

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: 1u

Bond precision:	C-C = 0.0085 A	Wavelength=0.71073
Cell:	a=23.8568(9)	b=12.7232(5) c=17.6759(7)
	alpha=90	beta=112.562(2) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	4954.6(3)	4954.6(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C22 H17 Cu I N3 O, C7 H7	C7 H7, C22 H17 Cu I N3 O
Sum formula	C29 H24 Cu I N3 O	C29 H24 Cu I N3 O
Mr	620.96	620.95
Dx,g cm-3	1.665	1.665
Z	8	8
Mu (mm-1)	2.156	2.156
F000	2472.0	2472.0
F000'	2471.45	
h,k,lmax	31,17,23	0,0,0
Nref	6202	6150
Tmin,Tmax	0.685,0.772	0.685,0.772
Tmin'	0.672	

Correction method= # Reported T Limits: Tmin=0.685 Tmax=0.772
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 28.377

R(reflections)= 0.0457(4691) wR2(reflections)= 0.1341(6150)

S = 1.074 Npar= 296

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

PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	2	Check
	C28 C29		
PLAT221_ALERT_2_C	Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range	5.3	Ratio
PLAT243_ALERT_4_C	High Solvent Ueq as Compared to Neighbors of	C28	Check
PLAT243_ALERT_4_C	High Solvent Ueq as Compared to Neighbors of	C29	Check
PLAT244_ALERT_4_C	Low Solvent Ueq as Compared to Neighbors of	C24	Check
PLAT244_ALERT_4_C	Low Solvent Ueq as Compared to Neighbors of	C26	Check
PLAT244_ALERT_4_C	Low Solvent Ueq as Compared to Neighbors of	C27	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C24	0.159	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00846	Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note
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
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	11.30	Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I1 --Cul .	13.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I1 --Cul_a .	17.3	s.u.
PLAT344_ALERT_2_G	Unusual sp? Angle Range in Solvent/Ion for		C28 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C24 ..C28	3.12	Ang.
	1-x,y,3/2-z =	2_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C28 ..C28	2.36	Ang.
	1-x,y,3/2-z =	2_656	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	1	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
9 **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
9 **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
7 **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.

