

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: 1

Bond precision: C-C = 0.0033 A Wavelength=0.71073
Cell: a=9.9440(4) b=9.3620(4) c=18.5299(7)
alpha=90 beta=95.626(3) gamma=90
Temperature 150 K
:
Calculated Reported
Volume 1716.75(12) 1716.75(12)
Space group P 21/c P 21/c
Hall group -P 2ybc -P 2ybc
Moiety formula C12 H18 Cl Cu N4 O, B F4 ?
Sum formula C12 H18 B Cl Cu F4 N4 O C12 H18 B Cl Cu F4 N4 O
Mr 420.11 420.10
Dx,g cm-3 1.625 1.625
Z 4 4
Mu (mm-1) 1.475 1.475
F000 852.0 852.0
F000' 854.27
h,k,lmax 12,12,24 12,12,24
Nref 3933 3931
Tmin,Tmax 0.370,0.642 0.696,1.000
Tmin' 0.342
Correction method= # Reported T Limits: Tmin=0.696
Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.999 Theta(max)= 27.483
R(reflections)= 0.0334(3327) wR2(reflections)= 0.0858(3931)
S = 1.050 Npar= 249

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

PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	B1 Check
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F3BB Check
	F3BB	B1 F1B	
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F3BB Check
	F3BB	B1 F2B	
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F1BB Check
	F1BB	B1 F2B	
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F2AA Check
	F2AA	B1 F1A	
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F3BB Check
	F3BB	B1 F4	
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F1BB Check
	F1BB	B1 F4	
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F2AA Check
	F2AA	B1 F4	
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F2BB Check
	F2BB	B1 F4	
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F1AA Check
	F1AA	B1 F4	
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F2AA Check
	F2AA	B1 F3A	
PLAT712_ALERT_1_C	ANGLE	Unknown or Inconsistent Label	F1AA Check
	F1AA	B1 F3A	

● Alert level G

PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.70 mm
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	60% Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3 Note

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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
 - 12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 5 **ALERT level G** = General information/check it is not something unexpected
-
- 12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 1 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
 - 3 ALERT type 4 Improvement, methodology, query or suggestion
 - 0 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

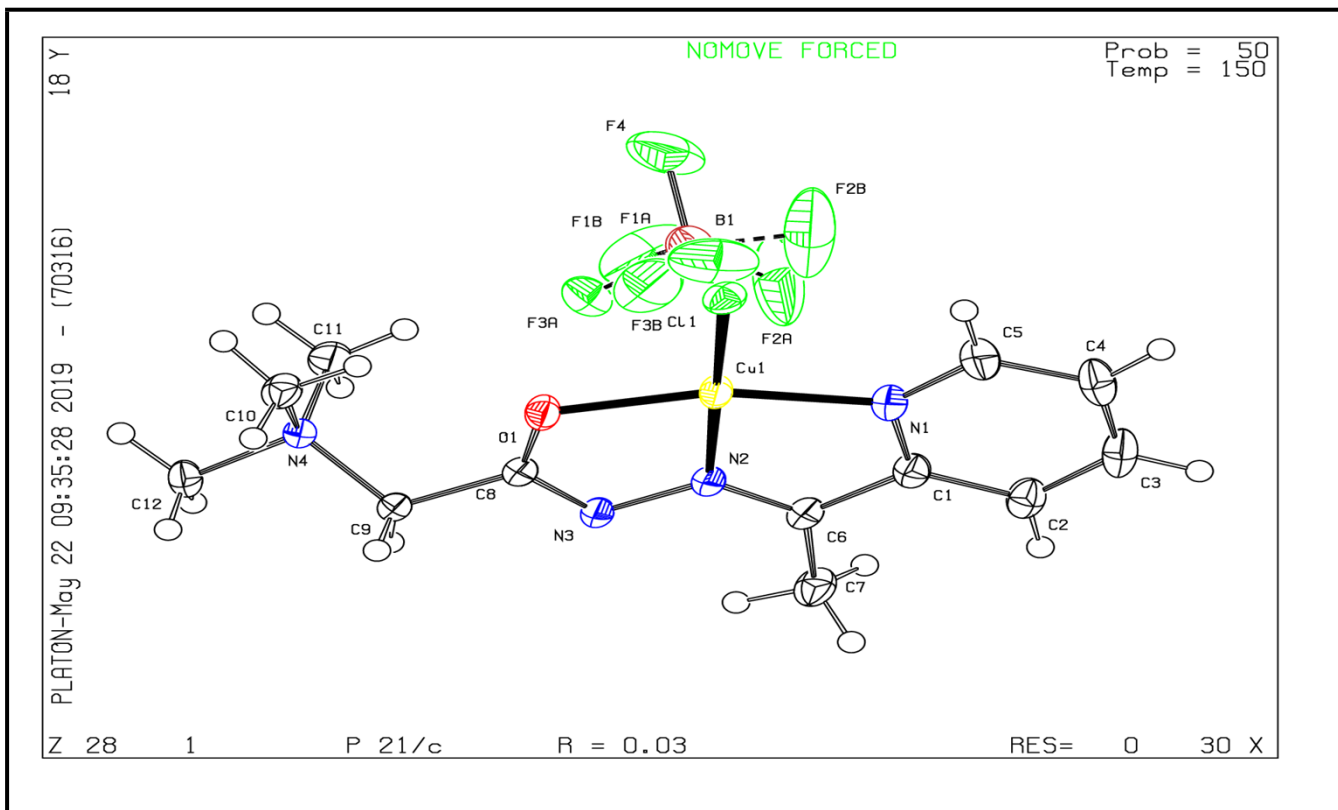
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

Datablock 1 - ellipsoid plot



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