checkCIF/PLATON report

Structure factors have been supplied for datablock(s) olsn16

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: olsn16

```
Bond precision:  C-C = 0.0076 A          Wavelength=0.71073

Cell:          a=11.8690(4)       b=13.0006(5)     c=16.0853(5)
               alpha=110.653(3)   beta=94.658(3)   gamma=114.343(4)
Temperature:   100 K
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	Calculated	Reported
Volume	2039.92(16)	2039.91(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C33 H5 F33 O8 P Tb	C33 H5 F33 O8 P Tb
Sum formula	C33 H5 F33 O8 P Tb	C33 H5 F33 O8 P Tb
Mr	1346.27	1346.22
Dx,g cm-3	2.192	2.192
Z	2	2
Mu (mm-1)	1.976	1.976
F000	1288.0	1288.0
F000’	1289.24	
h,k,lmax	14,15,19	14,15,19
Nref	7484	7470
Tmin,Tmax	0.360,0.655	0.549,1.000
Tmin’	0.225	

```
Correction method= # Reported T Limits: Tmin=0.549 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 25.349

R(reflections)= 0.0396( 6396)     wR2(reflections)= 0.0818( 7470)

S = 1.028                 Npar= 686
```

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Th(Min) ... 12 Report

Author Response: Reduction of beam stop mask did not yield significant improvement. Most of those missing strong reflections appeared to be very strong and were treated as overflows.

Alert level C

```
PLAT213_ALERT_2_C Atom F8              has ADP max/min Ratio .....       3.4 prolat
PLAT220_ALERT_2_C Large Non-Solvent  F     Ueq(max)/Ueq(min) Range      3.2 Ratio
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600        3 Report
PLAT973_ALERT_2_C Check Calcd Positive Residual Density on     Tb1      1.44 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density  0.99A From     O8       0.53 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density  1.08A From     O8      -0.66 eA-3
PLAT977_ALERT_2_C Check Negative Residual Density on ......    H8B     -0.65 eA-3
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............        2 Report
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....     0.73 mm
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...        2 Units
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C9 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C10 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C14 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F11    ..  C19     ..     2.96 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F1     ..  F28     ..     2.69 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F14    ..  F31     ..     2.84 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F18    ..  F27     ..     2.81 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F20    ..  F29     ..     2.65 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F23    ..  F25     ..     2.77 Ang.
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   7 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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  15 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
   1 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 19/11/2015; check.def file version of 17/11/2015

Datablock olsn16 - ellipsoid plot