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: Dongxiaoyu_Pb2Ba3B3O9Br

```
Bond precision:    O- B = 0.0156 A           Wavelength=0.71073

Cell:           a=10.5385(13)      b=14.2877(17)      c=8.1074(10)
                alpha=90           beta=90            gamma=90
Temperature:    296 K

                Calculated                 Reported
Volume          1220.7(3)                  1220.7(3)
Space group     C 2 2 21                   C222(1)
Hall group      C 2c 2                     ?
Moiety formula  B3 Br O9 Pb2, 3(Ba)        ?
Sum formula     B3 Ba3 Br O9 Pb2           B3 Ba3 Br O9 Pb2
Mr              1082.72                    1082.74
Dx,g cm-3       5.891                      5.891
Z               4                          4
Mu (mm-1)       40.325                     40.324
F000            1816.0                     1816.0
F000'           1787.52
h,k,lmax        13,18,10                   13,18,10
Nref            822[ 1415]                 1412
Tmin,Tmax       0.047,0.298                0.102,0.398
Tmin'           0.013

Correction method= MULTI-SCAN

Data completeness= 1.72/1.00       Theta(max)= 27.470

R(reflections)= 0.0261( 1336)      wR2(reflections)= 0.0637( 1412)

S = 1.080                   Npar= 86
```

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

```
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:    PB1    -- BA3    ..    3.89 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:    PB1    -- BA1    ..    3.92 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:    PB1    -- BA2    ..    3.95 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:    BA1    -- PB1    ..    3.92 Ang.
```

```
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   BA2    -- PB1    ..       3.95 Ang.
```

 Alert level G

```
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
            correct. If it is not, please give the correct count in the
            _publ_section_exptl_refinement section of the submitted CIF.
            From the CIF: _diffrn_reflns_theta_max          27.47
            From the CIF: _reflns_number_total              1412
            Count of symmetry unique reflns        822
            Completeness (_total/calc)          171.78%
            TEST3: Check Friedels for noncentro structure
            Estimate of Friedel pairs measured       590
            Fraction of Friedel pairs measured     0.718
            Are heavy atom types Z>Si present         yes
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension .        2
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....        ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      5.48
PLAT158_ALERT_4_G The Input Unitcell is NOT Standard/Reduced .....        ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1    -- Br1_a   ..       14.9 su
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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
   5 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

   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
   0 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
```

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 19/04/2012; check.def file version of 14/04/2012