

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: 1v

Bond precision:	C-C = 0.0219 A	Wavelength=0.71073
Cell:	a=23.9180(9)	b=12.7420(5) c=17.8041(7)
	alpha=90	beta=112.848(2) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	5000.3(3)	5000.3(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C22 H17 Cu I N3 O), C12 H8 Cl3	C22 H17 Cu I N3 O, C6 H4 Cl1.5
Sum formula	C56 H42 Cl3 Cu2 I2 N6 O2	C28 H21 Cl1.50 Cu I N3 O
Mr	1318.21	659.09
Dx,g cm-3	1.751	1.751
Z	4	8
Mu (mm-1)	2.296	2.296
F000	2604.0	2604.0
F000'	2605.24	
h,k,lmax	28,15,21	28,15,21
Nref	4713	4660
Tmin,Tmax	0.396,0.502	0.519,0.745
Tmin'	0.342	

Correction method= # Reported T Limits: Tmin=0.519 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.989 Theta(max)= 25.579

R(reflections)= 0.0812(3646) wR2(reflections)= 0.2560(4660)

S = 1.035 Npar= 287

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

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.02193 Ang.

Author Response: This alert is coming due to poor data quality.



Alert level C

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.26 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1 Check
C11
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C24 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C11 0.248 Check
PLAT336_ALERT_2_C Long Bond Distance for C24 -C11 1.940 Ang.



Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 7 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF Please Check
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 101.03 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 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
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 3 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 21 Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
6 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.

