checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C__Crystal_Vrac_79_3_ZnBrN3H8

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: C__Crystal_Vrac_79_3_ZnBrN3H8

```
Bond precision:  Zn- N = 0.0220 A        Wavelength=0.71073

Cell:            a=7.6055(4)    b=5.9772(4)        c=12.5722(8)
                 alpha=90       beta=93.475(4)     gamma=90
Temperature:     298 K
```

	Calculated	Reported
Volume	570.48(6)	570.48(6)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	H16 N6 Zn2, 2(Br)	?
Sum formula	Br2 H16 N6 Zn2	B2R H16 N6 Zn2
Mr	390.77	390.77
Dx,g cm-3	2.275	2.275
Z	2	2
Mu (mm-1)	11.165	11.165
F000	376.0	376.0
F000’	376.22	
h,k,lmax	9,7,16	9,7,16
Nref	1312	1298
Tmin,Tmax		
Tmin’		

```
Correction method= Not given

Data completeness= 0.989          Theta(max)= 27.491

R(reflections)= 0.0344( 1085)     wR2(reflections)= 0.0864( 1298)

S = 1.047                 Npar= 71
```

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

```
EXPT005_ALERT_1_A  _exptl_crystal_description is missing
            Crystal habit description.
            The following tests will not be performed.
            CRYSR_01
DIFF003_ALERT_1_A  _diffrn_measurement_device_type is missing
            Diffractometer make and type. Replaces _diffrn_measurement_type.
ABSMU01_ALERT_1_A  The ratio of given/expected absorption coefficient lies
               outside the range 0.90 <> 1.10
            Calculated value of mu =     4.158
            Value of mu given      =    11.165
CHEMW01_ALERT_1_A  The ratio of given/expected molecular weight as calculated
            from the _chemical_formula_sum lies outside
            the range 0.90 <> 1.10
            Calculated formula weight =   252.5466
            Formula weight given      =   390.7700
SHFSU01_ALERT_2_A  The absolute value of parameter shift to su ratio > 0.20
            Absolute value of the parameter shift to su ratio given   1.140
            Additional refinement cycles may be required.
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .      0.573 Note
PLAT080_ALERT_2_A Maximum Shift/Error ............................       1.14 Why ?
PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used value ....     Please Do !
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min value ......     Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max value ......     Please Do !
PLAT211_ALERT_2_A ADP of Atom N2      is N.P.D. or (nearly) 2D ...     Please Check
```

Alert level B

```
PLAT031_ALERT_4_B Refined Extinction Parameter within Range ......      1.923 Sigma
PLAT911_ALERT_3_B Missing # FCF Refl Between THmin & STh/L=  0.600        440 Report
```

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT213_ALERT_2_C Atom N1              has ADP max/min Ratio .....        3.3 prolat
PLAT420_ALERT_2_C D-H Without Acceptor       N3     --  H3B    ...     Please Check
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:H16 B2 N6 Zn2
            Atom count from the _atom_site data:  H16 Br2 N6 Zn2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  B2r H16 N6 Zn2
           TEST: Compare cell contents of formula and atom_site data
           WARNING: Unexpected atom type is in site list: Br
           WARNING: Formula and atom_type_symbol element names mismatch.

           atom    Z*formula  cif sites diff
           B          4.00      0.00    4.00
           r          2.00      0.00    2.00
           H         32.00     32.00    0.00
           N         12.00     12.00    0.00
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          Zn         4.00      4.00    0.00
           WARNING: Site labels do not match formula elements
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         11 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          8 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          8 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        122 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
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  11 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

  14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
   4 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* or *IUCrData*, 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 11/08/2016; check.def file version of 04/08/2016

Datablock C__Crystal_Vrac_79_3_ZnBrN3H8 - ellipsoid plot