

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: Compound2

Bond precision: C-C = 0.0032 A Wavelength=0.71069

Cell: a=14.0661(18) b=6.9184(12) c=24.300(2)
 alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2364.8(5)	2364.7(6)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C22 H22 Cu N8 O6	?
Sum formula	C22 H22 Cu N8 O6	C22 H22 Cu N8 O6
Mr	558.03	558.01
Dx,g cm-3	1.567	1.567
Z	4	4
Mu (mm-1)	0.981	0.981
F000	1148.0	1148.0
F000'	1149.71	
h,k,lmax	17,8,30	17,8,30
Nref	2440	2435
Tmin,Tmax	0.855,0.907	0.456,0.746
Tmin'	0.855	

Correction method= # Reported T Limits: Tmin=0.456 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 0.998 Theta(max)= 26.430

R(reflections)= 0.0335(1850) wR2(reflections)= 0.0806(2435)

S = 1.032 Npar= 169

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

PLAT213_ALERT_2_C	Atom C7	has ADP max/min Ratio	3.4	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 1	C Ueq(max)/Ueq(min) Range		3.3	Ratio

● Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		4	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1	-- O1W	..	6.7	s.u.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		4	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1	(II)	2.17	Note

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

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

