checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: tm10

Bond precision: C-C = 0.0047 A Wavelength=0.71073

Cell: **a=10.6287(2) b=17.3801(5) c=10.9153(3)**
alpha=90 beta=113.0391(11) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1855.53(8)	1855.53(8)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H20 Br N O	C22 H20 Br1 N1 O1
Sum formula	C22 H20 Br N O	C22 H20 Br N O
Mr	394.29	394.30
Dx,g cm-3	1.411	1.411
Z	4	4
Mu (mm-1)	2.224	2.224
F000	808.0	808.0
F000'	807.13	
h,k,lmax	13,22,14	13,22,14
Nref	4259	4186
Tmin,Tmax	0.766,0.935	0.757,0.831
Tmin'	0.641	

Correction method= MULTI-SCAN

Data completeness= 0.983 Theta(max)= 27.480

R(reflections)= 0.0479(2497) wR2(reflections)= 0.1090(4186)

S = 1.023 Npar= 254

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

PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uso(min) ... 4.64 Ratio
PLAT245_ALERT_2_C U(iso) H2A Smaller than U(eq) C2 by ... 0.01 AngSq
PLAT391_ALERT_3_C Deviating Methyl C22 H-C-H Bond Angle ..... 101.00 Deg.

Alert level G

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PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......      P21/n
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.          6
PLAT199_ALERT_1_G Check the Reported _cell_measurement_temperature        293 K
PLAT200_ALERT_1_G Check the Reported   _diffrn_ambient_temperature        293 K
PLAT793_ALERT_4_G The Model has Chirality at C3      (Verify) ....          R
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   0 ALERT level A = In general: serious problem
   0 ALERT level B = Potentially serious problem
   3 ALERT level C = Check and explain
   5 ALERT level G = General alerts; check

   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
   2 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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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 22/10/2010; check.def file version of 11/10/2010

Datablock tm10 - ellipsoid plot