

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu_240116lu_lgpz130644_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_240116lu_lgpz130644_0m

Bond precision: C-C = 0.0027 Å Wavelength=1.54178

Cell: a=10.5994 (2) b=9.7322 (2) c=19.1707 (4)
 alpha=90 beta=93.164 (1) gamma=90

Temperature: 193 K

	Calculated	Reported
Volume	1974.55 (7)	1974.55 (7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C24 H12, 0.5 (C12 H2 F2 N4)	C12 H2 F2 N4, 2 (C24 H12)
Sum formula	C30 H13 F N2	C60 H26 F2 N4
Mr	420.42	840.85
Dx, g cm ⁻³	1.414	1.414
Z	4	2
Mu (mm ⁻¹)	0.719	0.719
F000	864.0	864.0
F000'	866.57	
h, k, lmax	13, 12, 24	13, 12, 24
Nref	4325	4013
Tmin, Tmax	0.917, 0.937	0.656, 0.754
Tmin'	0.917	

Correction method= # Reported T Limits: Tmin=0.656 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.928 Theta (max)= 79.954

R(reflections)= 0.0652 (3187)	wR2(reflections)=
S = 1.080	0.1911 (4013)
Npar= 525	

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 B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 7.64 Note

Author Response: Structural disorder of the sample lead to the poor data / parameter ratio.



Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C24 H12, 0.5(C12 H2 F2 N4)
Rep.: C12 H2 F2 N4, 2(C24 H12)

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.18 Report

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.1 Note

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.620 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.376 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 35 Report

2 0 0, 3 1 0, 6 1 0, 6 2 0, -11 2 1, -3 0 1,
3 0 1, 3 1 1, 5 1 1, 6 1 1, 6 2 1, -10 0 2,
5 1 2, 6 2 2, -12 0 4, -12 3 5, 8 6 5, -12 0 6,
-12 1 6, -12 1 7, -12 2 7, -9 0 7, -2 11 7, -12 0 8,
-12 1 8, -8 0 8, -6 1 8, -9 0 9, -5 3 20, -5 0 21,
-5 1 21, -5 2 21, -4 3 21, -4 0 22, -4 1 22,

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 4 Note

3 1 0, -3 0 1, 3 0 1, 3 1 1,



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 48 Note

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 48 Report

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2 Check

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report

PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 1 Report

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report

PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT230_ALERT_2_G Hirshfeld Test Diff for C14A --C15A . 10.7 s.u.

PLAT230_ALERT_2_G Hirshfeld Test Diff for C17A --C18A . 8.3 s.u.

PLAT230_ALERT_2_G Hirshfeld Test Diff for C29A --C30A . 5.2 s.u.

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 100% Note

PLAT301_ALERT_3_G Main Residue Disorder(Resd 2) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 11% Note

PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 1) 23.26 Check

PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 12.74 Check

PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C7A -C12A . 1.42 Ang.

PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C7 -C16 0.20 Ang.

PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints 996 Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 276 Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.8 Low

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 5.41 Note

Predicted wR2: Based on SigI**2 3.53 or SHELX Weight 18.98
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 15 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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

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

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.

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