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: 1

```
Bond precision:  O- C = 0.0059 A         Wavelength=0.71073

Cell:            a=8.018(3)    b=15.929(5)          c=13.950(5)
                 alpha=90      beta=101.425(6)      gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	1746.4(11)	1746.4(11)
Space group	C c	Cc
Hall group	C -2yc	?
Moiety formula	C6 F2 Na8 O18 Yb2	?
Sum formula	C6 F2 Na8 O18 Yb2	C6 F2 Na8 O18 Yb2
Mr	928.06	928.06
Dx,g cm-3	3.530	3.530
Z	4	4
Mu (mm-1)	10.968	10.968
F000	1704.0	1704.0
F000’	1703.07	
h,k,lmax	10,20,18	10,20,18
Nref	4022[2016]	3946
Tmin,Tmax	0.210,0.334	0.844,1.000
Tmin’	0.177	

```
Correction method= # Reported T Limits: Tmin=0.844 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.96/0.98      Theta(max)= 27.470

R(reflections)= 0.0171( 3881)     wR2(reflections)= 0.0350( 3946)

S = 1.077                 Npar= 325
```

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

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as Multi-scan
PLAT036_ALERT_1_C No s.u. Given for Flack Parameter ..............     Please Do !
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       6.20 Note
PLAT213_ALERT_2_C Atom C4              has ADP max/min Ratio .....        3.3 oblate
PLAT213_ALERT_2_C Atom C5              has ADP max/min Ratio .....        3.1 oblate
```

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
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem       sub         86 %Fit
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Yb1      --O18_k     .       11.6 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Yb1       (III)     .       2.86 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Yb2       (III)     .       2.93 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         14 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2018 Note
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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
  12 **ALERT level G** = General information/check it is not something unexpected

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   4 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 14/07/2018; check.def file version of 05/06/2018

Datablock 1 - ellipsoid plot