

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CuL2, L1, L2

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: L1

Bond precision:	C-C = 0.0032 A	Wavelength=0.71073
Cell:	a=12.2207(13) b=8.2084(9) c=14.7380(16)	
	alpha=90 beta=105.6968(19) gamma=90	
Temperature:	293 K	
	Calculated	Reported
Volume	1423.3(3)	1423.3(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H13 N	C21 H13 N
Sum formula	C21 H13 N	C21 H13 N
Mr	279.32	279.32
Dx,g cm-3	1.304	1.304
Z	4	4
Mu (mm-1)	0.076	0.072
F000	584.0	584.0
F000'	584.21	
h,k,lmax	15,10,19	15,10,19
Nref	3279	3274
Tmin,Tmax	0.985,0.999	0.454,0.744
Tmin'	0.972	

Correction method= # Reported T Limits: Tmin=0.454 Tmax=0.744
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.531

R(reflections)= 0.0543(1561) wR2(reflections)= 0.1669(3274)

S = 0.986 Npar= 199

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

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies
outside the range 0.99 <> 1.01
Calculated value of mu = 0.076
Value of mu given = 0.072

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 48% Check
PLAT230_ALERT_2_C Hirshfeld Test Diff for C9 --C10 . 5.5 s.u.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -10.358 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -1.095 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

● Alert level G

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 6 Note

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

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

Datablock: L2

Bond precision: C-C = 0.0024 Å Wavelength=0.71073

Cell: a=8.2054(10) b=9.7248(12) c=10.4571(12)
alpha=85.133(2) beta=79.400(2) gamma=74.341(2)

Temperature: 296 K

	Calculated	Reported
Volume	789.21(16)	789.21(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C23 H17 N	C23 H17 N
Sum formula	C23 H17 N	C23 H17 N
Mr	307.38	307.38
Dx,g cm-3	1.293	1.293
Z	2	2
Mu (mm-1)	0.075	0.075
F000	324.0	324.0
F000'	324.11	
h,k,lmax	10,12,13	10,12,13
Nref	3511	3494
Tmin,Tmax	0.982,0.994	0.681,0.746
Tmin'	0.963	

Correction method= # Reported T Limits: Tmin=0.681 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 27.140

R(reflections)= 0.0494(2140) wR2(reflections)= 0.1530(3494)

S = 1.042 Npar= 236

The following ALERTS were generated. Each ALERT has the format

```
test-name ALERT alert-type alert-level.
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Click on the hyperlinks for more details of the test.

- Alert level C

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N1	--C21	.	5.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C20	--C21	.	5.5 s.u.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H13	..H18D	.	1.97 Ang.
			x,y,z =	1_555	Check
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.				0 Info

- Alert level G

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002 Degree
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	8% Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STH/L= 0.600	17 Note

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## Datablock: CuL2

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Bond precision: C-C = 0.0038 Å                      Wavelength=0.71073

Cell:                      a=20.4752(9)              b=4.5020(2)              c=20.2080(9)  
                            alpha=90              beta=103.158(1)              gamma=90

Temperature:              296 K

|                | Calculated     | Reported       |
|----------------|----------------|----------------|
| Volume         | 1813.86(14)    | 1813.85(14)    |
| Space group    | P 21/c         | P 21/c         |
| Hall group     | -P 2ybc        | -P 2ybc        |
| Moiety formula | C23 H17 Cu I N | C23 H17 Cu I N |
| Sum formula    | C23 H17 Cu I N | C23 H17 Cu I N |
| Mr             | 497.83         | 497.82         |
| Dx,g cm-3      | 1.823          | 1.823          |
| Z              | 4              | 4              |
| Mu (mm-1)      | 2.912          | 2.912          |
| F000           | 976.0          | 976.0          |
| F000'          | 975.64         |                |
| h,k,lmax       | 30,6,30        | 30,6,29        |
| Nref           | 6440           | 6174           |
| Tmin,Tmax      | 0.598,0.865    | 0.593,0.746    |
| Tmin'          | 0.357          |                |

Correction method= # Reported T Limits: Tmin=0.593 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.959                      Theta(max)= 32.255

R(reflections)= 0.0333( 4762)              wR2(reflections)= 0.0844( 6174)

S = 1.023                      Npar= 235

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**test-name\_ALERT\_alert-type\_alert-level.**  
Click on the hyperlinks for more details of the test.

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### Alert level C

|                                                                   |           |
|-------------------------------------------------------------------|-----------|
| PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of  | Cu1 Check |
| PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # | 1 Note    |
| C23 H17 Cu I N                                                    |           |

**Alert level G**

|                   |                                                  |       |       |
|-------------------|--------------------------------------------------|-------|-------|
| PLAT004_ALERT_5_G | Polymeric Structure Found with Maximum Dimension | 1     | Info  |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) I1 --Cul .             | 41.3  | s.u.  |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) I1 --Cul_a .           | 65.3  | s.u.  |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) I1 --Cul_b .           | 211.7 | s.u.  |
| PLAT764_ALERT_4_G | Overcomplete CIF Bond List Detected (Rep/Expd) . | 1.13  | Ratio |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min). | 1     | Note  |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600  | 255   | Note  |
| PLAT933_ALERT_2_G | Number of OMIT Records in Embedded .res File ... | 1     | Note  |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 14    | Info  |

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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.





