

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: 2

Bond precision:	C-C = 0.0129 Å	Wavelength=0.71073
Cell:	a=11.172(2)	b=15.205(3) c=15.890(3)
	alpha=78.94(3)	beta=85.98(3) gamma=70.21(3)
Temperature:	113 K	
	Calculated	Reported
Volume	2492.6(10)	2492.6(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C37 H23 Cu2 F24 N4 O10 [+ solvent]	C37 H23 Cu2 F24 N4 O10
Sum formula	C37 H23 Cu2 F24 N4 O10 [+ solvent]	C37 H23 Cu2 F24 N4 O10
Mr	1266.70	1266.67
Dx, g cm ⁻³	1.688	1.688
Z	2	2
Mu (mm ⁻¹)	0.998	0.998
F000	1254.0	1254.0
F000'	1256.41	
h,k,lmax	13,18,18	13,18,18
Nref	8789	8784
Tmin,Tmax	0.705,0.819	0.758,1.000
Tmin'	0.601	

Correction method= # Reported T Limits: Tmin=0.758 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.009

R(reflections)= 0.0927(6655) wR2(reflections)= 0.2363(8784)

S = 1.007 Npar= 701

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as Multi-scan

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 3.14 Report

PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 2.62 eA-3

PLAT213_ALERT_2_C Atom F11 has ADP max/min Ratio 3.1 oblate

PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.0 Ratio

PLAT220_ALERT_2_C Non-Solvent Resd 1 F Ueq(max)/Ueq(min) Range 3.3 Ratio

PLAT230_ALERT_2_C Hirshfeld Test Diff for F9 --C27 . 5.5 s.u.

PLAT230_ALERT_2_C Hirshfeld Test Diff for F10 --C24 . 5.5 s.u.

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu1 --O10 . 5.7 s.u.

PLAT234_ALERT_4_C Large Hirshfeld Difference F7 --C27 . 0.17 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference F11 --C24 . 0.23 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference F12 --C24 . 0.22 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference F13 --C32 . 0.19 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference F14 --C32 . 0.17 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference F17 --C29 . 0.19 Ang.

PLAT234_ALERT_4_C Large Hirshfeld Difference O7 --C31 . 0.18 Ang.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 02 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 07 Check

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.01287 Ang.



Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 61 Report

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 46.00 Why ?

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree

PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 5 Report

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 4 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report

PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C19 Check

PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C22 Check

PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C24 Check

PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C27 Check

PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C29 Check

PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C32 Check

PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C34 Check

PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C37 Check

PLAT343_ALERT_2_G Unusual sp3 Angle Range in Main Residue for C24 Check

PLAT434_ALERT_2_G Short Inter HL..HL Contact F1 ..F20 2.73 Ang.

-1+x,1+y,-1+z = 1_464 Check

PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 184 A**3

PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.18 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Cu2 (II) . 2.21 Info

PLAT794_ALERT_5_G Tentative Bond Valency for Cu3 (II) . 2.26 Info

PLAT860_ALERT_3_G Number of Least-Squares Restraints 641 Note

PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info

0 ALERT level A = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully
20 **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

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

