

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CuLphen\_0ma

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: CuLphen\_0ma

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Bond precision:	C-C = 0.0038 A	Wavelength=0.71073	
Cell:	a=25.1157(11)	b=11.2432(4)	c=15.2228(5)
	alpha=90	beta=94.727(3)	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	4284.0(3)	4284.0(3)	
Space group	C 2/c	C2/c	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C25 H18 Cu N4 O2	C25 H18 Cu N4 O2	
Sum formula	C25 H18 Cu N4 O2	C25 H18 Cu N4 O2	
Mr	469.98	469.97	
Dx,g cm-3	1.457	1.457	
Z	8	8	
Mu (mm-1)	1.050	1.050	
F000	1928.0	1928.0	
F000'	1931.15		
h,k,lmax	32,14,19	32,14,19	
Nref	4687	4620	
Tmin,Tmax	0.748,0.811	0.661,0.746	
Tmin'	0.737		

Correction method= # Reported T Limits: Tmin=0.661 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.986      Theta(max)= 27.000

R(reflections)= 0.0292( 3839)      wR2(reflections)= 0.0882( 4620)

S = 0.927      Npar= 290

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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

PLAT220_ALERT_2_C	Large Non-Solvent C	Ueq(max)/Ueq(min) Range	3.3	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C16 -- C17 ..	5.7	su
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for .....	C16	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for .....	C18	Check
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .		58	Ang3

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### ● Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details	in the CIF		Please Do !
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1	(II) .....	2.41	Note
PLAT899_ALERT_4_G	SHELXL97	is Deprecated and Succeeded by SHELXL		2014 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  
5 **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
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
5 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
1 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*, 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.

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