checkCIF/PLATON report

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

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: ME4NDCNM.CIF

```
Bond precision:  C-C = 0.0055 A          Wavelength=0.71073

Cell:            a=8.6630(17)    b=6.5838(13)       c=9.0253(18)
                 alpha=90        beta=116.56(3)     gamma=90
Temperature:     123 K
```

	Calculated	Reported
Volume	460.4(2)	460.4(2)
Space group	P 21/m	P21/m
Hall group	-P 2yb	?
Moiety formula	C3 N3 O, C4 H12 N	C3 N3 O, C4 H12 N
Sum formula	C7 H12 N4 O	C7 H12 N4 O
Mr	168.27	168.21
Dx,g cm-3	1.214	1.213
Z	2	2
Mu (mm-1)	0.086	0.086
F000	180.1	180.0
F000’	180.12	
h,k,lmax	11,8,11	11,8,11
Nref	1146	1137
Tmin,Tmax	0.980,0.991	0.975,0.983
Tmin’	0.975	

```
Correction method= EMPIRICAL

Data completeness= 0.992          Theta(max)= 27.490

R(reflections)= 0.0691( 879)      wR2(reflections)= 0.1954( 1137)

S = 1.140                 Npar= 86
```

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

```
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....         N4 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.0055 Ang.
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C7 H12 N4 O1
           Atom count from the _atom_site data:  C7 H13 N4 O1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C7 H12 N4 O
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         14.00     14.00    0.00
          H         24.00     26.00   -2.00
          N          8.00      8.00    0.00
          O          2.00      2.00    0.00
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.20
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          9 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         12
             N1A  -C1   -N1B     1.555   1.555   1.555            36.30 Deg.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
```

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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
   2 **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

   2 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
   2 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 18/09/2013; check.def file version of 12/09/2013

Datablock ME4NDCNM.CIF - ellipsoid plot