	C12 H12 O5
Mr	236.22	236.22
Dx,g cm-3	1.450	1.450
Z	4	4
Mu (mm-1)	0.964	0.964
F000	496.0	496.0
F000'	497.80	
h,k,lmax	10,24,7	10,24,7
Nref	2001[ 1192]	1997
Tmin,Tmax		0.503,0.753
Tmin'		

Correction method= # Reported T Limits: Tmin=0.503 Tmax=0.753  
AbsCorr = NONE

Data completeness= 1.68/1.00                      Theta(max)= 68.367

R(reflections)= 0.0564( 1831)                      wR2(reflections)= 0.1519( 1997)

S = 1.070    Npar= 156

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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 A**

EXPT005\_ALERT\_1\_A \_exptl\_crystal\_description is missing  
Crystal habit description.  
The following tests will not be performed.  
CRYSR\_01  
PLAT414\_ALERT\_2\_A Short Intra D-H..H-X H003 ..H00B 1.66 Ang.  
x,y,z = 1\_555 Check  
PLAT699\_ALERT\_1\_A Missing \_exptl\_crystal\_description Value ..... Please Do !

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**Alert level B**

PLAT035\_ALERT\_1\_B \_chemical\_absolute\_configuration Info Not Given Please Do !  
PLAT420\_ALERT\_2\_B D-H Without Acceptor O003 --H003 . Please Check  
PLAT430\_ALERT\_2\_B Short Inter D...A Contact O005 ..0005 . 2.77 Ang.  
1-x,1-y,z = 2\_665 Check

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**Alert level C**

PLAT053\_ALERT\_1\_C Minimum Crystal Dimension Missing (or Error) ... Please Check  
PLAT054\_ALERT\_1\_C Medium Crystal Dimension Missing (or Error) ... Please Check  
PLAT055\_ALERT\_1\_C Maximum Crystal Dimension Missing (or Error) ... Please Check  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00483 Ang.  
PLAT415\_ALERT\_2\_C Short Inter D-H..H-X H003 ..H00F . 2.11 Ang.  
-1+x,y,z = 1\_455 Check  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 1.06A From O003 -0.43 eA-3  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.89A From O004 -0.42 eA-3  
PLAT977\_ALERT\_2\_C Check Negative Difference Density on H003 -0.36 eA-3  
PLAT977\_ALERT\_2\_C Check Negative Difference Density on H004 -0.42 eA-3

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**Alert level G**

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 2 Report  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 29 Note  
PLAT791\_ALERT\_4\_G Model has Chirality at C00C (Sohnke SpGr) S Verify  
PLAT791\_ALERT\_4\_G Model has Chirality at C00E (Sohnke SpGr) R Verify  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 1 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 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  
4 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.

### Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_EXPT005_cu_20200610_0ma_a
;
PROBLEM: _exptl_crystal_description is missing
RESPONSE: ...
;
_vrf_PLAT414_cu_20200610_0ma_a
;
PROBLEM: Short Intra D-H..H-X          H003      ..H00B          1.66 Ang.
RESPONSE: ...
;
_vrf_PLAT699_cu_20200610_0ma_a
;
PROBLEM: Missing _exptl_crystal_description Value ..... Please Do !
RESPONSE: ...
;
_vrf_PLAT035_cu_20200610_0ma_a
;
PROBLEM: _chemical_absolute_configuration Info Not Given Please Do !
RESPONSE: ...
;
_vrf_PLAT420_cu_20200610_0ma_a
;
PROBLEM: D-H Without Acceptor          0003      --H003      .      Please Check
RESPONSE: ...
;
_vrf_PLAT430_cu_20200610_0ma_a
```

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;
PROBLEM: Short Inter D...A Contact  O005      ..0005      .      2.77 Ang.
RESPONSE: ...
;
_vrf_PLAT053_cu_20200610_0ma_a
;
PROBLEM: Minimum Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT054_cu_20200610_0ma_a
;
PROBLEM: Medium Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT055_cu_20200610_0ma_a
;
PROBLEM: Maximum Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT340_cu_20200610_0ma_a
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.00483 Ang.
RESPONSE: ...
;
_vrf_PLAT415_cu_20200610_0ma_a
;
PROBLEM: Short Inter D-H..H-X      H003      ..H00F      .      2.11 Ang.
RESPONSE: ...
;
_vrf_PLAT976_cu_20200610_0ma_a
;
PROBLEM: Check Calcd Resid. Dens.  1.06A      From O003      -0.43 eA-3
RESPONSE: ...
;
_vrf_PLAT977_cu_20200610_0ma_a
;
PROBLEM: Check Negative Difference Density on H003      -0.36 eA-3
RESPONSE: ...
;
# end Validation Reply Form

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**PLATON version of 05/12/2020; check.def file version of 05/12/2020**

