checkCIF/PLATON report

Structure factors have been supplied for datablock(s) vdj_917_teply_uochb_sqd

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: vdj_917_teply_uochb_sqd

```
Bond precision:  C-C = 0.0046 A          Wavelength=0.71073

Cell:            a=45.657(4)     b=12.2162(12)       c=7.4051(6)
                 alpha=90        beta=93.046(3)      gamma=90
Temperature:     150 K
```

	Calculated	Reported
Volume	4124.4(6)	4124.4(7)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C42 H42 N2 O4, 2(Br)	C42 H42 N2 O4, 2(Br)
Sum formula	C42 H42 Br2 N2 O4	C42 H42 Br2 N2 O4
Mr	798.58	798.60
Dx,g cm-3	1.286	1.286
Z	4	4
Mu (mm-1)	2.005	2.005
F000	1640.0	1640.0
F000’	1638.33	
h,k,lmax	56,15,9	56,15,9
Nref	4056	4050
Tmin,Tmax	0.655,0.887	0.515,0.896
Tmin’	0.462	

```
Correction method= # Reported T Limits: Tmin=0.515 Tmax=0.896
AbsCorr = NUMERICAL

Data completeness= 0.999          Theta(max)= 26.000

R(reflections)= 0.0478( 2859)     wR2(reflections)= 0.1159( 4050)

S = 1.010                 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 ....       2.21 Report
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      7.738 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600          4 Report
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .        171 A**3
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          1 Report
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
```

```
   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
   6 ALERT level G = General information/check it is not something unexpected

   0 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
   3 ALERT type 3 Indicator that the structure quality may be low
   3 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 21/06/2015; check.def file version of 21/06/2015

Datablock vdj_917_teply_uochb_sqd - ellipsoid plot