checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: joe135as

```
Bond precision:  C-C = 0.0043 A          Wavelength=0.71073

Cell:            a=8.7385(9)     b=11.4473(12)     c=15.1957(16)
                 alpha=90        beta=90           gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	1520.1(3)	1520.1(3)
Space group	P 21 21 21	P 2(1)2(1)2
Hall group	P 2ac 2ab	?
Moiety formula	C16 H21 N O5	?
Sum formula	C16 H21 N O5	C16 H21 N O5
Mr	307.34	307.34
Dx,g cm-3	1.343	1.343
Z	4	4
Mu (mm-1)	0.100	0.100
F000	656.0	656.0
F000’	656.36	
h,k,lmax	10,14,18	10,14,18
Nref	1784[3097]	1780
Tmin,Tmax	0.977,0.990	0.830,0.990
Tmin’	0.977	

```
Correction method= MULTI-SCAN

Data completeness= 1.00/0.57      Theta(max)= 26.380

R(reflections)= 0.0466( 1700)     wR2(reflections)= 0.1214( 1780)

S = 1.142                 Npar= 206
```

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

```
STRVA01_ALERT_4_C          Flack parameter is too small
          From the CIF: _refine_ls_abs_structure_Flack   -1.200
          From the CIF: _refine_ls_abs_structure_Flack_su    1.800
PLAT033_ALERT_4_C Flack x Parameter Value Deviates from Zero .....     -1.200
```

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.19
PLAT222_ALERT_3_C Large Non-Solvent    H    Uiso(max)/Uiso(min) ..        6.4 Ratio
PLAT245_ALERT_2_C U(iso) H03     Smaller than U(eq) N3      by ...      0.011 AngSq
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0043 Ang
```

Alert level G

```
HYDTR01_ALERT_1_G  Extra text has been found in the _refine_ls_hydrogen_treatment fi
           Explanatory text should be in the _publ_section_refinement field.
           Hydrogen treatment given as NH free with DFIX, rigid methyls, others
           Hydrogen treatment identified as  riding
REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
           correct. If it is not, please give the correct count in the
           _publ_section_exptl_refinement section of the submitted CIF.
          From the CIF: _diffrn_reflns_theta_max           26.38
          From the CIF: _reflns_number_total               1780
          Count of symmetry unique reflns         1784
          Completeness (_total/calc)             99.78%
          TEST3: Check Friedels for noncentro structure
          Estimate of Friedel pairs measured         0
          Fraction of Friedel pairs measured     0.000
          Are heavy atom types Z>Si present         no
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          2
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ....          ?
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      1.800
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          1
PLAT791_ALERT_4_G Note: The Model has Chirality at C5     (Verify)          S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......          1
```

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

1 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
3 ALERT type 3 Indicator that the structure quality may be low
6 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 19/04/2012; check.def file version of 14/04/2012

Datablock joe135as - ellipsoid plot