Datablock: 3

Bond precision: C-C = 0.0053 A Wavelength=0.71073
Cell: a=7.2915(3) b=28.1816(13) c=8.9402(5)
alpha=90 beta=112.196(6) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	1700.95(16)	1700.95(16)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C24 H36 Cl2 Cu2 N8 O2, 2(B F4)	?
Sum formula	C24 H36 B2 Cl2 Cu2 F8 N8 O2	C24 H36 B2 Cl2 Cu2 F8 N8 O2
Mr	840.23	840.21
Dx,g cm-3	1.640	1.640
Z	2	2
Mu (mm-1)	1.489	1.489
F000	852.0	852.0
F000'	854.27	
h,k,lmax	9,36,11	9,36,11
Nref	3912	3910
Tmin,Tmax	0.494,0.742	0.563,1.000
Tmin'	0.301	

Correction method= # Reported T Limits: Tmin=0.563
Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.999 Theta(max)= 27.485
R(reflections)= 0.0490(3365) wR2(reflections)= 0.1256(3910)
S = 1.107 Npar= 221

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.15 Report
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.253 Check

Alert level G

PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.80 mm
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	B1 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # B F4	2 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II) .	2.22 Info
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).	2 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	5 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
3 ALERT type 4 Improvement, methodology, query or suggestion
1 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

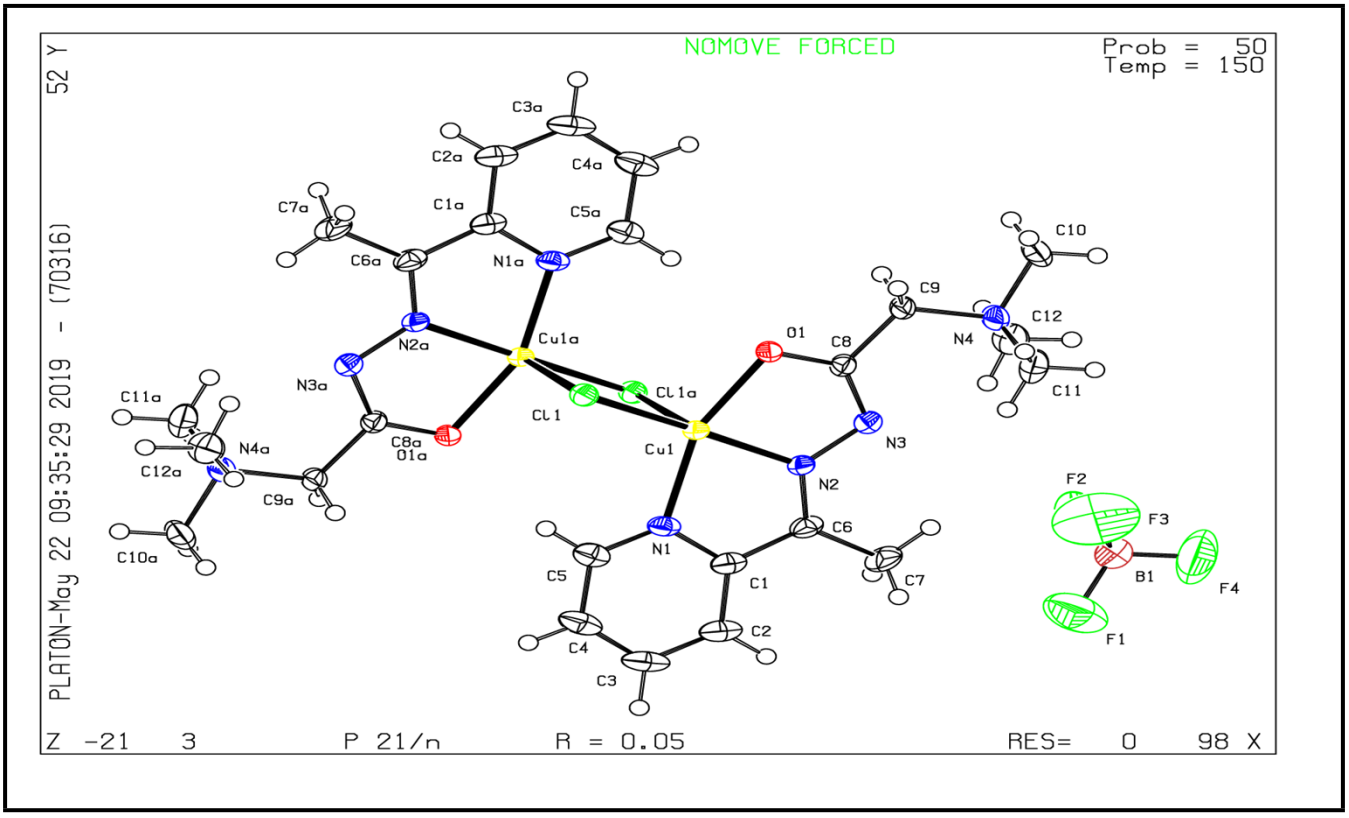
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 03/05/2019; check.def file version of 29/04/2019

Datablock 3 - ellipsoid plot



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