checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: 11

Bond precision: C-C = 0.0070 A   Wavelength=0.71073

Cell: a=9.720(2)   b=15.939(3)   c=11.457(2)
                   alpha=90   beta=94.909(4)   gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1768.5(6)	1768.7(6)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C24 H22 N4, 2(C8 H7 Br O2)	C24 H22 N4, 2(C8 H7 Br O2)
Sum formula	C40 H36 Br2 N4 O4	C40 H36 Br2 N4 O4
Mr	796.53	796.55
Dx,g cm-3	1.496	1.496
Z	2	2
Mu (mm-1)	2.340	2.340
F000	812.0	812.0
F000'	811.16	
h,k,lmax	11,18,13	11,18,13
Nref	3125	3120
Tmin,Tmax	0.663,0.704	0.649,0.701
Tmin'	0.620	

Correction method= MULTI-SCAN

Data completeness= 0.998   Theta(max)= 25.010

R(reflections)= 0.0666(2014)   wR2(reflections)= 0.1783(3120)

S = 1.076   Npar= 228

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
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.29
PLAT230_ALERT_2_C Hirshfeld Test Diff for   C3   -- C4   ..   6.3 su
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.0070 Ang

Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF         ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms ............         1
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......      P21/n
PLAT194_ALERT_1_G Missing _cell_measurement_reflns_used datum ....         ?
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....         ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....         ?
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 C6       (Verify) ....        R
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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
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   2 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*, 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 05/11/2012; check.def file version of 05/11/2012