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: 1p

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Bond precision:  C-C = 0.0198 A          Wavelength=0.71073

Cell:            a=24.282(3)    b=12.4370(14)       c=17.961(2)
                 alpha=90       beta=112.100(4)     gamma=90
Temperature:     109 K
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	Calculated	Reported
Volume	5025.6(10)	5025.5(10)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C22 H15.95 Cu I N3 O, 0.561(C Cl4), 0.44(C Cl3), 0.44(Cl)	C22 H15.95 Cu I N3 O, C1 Cl4
Sum formula	C23 H15.95 Cl4 Cu I N3 O	C23 H15.95 Cl4 Cu I N3 O
Mr	682.58	682.57
Dx,g cm-3	1.804	1.804
Z	8	8
Mu (mm-1)	2.545	2.545
F000	2663.6	2664.0
F000’	2667.72	
h,k,lmax	29,15,21	29,15,21
Nref	4662	4644
Tmin,Tmax	0.262,0.318	0.474,0.745
Tmin’	0.221	

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Correction method= # Reported T Limits: Tmin=0.474 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 25.476

R(reflections)= 0.0983( 4087)     wR2(reflections)= 0.2385( 4644)

S = 1.266                 Npar= 348
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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

PLAT241_ALERT_2_C High ’MainMol’ Ueq as Compared to Neighbors of C18 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl1A 0.123 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl4A 0.113 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01976 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
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 412.99 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 7 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of O1B Constrained at 0.5265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1A Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19B Constrained at 0.5265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20B Constrained at 0.5265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21B Constrained at 0.5265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22B Constrained at 0.5265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19A Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20A Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21A Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22A Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19B Constrained at 0.5265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21B Constrained at 0.5265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22D Constrained at 0.5265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22E Constrained at 0.5265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22F Constrained at 0.5265 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17 Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18 Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H19A Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21A Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22A Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22B Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22C Constrained at 0.4735 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1B Constrained at 0.5605 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2B Constrained at 0.5605 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3B Constrained at 0.5605 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4B Constrained at 0.5605 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C0AA Constrained at 0.5605 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1A Constrained at 0.4395 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2A Constrained at 0.4395 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3A Constrained at 0.4395 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23A Constrained at 0.4395 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4A Constrained at 0.4395 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 18% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT434_ALERT_2_G Short Inter HL..HL Contact I001 ..Cl4A 3.46 Ang.
1-x,2-y,1-z = 5_676 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact I001 ..Cl2B 3.53 Ang.
x,1+y,z = 1_565 Check

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          3 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  50 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
  38 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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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.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

Datablock 1p - ellipsoid plot