

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0054 Å Wavelength=0.71073

Cell: a=17.421(7) b=15.653(6) c=23.368(9)
 alpha=90 beta=105.588(5) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	6138(4)	6138(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C56 H56 Cu4 I4 N16	C56 H56 Cu4 I4 N16
Sum formula	C56 H56 Cu4 I4 N16	C56 H56 Cu4 I4 N16
Mr	1714.97	1714.92
Dx,g cm-3	1.856	1.856
Z	4	4
Mu (mm-1)	3.430	3.430
F000	3328.0	3328.0
F000'	3326.29	
h,k,lmax	23,21,31	23,21,31
Nref	15640	15604
Tmin,Tmax	0.669,0.872	0.628,0.746
Tmin'	0.656	

Correction method= # Reported T Limits: Tmin=0.628 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 0.998 Theta(max)= 28.553

R(reflections)= 0.0313(9748) wR2(reflections)= 0.0715(15604)

S = 1.005 Npar= 721

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

PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C4	Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1	Note
	C56 H56 Cu4 I4 N16		
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-0.607	Report
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	2	Report



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.23	Why ?
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	36	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density	2	Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **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
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

PLATON version of 11/08/2016; check.def file version of 04/08/2016

Datablock shelx - ellipsoid plot

