

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SH5

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: SH5

Bond precision: C-C = 0.0029 Å Wavelength=1.54184

Cell: a=8.9894 (2) b=11.4187 (3) c=26.2615 (7)
 alpha=90 beta=99.8189 (19) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	2656.18 (12)	2656.18 (12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ycb
Moiety formula	C22 H30 Cu2 N5 O7, N O3	C22 H30 Cu2 N5 O7, N O3
Sum formula	C22 H30 Cu2 N6 O10	C22 H30 Cu2 N6 O10
Mr	665.62	665.60
Dx, g cm ⁻³	1.664	1.664
Z	4	4
Mu (mm ⁻¹)	2.562	2.559
F000	1368.0	1368.0
F000'	1356.27	
h, k, lmax	10, 13, 31	10, 13, 31
Nref	4785	4764
Tmin, Tmax	0.501, 0.802	0.502, 0.826
Tmin'	0.249	

Correction method= # Reported T Limits: Tmin=0.502 Tmax=0.826
AbsCorr = ANALYTICAL

Data completeness= 0.996 Theta(max)= 67.340

R(reflections)= 0.0271 (4340)	wR2(reflections)=
S = 1.470	0.0821 (4764)
Npar= 386	

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

PLAT127_ALERT_1_C	Implicit Hall Symbol Inconsistent with Explicit	-P 2ycb
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.599	22 Report



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1A --N2A .	6.4 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1B --N1B .	5.3 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cu1B --N2B .	5.3 s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100% Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	30 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1A (II) .	2.21 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1B (II) .	2.21 Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	2 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	15 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	91% Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	1 Check
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0 Sig(I)
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	8 Info

- 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
16 **ALERT level G** = General information/check it is not something unexpected

- 2 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
4 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
4 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. 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.

