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: ya327

```
Bond precision:  C-C = 0.0054 A          Wavelength=1.54184

Cell:            a=9.0162(2)    b=17.4431(4)       c=11.6043(3)
                 alpha=90       beta=95.066(2)     gamma=90
Temperature:     293 K

                Calculated                Reported
Volume          1817.89(7)                1817.88(7)
Space group     P 21/n                    P 1 21/n 1
Hall group      -P 2yn                    -P 2yn
Moiety formula  C14 H15 N O7 Y [+ solvent]C14 H15 N O7 Y
Sum formula     C14 H15 N O7 Y [+ solvent]C14 H15 N O7 Y
Mr              398.18                    398.18
Dx,g cm-3       1.455                     1.455
Z               4                         4
Mu (mm-1)       4.812                     4.812
F000            804.0                     804.0
F000'           805.32
h,k,lmax        11,21,14                  11,21,14
Nref            3609                      3516
Tmin,Tmax       0.399,0.421               0.409,0.470
Tmin'           0.302

Correction method= # Reported T Limits: Tmin=0.409 Tmax=0.470
AbsCorr = MULTI-SCAN

Data completeness= 0.974          Theta(max)= 72.458

R(reflections)= 0.0587( 3287)     wR2(reflections)= 0.1658( 3516)

S = 1.083                 Npar= 267
```

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

```
PLAT213_ALERT_2_C Atom O4              has ADP max/min Ratio .....       3.1 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range       3.8 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range       4.7 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Y1 Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        14 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         2 Info
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......    Please Check
PLAT014_ALERT_1_G No       _shelx_fab_checksum Found in CIF ......    Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.11 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       30% Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure       117 A**3
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .      1.28 Ratio
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       319 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed          ! Info
PLAT883_ALERT_1_G No Info for _atom_sites_solution_primary .......    Please Do !
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
15 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
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 ya327 - ellipsoid plot