checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Fraser36

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: Fraser36

```
Bond precision:  C-C = 0.0025 A          Wavelength=0.71073

Cell:          a=10.8234(16)      b=10.8522(16)    c=18.325(3)
               alpha=103.661(2)   beta=92.755(3)   gamma=91.456(3)
Temperature:   153 K
```

	Calculated	Reported
Volume	2087.6(6)	2087.6(5)
Space group	P -1	P -1
Hall group	: -P 1	-P 1
Moiety formula	C23 H28 O6	?
Sum formula	C23 H28 O6	C23 H28 O6
Mr	400.45	400.45
Dx,g cm-3	1.274	1.274
Z	4	4
Mu (mm-1)	0.091	0.091
F000	856.0	856.0
F000’	856.46	
h,k,lmax	15,15,25	15,15,25
Nref	11758	11643
Tmin,Tmax	0.985,0.987	0.920,0.990
Tmin’	0.958	

```
Correction method= # Reported T Limits: Tmin=0.920 Tmax=0.990
AbsCorr = MULTI-SCAN

Data completeness= 0.990          Theta(max)= 29.630

R(reflections)= 0.0510( 9205)     wR2(reflections)= 0.1441( 11643)

S = 1.042                 Npar= 546
```

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 Theta(Min). 16 Note

Alert level C

PLAT303_ALERT_2_C Full Occupancy Atom H1 with # Connections 2.00 Check
PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O8 - H8 . 1.02 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 17 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for O11A --C41 . 6.3 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 7% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 81 Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law (1 0 0) Est.d BASF 0.22 Check

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
4 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* 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 26/09/2018; check.def file version of 13/09/2018

Datablock Fraser36 - ellipsoid plot