

## 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: nzf-34-300k

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Bond precision:	C-C = 0.0039 A	Wavelength=0.71073	
Cell:	a=21.8874(6)	b=13.7262(4)	c=14.1778(5)
	alpha=90	beta=101.336(3)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	4176.4(2)	4176.4(2)	
Space group	C 2/c	C 1 2/c 1	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C40 H20 Cl4 Cu N6 O16	C26 H14 Cl2 Cu N4 O8, 2(C7 H3 Cl N O4)	
Sum formula	C40 H20 Cl4 Cu N6 O16	C40 H20 Cl4 Cu N6 O16	
Mr	1045.97	1045.96	
Dx, g cm-3	1.663	1.664	
Z	4	4	
Mu (mm-1)	0.862	0.862	
F000	2108.0	2108.0	
F000'	2112.68		
h,k,lmax	26,16,16	26,16,16	
Nref	3695	3692	
Tmin,Tmax	0.772,0.886	0.776,0.889	
Tmin'	0.766		

Correction method= # Reported T Limits: Tmin=0.776 Tmax=0.889  
AbsCorr = MULTI-SCAN

Data completeness= 0.999      Theta(max)= 25.000

R(reflections)= 0.0385( 3342)      wR2(reflections)= 0.1240( 3692)

S = 1.104      Npar= 310

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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 C**

PLAT220_ALERT_2_C	NonSolvent	Resd 1	O	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of		03	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		N2	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)					04 Check

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**Alert level G**

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF					Please Do !
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ					Please Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical					? Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature				293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature				293	Check
PLAT301_ALERT_3_G	Main Residue Disorder					6% Note
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O7B				46.3	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O8B				42.8	Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O8B		..C13		3.01 Ang.
				1/2-x,1/2-y,1-z =	7_556	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF					# 13 Check
	O7B -N2 -O7A	1.555	1.555	1.555		33.40 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF					# 61 Check
	N2 -O8B -O7B	1.555	1.555	1.555		42.80 Deg.
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1			(II)		. 2.20 Info

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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

4 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  
2 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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## 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_PLAT220_nzf-34-300k
;
PROBLEM: NonSolvent  Resd 1  O  Ueq(max)/Ueq(min) Range          3.5 Ratio
RESPONSE: ...
;
_vrf_PLAT241_nzf-34-300k
;
PROBLEM: High  'MainMol' Ueq as Compared to Neighbors of          03 Check
RESPONSE: ...
;
_vrf_PLAT242_nzf-34-300k
;
PROBLEM: Low  'MainMol' Ueq as Compared to Neighbors of          N2 Check
RESPONSE: ...
```

```
;
_vrf_PLAT309_nzf-34-300k
;
PROBLEM: Single Bonded Oxygen (C-O > 1.3 Ang) ..... O4 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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

