checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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:  C-C = 0.0031 A          Wavelength=0.71073

Cell:            a=4.5333(7)     b=21.946(4)         c=15.968(3)
                 alpha=90        beta=95.627(4)      gamma=90
Temperature:     120 K
```

	Calculated	Reported
Volume	1581.0(5)	1581.0(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C18 H18 N2 O5	C18 H18 N2 O5
Sum formula	C18 H18 N2 O5	C18 H18 N2 O5
Mr	342.34	342.34
Dx,g cm-3	1.438	1.438
Z	4	4
Mu (mm-1)	0.106	0.106
F000	720.0	720.0
F000’	720.38	
h,k,lmax	6,31,22	6,31,22
Nref	4888	4876
Tmin,Tmax	0.995,0.996	0.598,0.746
Tmin’	0.974	

```
Correction method= # Reported T Limits: Tmin=0.598 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 30.619

R(reflections)= 0.0636( 3049)     wR2(reflections)= 0.1635( 4876)

S = 1.030                 Npar= 264
```

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 C7              has ADP max/min Ratio .....        3.3 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       3.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C10      --C15      .        6.8 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     6.642 Check
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          2 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C6       --C7       .       15.7 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C6       --C7'      .        6.8 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C8       --C9       .        5.7 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        16% Note
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O1            105.9 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O2            105.1 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O4            105.6 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O5            105.2 Degree
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        12 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        11 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          7 Info
```

```
   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
  15 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 22/03/2021; check.def file version of 19/03/2021

Datablock 1 - ellipsoid plot