checkCIF/PLATON report

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

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: mxf-20181217

```
Bond precision:  C-C = 0.0110 A          Wavelength=1.54184

Cell:         a=6.7743(3)       b=11.1591(6)     c=13.7721(4)
              alpha=100.881(3)  beta=102.221(3)  gamma=105.571(4)
Temperature:  295 K
```

	Calculated	Reported
Volume	946.23(8)	946.23(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H16 Ba2 O13	C16 H16 Ba2 O13
Sum formula	C16 H16 Ba2 O13	C16 H16 Ba2 O13
Mr	690.95	690.97
Dx,g cm-3	2.425	2.425
Z	2	2
Mu (mm-1)	32.846	32.846
F000	656.0	656.0
F000’	654.53	
h,k,lmax	8,13,16	8,13,16
Nref	3669	3510
Tmin,Tmax		0.046,1.000
Tmin’		

```
Correction method= # Reported T Limits: Tmin=0.046 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.957          Theta(max)= 71.343

R(reflections)= 0.0747( 3190)     wR2(reflections)= 0.2120( 3510)

S = 1.043                 Npar= 273
```

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 B

```
PLAT420_ALERT_2_B D-H Without Acceptor       O3       --H3       .     Please Check
PLAT420_ALERT_2_B D-H Without Acceptor       O11      --H11B     .     Please Check
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Alert level C

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.975 Why?
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
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       4.79 eA-3
PLAT213_ALERT_2_C Atom O3              has ADP max/min Ratio .....       3.4 oblate
PLAT213_ALERT_2_C Atom O6              has ADP max/min Ratio .....       3.1 oblate
PLAT213_ALERT_2_C Atom C9              has ADP max/min Ratio .....       3.8 oblate
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range       5.2 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O9 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O13 Check
PLAT245_ALERT_2_C U(iso) H3        Smaller than U(eq) O3        by      0.023 Ang**2
PLAT314_ALERT_2_C Small Angle for H2O: Metal-O11      -H11A      .      54.01 Degree
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............      0.011 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H5       ..H10      .       1.95 Ang.
                                                    x,y,z  =      1_555 Check
PLAT751_ALERT_4_C Bond    Calc     2.24000, Rep    2.243(7) ......  Senseless s.u.
             BA1      -H3             1.555   2.665 ........     #    4 Check
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Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          2 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         10 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.17 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: Ba1      --Ba2       ..       4.37 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         12 Note
PLAT883_ALERT_1_G No Info for _atom_sites_solution_primary .......     Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         91 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  17 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 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* 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 18/02/2019; check.def file version of 18/02/2019

Datablock mxf-20181217 - ellipsoid plot