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: 1o

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Bond precision:  C-C = 0.0208 A          Wavelength=0.71073

Cell:           a=24.6615(9)    b=12.0846(5)        c=18.0322(7)
                alpha=90        beta=113.580(2)     gamma=90
Temperature:    100 K
```

	Calculated	Reported
Volume	4925.3(3)	4925.3(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, C H2 Cl2	C22 H17 Cu I N3 O, C H2 Cl2
Sum formula	C23 H19 Cl2 Cu I N3 O	C23 H19 Cl2 Cu I N3 O
Mr	614.76	614.75
Dx,g cm-3	1.658	1.658
Z	8	8
Mu (mm-1)	2.377	2.377
F000	2416.0	2416.0
F000’	2417.75	
h,k,lmax	29,14,21	29,14,21
Nref	4517	4515
Tmin,Tmax	0.442,0.467	0.515,0.745
Tmin’	0.409	

```
Correction method= # Reported T Limits: Tmin=0.515 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.000          Theta(max)= 25.349

R(reflections)= 0.1075( 3453)     wR2(reflections)= 0.2519( 4515)

S = 1.157                 Npar= 269
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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 B

PLAT260_ALERT_2_B Large Average Ueq of Residue Including Cl1 0.334 Check

Author Response: The CH2Cl2 were present as a lattice occluded guest in the crystal lattice and the thermal parameter associated with one Cl atom were high for better model EADP command were used thats why the alaert is comming.

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02076 Ang.

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

Alert level C

PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.53 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.5 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference N1 --C1 . 0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C23 Check
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 72 Ang**3

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 306.36 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 3 Note

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

1 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
2 ALERT type 3 Indicator that the structure quality may be low
4 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.

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

Datablock 1o - ellipsoid plot