No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: 1

Bond precision: C-C = 0.0046 A Wavelength=0.71073
Cell: a=9.9406(2) b=9.5650(2) c=18.8796(5)
alpha=90 beta=94.712(1) gamma=90
Temperature : 293 K

	Calculated	Reported
Volume	1789.04(7)	1789.04(7)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C12 H18 Cl2 Cu N4 O5	?
Sum formula	C12 H18 Cl2 Cu N4 O5	C12 H18 Cl2 Cu N4 O5
Mr	432.75	432.74
Dx,g cm-3	1.607	1.607
Z	4	4
Mu (mm-1)	1.549	1.549
F000	884.0	884.0
F000'	886.77	
h,k,lmax	12,12,24	12,12,24
Nref	4099	4065
Tmin,Tmax	0.911,0.925	0.801,0.927
Tmin'	0.793	

Correction method= # Reported T Limits: Tmin=0.801
Tmax=0.927 AbsCorr = MULTI-SCAN
Data completeness= 0.992 Theta(max)= 27.469
R(reflections)= 0.0432(3215) wR2(reflections)= 0.1328(4065)
S = 1.089 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 B

PLAT242_ALERT_2_B	Low 'MainMol' Ueq as Compared to Neighbors of	Cl Check
PLAT910_ALERT_3_B	Missing # of FCF Reflection(s) Below Theta(Min).	11 Note

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Alert level C

PLAT220_ALERT_2_C	Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range	4.2 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference Cl --O4A .	0.20 Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Cu1 Check
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O5BB Check
	O5BB CL O3B	
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O4AA Check
	O4AA CL O5A	
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O5BB Check
	O5BB CL O4B	
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O3BB Check
	O3BB CL O4B	
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O5BB Check
	O5BB CL O2	
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O3BB Check
	O3BB CL O2	
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O4AA Check
	O4AA CL O2	
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O5AA Check
	O5AA CL O2	
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O4BB Check
	O4BB CL O2	
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O4AA Check
	O4AA CL O3A	
PLAT712_ALERT_1_C	ANGLE Unknown or Inconsistent Label	O5AA Check
	O5AA CL O3A	

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 23 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 4 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 17.18 Check

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 13% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 44 Note
PLAT883_ALERT_1_G No Info for _atom_sites_solution_primary ..... Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 16 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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

15 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
8 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

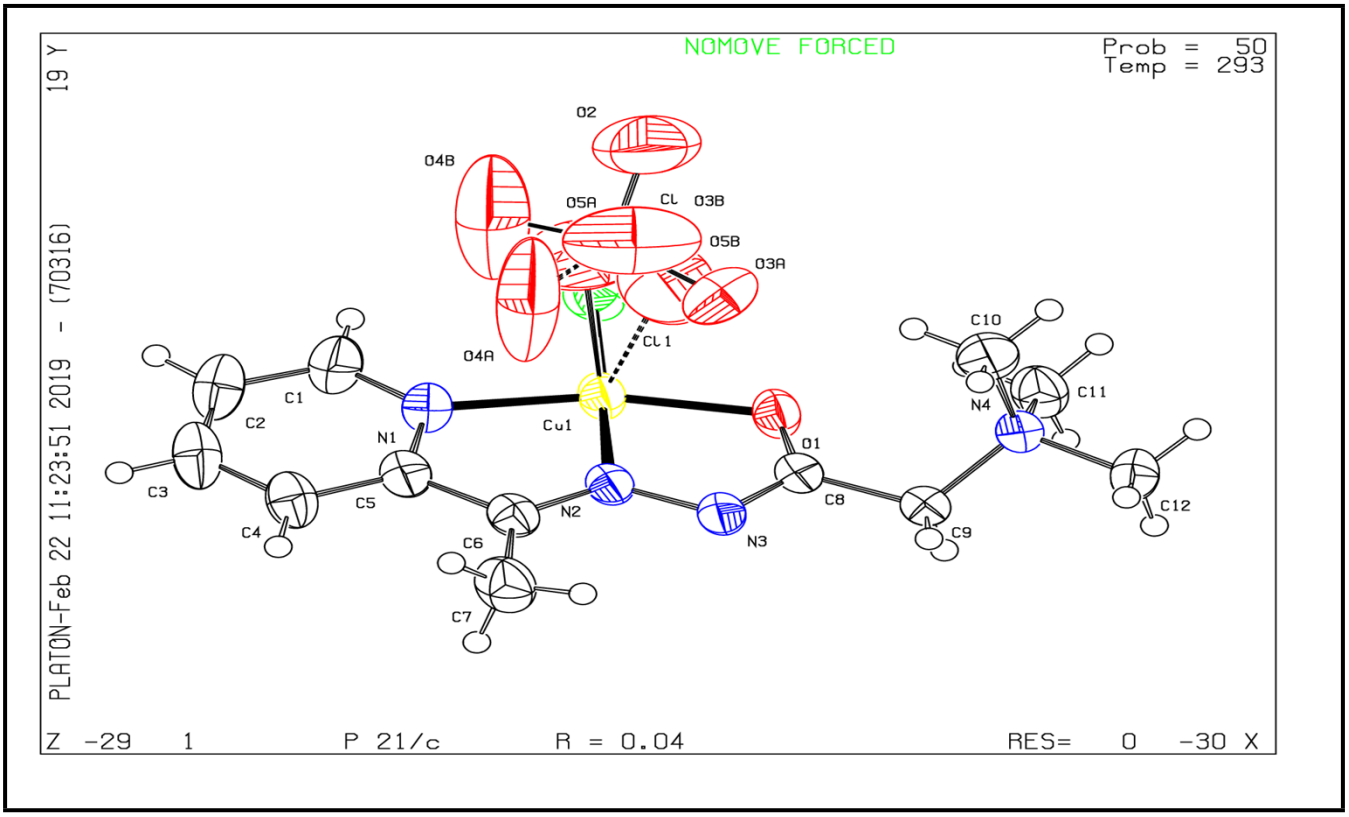
Publication of your CIF in IUCr journals

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.

Datablock 1 - ellipsoid plot



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