

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_20220424_ny_phdwg_1_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_20220424_ny_phdwg_1_0m

Bond precision: C-C = 0.0052 Å Wavelength=1.54178

Cell: a=11.3411(2) b=12.2038(3) c=15.3609(3)
 alpha=108.401(1) beta=98.498(1) gamma=108.462(1)
Temperature: 193 K

	Calculated	Reported
Volume	1839.58(7)	1839.58(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C50 H32, C H2 Cl2	C H2 Cl2, C50 H32
Sum formula	C51 H34 Cl2	C51 H34 Cl2
Mr	717.68	717.68
Dx, g cm ⁻³	1.296	1.296
Z	2	2
Mu (mm ⁻¹)	1.858	1.858
F000	748.0	748.0
F000'	751.23	
h, k, lmax	13, 14, 18	13, 14, 18
Nref	6764	6722
Tmin, Tmax	0.748, 0.800	0.377, 0.467
Tmin'	0.729	

Correction method= # Reported T Limits: Tmin=0.377 Tmax=0.467
AbsCorr = MULTI-SCAN

Data completeness= 0.994 Theta(max)= 68.402

R(reflections)= 0.0821(5077)	wR2(reflections)=
S = 1.079	0.2445(6722)
Npar= 478	

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	1.42 eA-3
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C51 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C11 0.221 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0052 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.138 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600 25 Report

Alert level G

PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ	Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.12 Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001 Degree
PLAT793_ALERT_4_G	Model has Chirality at C7 (Centro SPGR)	S Verify
PLAT793_ALERT_4_G	Model has Chirality at C20 (Centro SPGR)	S Verify
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600 17 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	9 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.1 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info

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

- 4 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
4 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

