# 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: sq13_se_pb

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```
Bond precision:  C-C = 0.0117 A          Wavelength=1.54175

Cell:           a=12.9142(5)    b=13.4373(2)         c=6.82870(13)
                alpha=90        beta=96.9271(17)     gamma=90
Temperature:    293 K

                Calculated                Reported
Volume          1176.35(5)                1176.35(5)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C11 H16 N2 O3             C22 H32 N4 O6
Sum formula     C11 H16 N2 O3             C22 H32 N4 O6
Mr              224.26                    448.00
Dx,g cm-3       1.266                     0.000
Z               4                         2
Mu (mm-1)       0.768                     0.000
F000            480.0                     0.0
F000'           481.55
h,k,lmax        9,9,5
Nref            505
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness= 0.000          Theta(max)=

R(reflections)=                   wR2(reflections)=

S =                        Npar=
```

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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.

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**Alert level A**

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**Alert level B**

PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for C4

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PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        C10
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for         N3
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for        N13
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ..............     0.0117 Ang
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## Alert level C

```
REFI015_ALERT_1_A  _refine_ls_shift/su_max is missing
           Maximum shift/s.u. ratio after final refinement cycle.
           The following tests will not be performed
           SHFSU_01
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        C15
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        O21
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C1     -   H31    ...       1.15 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C1     -   H32    ...       1.11 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C7     -   H8     ...       1.16 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C7     -   H9     ...       1.12 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C22    -   H28    ...       1.11 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C24    -   H27    ...       1.14 Ang.
PLAT353_ALERT_3_C Long    N-H Bond (0.87A)   N13    -   H14    ...       1.02 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H30    ..  H30     ..       2.00 Ang.
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## Alert level G

```
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms .............         1
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ          ?
PLAT045_ALERT_1_G Calculated and Reported Z Differ by .............      2.00 Ratio
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C1
PLAT343_ALERT_2_G Check sp?     Angle Range in Main Residue for ..        C2
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        87
PLAT950_ALERT_5_G Reported and Calculated Hmax Values Differ by ..         9
PLAT951_ALERT_5_G Reported and Calculated Kmax Values Differ by ..         9
PLAT952_ALERT_5_G Reported and Calculated Lmax Values Differ by ..         5
PLAT982_ALERT_1_G The  C-f'=     0.017 Deviates from the  IT-value      0.018
PLAT982_ALERT_1_G The  N-f'=     0.029 Deviates from the  IT-value      0.031
PLAT982_ALERT_1_G The  O-f'=     0.047 Deviates from the  IT-value      0.049
PLAT983_ALERT_1_G The  C-f"=     0.009 Deviates from the  IT-Value      0.009
PLAT983_ALERT_1_G The  O-f"=     0.032 Deviates from the  IT-Value      0.032
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  1 ALERT level A = Most likely a serious problem - resolve or explain
  5 ALERT level B = A potentially serious problem, consider carefully
 10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 14 ALERT level G = General information/check it is not something unexpected

  8 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
  9 ALERT type 3 Indicator that the structure quality may be low
  0 ALERT type 4 Improvement, methodology, query or suggestion
  4 ALERT type 5 Informative message, check
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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.

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**PLATON version of 04/07/2012; check.def file version of 28/06/2012**

**Datablock sq13_se_pb** - ellipsoid plot