



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_20230927_DZKD_ZHY_0m_a

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_20230927_DZKD_ZHY_0m_a

Bond precision:	C-C = 0.0050 Å	Wavelength=1.54178	
Cell:	a=36.234 (3)	b=8.6361 (7)	c=36.862 (3)
	alpha=90	beta=117.064 (5)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	10271.8 (15)	10271.7 (16)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	4 (C59 H41 N5), 4 (C6 H14), H2 Cl2 [+ solvent]	C 2 (C59 H41 N5), 2 (C6 H14), 0.5 (C H2 Cl2)	
Sum formula	C261 H222 Cl2 N20 [+ solvent]	C130.5 H111 Cl1 N10	
Mr	3709.49	1854.85	
Dx, g cm-3	1.199	1.199	
Z	2	4	
Mu (mm-1)	0.770	0.770	
F000	3924.0	3936.9	
F000'	3935.50		
h, k, lmax	43, 10, 44	43, 10, 43	
Nref	18389	18110	
Tmin, Tmax	0.955, 0.962	0.633, 0.753	
Tmin'	0.857		

Correction method= # Reported T Limits: Tmin=0.633 Tmax=0.753

AbsCorr = NONE

Data completeness= 0.985

Theta(max)= 67.140

R(reflections)= 0.0815(11664)

wR2(reflections)=
0.2148(18110)

S = 0.985

Npar= 1461

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

PLAT260_ALERT_2_C Large Average Ueq of Residue Including C11_9 0.143 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C11_10 0.171 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00498 Ang.
PLAT722_ALERT_1_C Angle Calc 111(7), Rep 109.50 Dev... 1.50 Degree
H6C_8 -C6_8 -H6A_8 1_555 1_555 1_555 # 538 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 5.346 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.022 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.598 274 Report
11 8 0, 12 8 0, 28 6 0, 36 0 0, -39 0 1, -35 0 1,
-34 5 1, -11 8 1, -10 9 1, -9 10 1, 9 10 1, 35 4 1,
-36 0 2, -29 7 2, -13 8 2, -12 8 2, -11 8 2, -10 9 2,
-10 10 2, -2 0 2, 0 0 2, 8 10 2, 29 6 2, -39 2 3,
-38 3 3, -35 0 3, -20 9 3, -10 9 3, -10 10 3, 34 4 3,
(244 More NOT listed: see .ckf listing file)



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 40 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 22 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula Strings Differ Please Check
Calc: C261 H222 Cl2 N20
Rep.: C130.5 H111 Cl1 N10
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: 4(C59 H41 N5), 4(C6 H14), C H2 Cl2
Rep.: 2(C59 H41 N5), 2(C6 H14), 0.5(C H2 Cl2)
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT073_ALERT_1_G H-atoms ref., but hydrogen treatment Reported as constr Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 17.36 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 13% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7) 100% Note

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PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 4) 10.54 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 5) 9.46 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 6) 1.65 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 7) 0.85 Check
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C9_2 -C14_2 . 1.44 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C9_1 -C14_1 . 1.44 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact N2_2 ..C1_9 . 2.98 Ang.
                                     x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C25_1 ..C34A_2 . 3.19 Ang.
                                     x,y,z = 1_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 70 A**3
PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data 4 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 15.30 Deg.
                C23A_-C19_2-C23_2 1_555 1_555 1_555 ..... # 265 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1467 Note
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 37% Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 2.32 Note
                -1 0 1,
PLAT948_ALERT_5_G Externally Supplied Scattering Factors CIF 4 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 4.472 Note
                Predicted wR2: Based on SigI**2 4.80 or SHELX Weight 21.80 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info
PLAT983_ALERT_1_G The Cl-f"= 0.7036 Deviates from IT-Value = 0.7018 Check
PLAT992_ALERT_5_G Repld & Actual _reflns_number_gt Values Differ by -12 Check

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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
7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
37 ALERT level G = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
17 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

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# start Validation Reply Form
_vrf_PLAT260_cu_20230927_DZKD_ZHY_0m_a
;
PROBLEM: Large Average Ueq of Residue Including C11_9 0.143 Check
RESPONSE: ...
;
_vrf_PLAT340_cu_20230927_DZKD_ZHY_0m_a
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.00498 Ang.
RESPONSE: ...
;
_vrf_PLAT722_cu_20230927_DZKD_ZHY_0m_a
;
PROBLEM: Angle Calc 111(7), Rep 109.50 Dev... 1.50 Degree

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RESPONSE: ...
;
_vrf_PLAT906_cu_20230927_DZKD_ZHY_0m_a
;
PROBLEM: Large K Value in the Analysis of Variance ..... 5.346 Check
RESPONSE: ...
;
_vrf_PLAT911_cu_20230927_DZKD_ZHY_0m_a
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.598 274 Report
RESPONSE: ...
;
# end Validation Reply Form
```

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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 23/04/2026; check.def file version of 30/03/2026

