checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dnba_300

No syntax errors found. CIF dictionary Interpreting this report

Datablock: dnba_300

```
Bond precision:  C-C = 0.0019 A          Wavelength=0.71073

Cell:             a=21.040(5)     b=8.730(5)          c=9.760(5)
                  alpha=90        beta=111.05(1)      gamma=90
Temperature:      300 K
```

	Calculated	Reported
Volume	1673.1(14)	1673.1(13)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C7 H4 N2 O6	?
Sum formula	C7 H4 N2 O6	C7 H4 N2 O6
Mr	212.12	212.00
Dx,g cm-3	1.684	1.683
Z	8	8
Mu (mm-1)	0.152	0.000
F000	864.0	68.0
F000’	864.63	
h,k,lmax	33,14,15	29,12,13
Nref	3644	1614
Tmin,Tmax		
Tmin’		

```
Correction method= Not given

Data completeness= 0.443          Theta(max)= 34.880

R(reflections)= 0.0431( 1181)     wR2(reflections)= 0.0801( 1614)

S = 1.300                 Npar= 173
```

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.
PLAT027_ALERT_3_A _diffrn_reflns_theta_full (too) Low ............       0.00 Deg.
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low .......      0.000
PLAT091_ALERT_1_A No Wavelength found in CIF - 0.71073 Ang Assumed          ?
```

Alert level B

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O5     ..  N1      ..       2.85 Ang.
```

Alert level C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.120
PLAT088_ALERT_3_C Poor Data / Parameter Ratio ...................       9.33
```

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 ....          ?
PLAT153_ALERT_1_G The su's on the Cell Axes   are Equal ..........    0.00500 Ang.
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3
PLAT195_ALERT_1_G Missing _cell_measurement_theta_max   datum ....          ?
PLAT196_ALERT_1_G Missing _cell_measurement_theta_min   datum ....          ?
PLAT432_ALERT_2_G Short Inter X...Y Contact  O6     ..  C7      ..       3.01 Ang.
PLAT950_ALERT_5_G Reported and Calculated Hmax Values Differ by ..          4
PLAT951_ALERT_5_G Reported and Calculated Kmax Values Differ by ..          2
PLAT952_ALERT_5_G Reported and Calculated Lmax Values Differ by ..          2
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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   4 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

  12 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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
   1 ALERT type 4 Improvement, methodology, query or suggestion
   4 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 19/04/2012; check.def file version of 14/04/2012

Datablock dnba_300 - ellipsoid plot