

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: I

Bond precision: C-C = 0.0037 Å

Wavelength=0.71073

Cell: a=8.8156(4) b=11.0165(6) c=13.0297(7)
 alpha=72.853(3) beta=83.183(3) gamma=89.275(3)
Temperature: 296 K

	Calculated	Reported
Volume	1200.28(11)	1200.28(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C56 H40 Cl4 Cu2 N4 O8	C56 H40 Cl4 Cu2 N4 O8
Sum formula	C56 H40 Cl4 Cu2 N4 O8	C56 H40 Cl4 Cu2 N4 O8
Mr	1165.82	1165.80
Dx, g cm-3	1.613	1.613
Z	1	1
Mu (mm-1)	1.173	1.173
F000	594.0	594.0
F000'	595.44	
h, k, lmax	11, 14, 16	11, 14, 16
Nref	5245	5187
Tmin, Tmax	0.678, 0.773	0.690, 0.780
Tmin'	0.664	

Correction method= # Reported T Limits: Tmin=0.690 Tmax=0.780
AbsCorr = MULTI-SCAN

Data completeness= 0.989

Theta(max)= 27.000

R(reflections)= 0.0373(4179)

wR2(reflections)= 0.0945(5187)

S = 1.017

Npar= 334

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 G

PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 24/11/2016; check.def file version of 23/11/2016

