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: 2020_07_21_dt_btmacubr2hbr-2to_n

Bond precision: C-C = 0.0067 A Wavelength=1.54184

Cell: a=9.1205(2) b=9.6086(3) c=28.8970(7)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2532.40(11)	2532.38(11)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	2(C10 H16 N), Br4 Cu	2(C10 H16 N), Br4 Cu
Sum formula	C20 H32 Br4 Cu N2	C20 H32 Br4 Cu N2
Mr	683.63	683.65
Dx,g cm-3	1.793	1.793
Z	4	4
Mu (mm-1)	8.661	8.661
F000	1340.0	1340.0
F000'	1322.95	
h,k,lmax	10,11,34	10,11,34
Nref	4524[2599]	4524
Tmin,Tmax	0.103,0.595	0.117,0.619
Tmin'	0.023	

Correction method= # Reported T Limits: Tmin=0.117 Tmax=0.619
AbsCorr = ANALYTICAL

Data completeness= 1.74/1.00 Theta(max)= 67.069

R(reflections)= 0.0226(4444) wR2(reflections)= 0.0567(4524)

S = 1.049 Npar= 250

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

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00671 Ang.

Alert level G

PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 10 Note
H7AA H7AB H9AA H9AB H9AC H7BA H7BB H9BA
H9BB H9BC
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.5 Low

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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
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

1 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
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

Datablock 2020_07_21_dt_btmacubr2hbr-2to_n - ellipsoid plot

