

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_20220621_zh_wx_tlc_top_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_20220621_zh_wx_tlc_top_0m

Bond precision:	C-C = 0.0022 A	Wavelength=1.54178	
Cell:	a=8.6768 (2)	b=14.2601 (3)	c=20.0588 (4)
	alpha=90	beta=92.113 (1)	gamma=90
Temperature:	193 K		
	Calculated	Reported	
Volume	2480.23 (9)	2480.23 (9)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C26 H32 N2 O6	C26 H32 N2 O6	
Sum formula	C26 H32 N2 O6	C26 H32 N2 O6	
Mr	468.54	468.53	
Dx, g cm ⁻³	1.255	1.255	
Z	4	4	
Mu (mm ⁻¹)	0.730	0.730	
F000	1000.0	1000.0	
F000'	1003.17		
h, k, lmax	10, 17, 24	10, 17, 24	
Nref	4544	4540	
Tmin, Tmax	0.892, 0.916	0.380, 0.467	
Tmin'	0.890		

Correction method= # Reported T Limits: Tmin=0.380 Tmax=0.467
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 68.299

R(reflections)= 0.0414 (3828)	wR2(reflections)= 0.1100 (4540)
S = 1.029	Npar= 312

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

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	0.66 eA-3
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C1 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2 Report

● Alert level G

PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C21 Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O4 .	107.5 Degree
PLAT432_ALERT_2_G	Short Inter X...Y Contact O1 ..C19 .	3.01 Ang.
	1+x,y,z =	1_655 Check
PLAT793_ALERT_4_G	Model has Chirality at C12 (Centro SPGR)	S Verify
PLAT793_ALERT_4_G	Model has Chirality at C16 (Centro SPGR)	R Verify
PLAT793_ALERT_4_G	Model has Chirality at C17 (Centro SPGR)	S Verify
PLAT793_ALERT_4_G	Model has Chirality at C19 (Centro SPGR)	R Verify
PLAT793_ALERT_4_G	Model has Chirality at C22 (Centro SPGR)	S Verify
PLAT793_ALERT_4_G	Model has Chirality at C23 (Centro SPGR)	R Verify
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	3 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	9 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	3 Check

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
8 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

