checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cs3_100

No syntax errors found. CIF dictionary Interpreting this report

Datablock: cs3_100

```
Bond precision:  C-C = 0.0032 A          Wavelength=0.71073

Cell:            a=14.430(6)     b=6.800(2)           c=16.760(8)
                 alpha=90        beta=99.450(16)      gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	1622.2(11)	1622.2(11)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	C9 H11 N O2, C7 H4 N2 O6	?
Sum formula	C16 H15 N3 O8	C16 H15 N3 O8
Mr	377.31	377.31
Dx,g cm-3	1.545	1.545
Z	4	4
Mu (mm-1)	0.126	0.002
F000	784.0	499.0
F000’	784.49	
h,k,lmax		19,9,21
Nref		3111
Tmin,Tmax	0.998,0.999	
Tmin’	0.996	

```
Correction method= Not given

Data completeness=                 Theta(max)= 0.000

R(reflections)= 0.0545( 2022)     wR2(reflections)= 0.1152( 3111)

S = 1.119                  Npar= 378
```

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 A

```
TYPE031_ALERT_1_A  _diffrn_radiation_wavelength is not of type numb.
RINTA01_ALERT_3_A  The value of Rint is greater than 0.25
            Rint given   0.251
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low .......      0.000
```

```
PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .    6214.39 Perc.
PLAT091_ALERT_1_A No Wavelength found in CIF - 0.71073 Ang Assumed          ?
```

Alert level B

```
DIFMN02_ALERT_2_B  The minimum difference density is < -0.1*ZMAX*1.00
            _refine_diff_density_min given =     -1.197
            Test value =     -0.800
DIFMX01_ALERT_2_B  The maximum difference density is > 0.1*ZMAX*1.00
            _refine_diff_density_max given =      0.998
            Test value =      0.800
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       1.00 eA-3
PLAT098_ALERT_2_B Large Reported Min.  (Negative) Residual Density      -1.20 eA-3
```

Alert level C

```
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
            The relevant atom site should be identified.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ....................       8.23
PLAT213_ALERT_2_C Atom O7              has ADP max/min Ratio .....        3.9 prola
PLAT213_ALERT_2_C Atom O8              has ADP max/min Ratio .....        3.4 prola
PLAT220_ALERT_2_C Large Non-Solvent    O     Ueq(max)/Ueq(min) ...        3.3 Ratio
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         N3
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.7
PLAT355_ALERT_3_C Long    O-H Bond (0.82A)   O1     -   H11    ...       1.02 Ang.
```

Alert level G

```
  ABSMU_01  Radiation type not identified. Calculation of
            _exptl_absorpt_correction_mu not performed.
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....       1.80 mm
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          4
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT981_ALERT_1_G No non-zero f" Anomalous Scattering Values Found          ?
PLAT982_ALERT_1_G The  C-f'=     0.000 Deviates from the  IT-value      0.003
PLAT982_ALERT_1_G The  N-f'=     0.000 Deviates from the  IT-value      0.006
PLAT982_ALERT_1_G The  O-f'=     0.000 Deviates from the  IT-value      0.011
PLAT983_ALERT_1_G The  C-f"=     0.000 Deviates from the  IT-Value      0.002
PLAT983_ALERT_1_G The  N-f"=     0.000 Deviates from the  IT-Value      0.003
PLAT983_ALERT_1_G The  O-f"=     0.000 Deviates from the  IT-Value      0.006
```

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   5 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  10 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

  15 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 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
   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 18/07/2011; check.def file version of 04/07/2011

Datablock cs3_100 - ellipsoid plot