

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ras1307

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: ras1307

Bond precision: C-C = 0.0052 Å Wavelength=0.71073

Cell: a=17.3344(3) b=17.3344(3) c=12.7924(2)
 alpha=90 beta=90 gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	3843.88(15)	3843.88(11)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C20 H28 Br10 Cu4 N8 O	C20 H28 Br10 Cu4 N8 O
Sum formula	C20 H28 Br10 Cu4 N8 O	C20 H28 Br10 Cu4 N8 O
Mr	1449.70	1449.72
Dx, g cm ⁻³	2.505	2.505
Z	4	4
Mu (mm ⁻¹)	12.608	12.608
F000	2712.0	2712.0
F000'	2707.89	
h, k, lmax	24, 24, 18	17, 24, 17
Nref	2823	2819
Tmin, Tmax	0.025, 0.091	0.055, 0.179
Tmin'	0.013	

Correction method= # Reported T Limits: Tmin=0.055 Tmax=0.179
AbsCorr = INTEGRATION

Data completeness= 0.999 Theta(max)= 30.032

R(reflections)= 0.0349(2335) wR2(reflections)= 0.0868(2819)

S = 0.989 Npar= 99

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 A

PLAT902_ALERT_1_A No (Interpretable) Reflections found in FCF Please Check

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.128

Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	20.94 Why ?
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	4 Units
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.21 Ratio

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 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*, 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 19/11/2015; check.def file version of 17/11/2015

Datablock ras1307 - ellipsoid plot

