

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: 1t

Bond precision:	C-C = 0.0164 A	Wavelength=0.71073
Cell:	a=23.696(4)	b=12.9253(19) c=17.710(3)
	alpha=90	beta=111.762(2) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	5037.6(14)	5037.4(13)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C22 H17 Cu I N3 O, C6 H5	C22 H17 Cu I N3 O, C6 H5
Sum formula	C28 H22 Cu I N3 O	C28 H22 Cu I N3 O
Mr	606.94	606.92
Dx,g cm-3	1.600	1.601
Z	8	8
Mu (mm-1)	2.118	2.118
F000	2408.0	2408.0
F000'	2407.44	
h,k,lmax	29,16,22	29,16,22
Nref	5360	5359
Tmin,Tmax	0.563,0.641	0.456,0.746
Tmin'	0.407	

Correction method= # Reported T Limits: Tmin=0.456 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 26.732

R(reflections)= 0.0641(4473) wR2(reflections)= 0.1507(5359)

S = 1.071 Npar= 269

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	4	Check
	C22S C23S C26S C27S		
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C27S	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C23S	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C25S	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C22S	0.279	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01644	Ang.

Alert level G

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
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	123.81	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) I001 --Cu02_a .	9.2	s.u.
PLAT344_ALERT_2_G	Unusual sp? Angle Range in Solvent/Ion for	C27S	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C27S ..C27S	2.72	Ang.
	2-x,y,1/2-z =	2_755	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	3	Note

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

1 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
2 ALERT type 3 Indicator that the structure quality may be low
5 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.

