



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 111

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: 111

Bond precision: C-C = 0.0030 Å

Wavelength=0.71073

Cell: a=9.1171 (4) b=11.7003 (4) c=12.4734 (5)
 alpha=77.205 (1) beta=77.943 (1) gamma=79.702 (1)
Temperature: 150 K

	Calculated	Reported
Volume	1256.60 (9)	1256.60 (9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H16 Cl Cu N4, B5 H4 O10	C20 H16 Cl Cu N4, B5 H4 O10
Sum formula	C20 H20 B5 Cl Cu N4 O10	C20 H20 B5 Cl Cu N4 O10
Mr	629.45	629.44
Dx, g cm ⁻³	1.664	1.664
Z	2	2
Mu (mm ⁻¹)	1.040	1.040
F000	638.0	638.0
F000'	639.22	
h, k, lmax	11, 14, 15	11, 14, 15
Nref	5207	5178
Tmin, Tmax	0.829, 0.883	0.011, 0.028
Tmin'	0.812	

Correction method= # Reported T Limits: Tmin=0.011 Tmax=0.028
AbsCorr = ?

Data completeness= 0.994

Theta(max)= 26.479

R(reflections)= 0.0261(4645)

wR2(reflections)=
0.0725(5178)

S = 1.054

Npar= 374

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

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report
-2 1 1, 1 1 1, 0 2 1, -2 2 2, -1 2 2, 1 1 3,
1 2 3,



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
H1A H3A H8A H10A
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu01 --N1 . 5.1 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 1 Note
Cu01
PLAT794_ALERT_5_G Tentative Bond Valency for Cu01 (II) . 2.28 Info
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 2.23 Note
0 1 0, 0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 20 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 2 Note
-2 2 2, -1 2 2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 4.166 Note
Predicted wR2: Based on SigI**2 1.74 or SHELX Weight 6.88 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 15 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
10 **ALERT level G** = General information/check it is not something unexpected
- 2 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
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
3 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 23/04/2026; check.def file version of 30/03/2026

duplicate check

No duplication found

Datablock 111 - ellipsoid plot

