

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu\_hku\_dicz\_p2\_0m

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: cu\_hku\_dicz\_p2\_0m

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Bond precision:      C-C = 0.0074 Å

Wavelength=1.54178

Cell:                      a=14.6091(3)                      b=15.3776(4)                      c=22.3624(5)  
                              alpha=92.706(2)                      beta=102.868(2)                      gamma=107.854(2)  
Temperature:              223 K

	Calculated	Reported
Volume	4625.5(2)	4625.50(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C92 H84 N4 [+ solvent]	C92 H84 N4
Sum formula	C92 H84 N4 [+ solvent]	C92 H84 N4
Mr	1245.64	1245.63
Dx, g cm <sup>-3</sup>	0.894	0.894
Z	2	2
Mu (mm <sup>-1</sup> )	0.390	0.390
F000	1328.0	1328.0
F000'	1331.38	
h,k,lmax	17,18,26	17,18,26
Nref	16352	16257
Tmin,Tmax	0.951,0.958	0.533,0.753
Tmin'	0.951	

Correction method= # Reported T Limits: Tmin=0.533 Tmax=0.753  
AbsCorr = MULTI-SCAN

Data completeness= 0.994

Theta(max)= 66.593

R(reflections)= 0.1085( 10661)

wR2(reflections)=  
0.2761( 16257)

S = 1.001

Npar= 914

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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.

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### Alert level C

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75

The relevant atom site should be identified.

PLAT082_ALERT_2_C	High R1 Value .....	0.11	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25) .....	0.28	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	0.70	eA-3
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.3	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.1	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C89 --C91 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C89 --C90A .	0.19	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C17	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C39	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C43	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C85	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C89	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00743	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	5.465	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.481	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	95	Report
	-3 1 0, -2 1 0, -1 1 0, 0 1 0, -3 2 0, 0 3 0,		
	-1 4 0, -12 11 0, 8-18 1, 5 -9 1, 2 -4 1, 1 -3 1,		
	5 -3 1, 2 -2 1, 3 -2 1, 4 -2 1, 2 -1 1, -2 2 1,		
	2 2 1, -4 3 1, -2 3 1, -2 4 1, 1 5 1, -6 8 1,		
	2 8 1, 8-18 2, -2 -7 2, -3 -6 2, 0 -3 2, 1 -3 2,		
	4 -3 2, -5 -2 2, 1 -2 2, 0 1 2, 2 3 2, -3 14 2,		
	4 -9 3, -1 0 3, -1 1 3, 2 1 3, 3 1 3, 3 2 3,		
	-2 3 3, 1 5 3, 2 5 3, 1 6 3, 3 -7 4, 1 -2 4,		
	1 -1 4, -2 2 4, 10 9 4, 9 10 4, 6 12 4, 2 -7 5,		
	1 -3 5, 1 0 5, -1 1 5, 3 1 5, 3 2 5, -9 4 5,		
	-7 7 5, 10 9 5, 9 10 5, 3 -7 6, 6 -3 6, 2 2 6,		
	-4 3 6, -7 7 6, 3 -8 7, 7 11 7, 4 -7 8, 15 -6 8,		
	-5 1 8, -8 2 8, 8 10 8, 7 11 8, 6 12 8, -8 5 9,		
	6 11 10, 2 -5 11, -1 0 11, 10 -7 12, 6 10 12, 5 11 12,		
	-11 13 13, -16 4 15, 4 10 15, -15 5 17, -15 6 17, -15 3 18,		
	-15 4 18, -15 5 18, -13 2 19, -11 -4 21, 2 -3 25,		
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1	Check

### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H Atoms	6	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	20.00	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0100	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for SecondPar	0.0200	Report
PLAT190_ALERT_3_G	A Non-default RIGU Restraint Value for First Par	0.0100	Report



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.

