

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: 1y

Bond precision:	C-C = 0.0207 Å	Wavelength=0.71073
Cell:	a=23.5760(19)	b=12.8738(11) c=17.7114(14)
	alpha=90	beta=110.880(2) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	5022.6(7)	5022.6(7)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C44 H34 Cu2 I2 N6 O2, C10 H8, C2 H3 N	C44 H34 Cu2 I2 N6 O2, C2 H3 N, C10 H8
Sum formula	C56 H45 Cu2 I2 N7 O2	C56 H45 Cu2 I2 N7 O2
Mr	1228.89	1228.87
Dx,g cm-3	1.625	1.625
Z	4	4
Mu (mm-1)	2.126	2.126
F000	2440.0	2440.0
F000'	2439.44	
h,k,lmax	28,15,21	28,15,21
Nref	9227	9191
Tmin,Tmax	0.581,0.640	0.571,0.745
Tmin'	0.570	

Correction method= # Reported T Limits: Tmin=0.571 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.371

R(reflections)= 0.0817(6320) wR2(reflections)= 0.2034(9191)

S = 1.091 Npar= 625

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 0.02074 Ang.

Author Response: The crystal was poorly diffracting at higher Bragg angles and this alert is coming due to poor data quality.



Alert level C

PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C01X	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C44	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C47	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C54	Check
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor	2.1	Note



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
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	165.38	Why ?
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	4	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
5 **ALERT level G** = General information/check it is not something unexpected

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

