

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: 1s

Bond precision:	C-C = 0.0313 A	Wavelength=0.71073
Cell:	a=18.180(2)	b=11.850(1) c=24.082(3)
	alpha=90	beta=109.299(8) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	4896.5(9)	4896.5(9)
Space group	I 2/c	I 1 2/c 1
Hall group	-I 2yc	-I 2yc
Moiety formula	C22 H17 Cu I N3 O, C H2 O, 0.5(C2 H6 O2)	C22 H17 Cu I N3 O, C H3 O, C H2 O
Sum formula	C24 H22 Cu I N3 O3	C24 H22 Cu I N3 O3
Mr	590.90	590.88
Dx,g cm-3	1.603	1.603
Z	8	8
Mu (mm-1)	2.182	2.182
F000	2344.0	2344.0
F000'	2343.52	
h,k,lmax	22,14,29	21,14,29
Nref	4702	4584
Tmin,Tmax	0.585,0.605	0.520,0.745
Tmin'	0.574	

Correction method= # Reported T Limits: Tmin=0.520 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.975 Theta(max)= 25.742

R(reflections)= 0.1348(3884) wR2(reflections)= 0.3017(4584)

S = 1.168 Npar= 266

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 0.0313 Ang.

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



Alert level C

CRYSC01_ALERT_1_C The word below has not been recognised as a standard
 identifier.
 dull

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
 Rint given 0.128

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12	0.128 Report
PLAT082_ALERT_2_C High R1 Value	0.13 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.30 Report
PLAT213_ALERT_2_C Atom O1 has ADP max/min Ratio	3.4 prolat
PLAT213_ALERT_2_C Atom C11 has ADP max/min Ratio	3.3 prolat
PLAT213_ALERT_2_C Atom C12 has ADP max/min Ratio	3.4 prolat
PLAT213_ALERT_2_C Atom C13 has ADP max/min Ratio	3.6 prolat
PLAT213_ALERT_2_C Atom C14 has ADP max/min Ratio	3.9 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max) / Ueq(min) Range	3.1 Ratio
PLAT223_ALERT_4_C Solv./Anion Resd 3 H Ueq(max)/Ueq(min) Range	4.1 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C9 --C10 .	5.6 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C11 --C12 .	5.5 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference O1 --C22 .	0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13 --C14 .	0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C19 --C20 .	0.21 Ang.
PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of	C10 Check
PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of	C12 Check
PLAT241_ALERT_2_C High MainMol Ueq as Compared to Neighbors of	C19 Check
PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of	C6 Check
PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of	C9 Check
PLAT242_ALERT_2_C Low MainMol Ueq as Compared to Neighbors of	C11 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor	2.7 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including 02	0.111 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including 03	0.118 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang)	02 Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C11 -C16	1.37 Ang.



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	1 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	1 Report
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	653.31 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	4 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) I001 --Cu03 .	5.2 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels	8 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints	1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	5 Note

0	ALERT level A	= Most likely a serious problem - resolve or explain
1	ALERT level B	= A potentially serious problem, consider carefully
28	ALERT level C	= Check. Ensure it is not caused by an omission or oversight
12	ALERT level G	= General information/check it is not something unexpected
3	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
24	ALERT type 2	Indicator that the structure model may be wrong or deficient
5	ALERT type 3	Indicator that the structure quality may be low
7	ALERT type 4	Improvement, methodology, query or suggestion
2	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.

