

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 10cu\_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: 10cu\_0m

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Bond precision:	C-C = 0.0079 Å	Wavelength=0.71073
Cell:	a=27.190 (5)      b=29.265 (6)      c=20.527 (4)	
	alpha=90      beta=112.081 (8)      gamma=90	
Temperature:	150 K	
	Calculated	Reported
Volume	15136 (5)	15136 (5)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C62 H50 Cu2 N2 O10 [+ solvent]	C62 H50 Cu2 N2 O10
Sum formula	C62 H50 Cu2 N2 O10 [+ solvent]	C62 H50 Cu2 N2 O10
Mr	1110.14	1110.12
Dx, g cm <sup>-3</sup>	0.974	0.974
Z	8	8
Mu (mm <sup>-1</sup> )	0.606	0.606
F000	4592.0	4592.0
F000'	4598.98	
h, k, lmax	32, 34, 24	32, 34, 24
Nref	13003	12917
Tmin, Tmax	0.702, 0.941	0.627, 0.745
Tmin'	0.648	

Correction method= # Reported T Limits: Tmin=0.627 Tmax=0.745

AbsCorr = MULTI-SCAN

Data completeness= 0.993

Theta(max)= 24.778

R(reflections)= 0.0751( 9234)

wR2(reflections)=  
0.2492( 12917)

S = 1.049

Npar= 598

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

PLAT934\_ALERT\_3\_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check

### Alert level C

THETM01\_ALERT\_3\_C The value of sine(theta\_max)/wavelength is less than 0.590

Calculated sin(theta\_max)/wavelength = 0.5897

PLAT218\_ALERT\_3\_C Constrained U(ij) Components(s) for N1S . 6 Check  
PLAT218\_ALERT\_3\_C Constrained U(ij) Components(s) for C1S . 6 Check  
PLAT218\_ALERT\_3\_C Constrained U(ij) Components(s) for C2S . 6 Check  
PLAT218\_ALERT\_3\_C Constrained U(ij) Components(s) for C3S . 6 Check  
PLAT218\_ALERT\_3\_C Constrained U(ij) Components(s) for C4S . 6 Check  
PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio  
PLAT222\_ALERT\_3\_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.3 Ratio  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of O2S Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Cu1 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Cu2 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of N1S Check  
PLAT341\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00789 Ang.  
PLAT412\_ALERT\_2\_C Short Intra XH3 .. XHn H2SA ..H4SB . 1.81 Ang.  
x,y,z = 1\_555 Check  
PLAT741\_ALERT\_1\_C Bond Calc 1.2453(3), Rep 1.24550 ..... Missing s.u.  
N1S -C1S 1\_555 1\_555 ..... # 29 Check  
PLAT741\_ALERT\_1\_C Bond Calc 1.5038(3), Rep 1.50460 ..... Missing s.u.  
N1S -C3S 1\_555 1\_555 ..... # 30 Check  
PLAT741\_ALERT\_1\_C Bond Calc 1.4429(3), Rep 1.44520 ..... Missing s.u.  
N1S -C4S 1\_555 1\_555 ..... # 31 Check  
PLAT741\_ALERT\_1\_C Bond Calc 1.5258(3), Rep 1.52510 ..... Missing s.u.  
C1S -C2S 1\_555 1\_555 ..... # 37 Check  
PLAT742\_ALERT\_1\_C Angle Calc 115.26(1), Rep 115.40 ..... Missing s.u.  
C1S -N1S -C3S 1\_555 1\_555 1\_555 # 41 Check  
PLAT742\_ALERT\_1\_C Angle Calc 127.55(1), Rep 127.50 ..... Missing s.u.  
C1S -N1S -C4S 1\_555 1\_555 1\_555 # 42 Check  
PLAT742\_ALERT\_1\_C Angle Calc 115.02(1), Rep 115.00 ..... Missing s.u.  
C4S -N1S -C3S 1\_555 1\_555 1\_555 # 43 Check  
PLAT742\_ALERT\_1\_C Angle Calc 110.64(1), Rep 110.60 ..... Missing s.u.  
N1S -C1S -C2S 1\_555 1\_555 1\_555 # 54 Check  
PLAT743\_ALERT\_1\_C Torsion Calc -179.72(1), Rep -179.70 ..... Missing s.u.  
C3S -N1S -C1S -C2S 1\_555 1\_555 1\_555 1\_555 # 32 Check  
PLAT743\_ALERT\_1\_C Torsion Calc -17.43(1), Rep -17.40 ..... Missing s.u.  
C4S -N1S -C1S -C2S 1\_555 1\_555 1\_555 1\_555 # 36 Check  
PLAT767\_ALERT\_4\_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check  
PLAT905\_ALERT\_3\_C Negative K value in the Analysis of Variance ... -0.748 Report  
PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min). 8 Note  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.590 75 Report  
PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 1.08Ang From C3S 1.86 eA-3

PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.23Ang From C4S	-1.60 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H4SC	-0.40 eA-3

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### ● Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..	0.70	mm
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.15	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	37.77	Why ?
PLAT169_ALERT_4_G	The CIF-Embedded .res File Contains AFIX 1 Recds	29	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	3	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C6SA Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6SB Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8SA Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8SB Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6SA Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6SB Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6SC Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6SD Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6SE Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6SF Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8SA Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8SB Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8SC Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8SD Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8SE Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8SF Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	3%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H7SB ..H8SF .	1.97	Ang.
	x,y,z =	1_555	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure .....	!	Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	28	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II) .	2.16	Info
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed	!	Info
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	42%	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	10	Note
PLAT953_ALERT_1_G	Reported (CIF) and Actual (FCF) Hmax Differ by .	1	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
1 **ALERT level B** = A potentially serious problem, consider carefully  
31 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
33 **ALERT level G** = General information/check it is not something unexpected
- 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
14 ALERT type 2 Indicator that the structure model may be wrong or deficient  
15 ALERT type 3 Indicator that the structure quality may be low  
23 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.

Datablock 10cu\_0m - ellipsoid plot

