



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: exp_807_auto

Bond precision:	C-C = 0.0061 Å		Wavelength=1.54184
Cell:	a=8.6582 (1)	b=24.7519 (3)	c=11.8844 (1)
	alpha=90	beta=91.136 (1)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2546.41 (5)	2546.41 (5)	
Space group	P 21	P 1 21 1	
Hall group	P 2yb	P 2yb	
Moiety formula	Cu ₈ N ₅₄ , 2 (C ₈ H ₂₀ N)	Cu ₈ N ₅₄ , 2 (C ₈ H ₂₀ N)	
Sum formula	C ₁₆ H ₄₀ Cu ₈ N ₅₆	C ₁₆ H ₄₀ Cu ₈ N ₅₆	
Mr	1525.44	1525.36	
Dx, g cm ⁻³	1.990	1.989	
Z	2	2	
Mu (mm ⁻¹)	4.313	4.313	
F000	1520.0	1520.0	
F000'	1491.81		
h, k, lmax	10, 31, 15	10, 30, 14	
Nref	10781 [5518]	8122	
Tmin, Tmax	0.856, 0.958	0.398, 1.000	
Tmin'	0.842		

Correction method= # Reported T Limits: Tmin=0.398 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.47/0.75

Theta(max)= 77.240

R(reflections)= 0.0253(8098)

wR2(reflections)=
0.0675(8122)

S = 1.067

Npar= 730

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

STRVA01_ALERT_4_C Flack test results are ambiguous.
 From the CIF: _refine_ls_abs_structure_Flack 0.420
 From the CIF: _refine_ls_abs_structure_Flack_su 0.020
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 7.56 Note
PLAT213_ALERT_2_C Atom N162 has ADP max/min Ratio 3.1 oblate
PLAT213_ALERT_2_C Atom N201 has ADP max/min Ratio 3.5 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00612 Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 1 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF Please Check
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * Sigma from Zero . 0.420 Note
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00010 Ang.
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (I) . 1.16 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2 (II) . 2.16 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu3 (I) . 1.18 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu4 (I) . 1.19 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu5 (I) . 1.17 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu6 (II) . 2.13 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu7 (I) . 1.16 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu8 (I) . 1.16 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 7 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
9 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 20/06/2026; check.def file version of 19/06/2026

duplicate check

No duplication found

Datablock exp_807_auto - ellipsoid plot

