# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) x

No syntax errors found.       CIF dictionary       Interpreting this report

## Datablock: x

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Bond precision:   C-C = 0.0037 A              Wavelength=0.71073

Cell:             a=12.208(5)      b=6.102(3)             c=13.056(5)
                  alpha=90         beta=111.438(7)        gamma=90
Temperature:      173 K

                  Calculated                 Reported
Volume            905.3(7)                   905.3(6)
Space group       P 21                       P 21
Hall group        P 2yb                      ?
Moiety formula    C18 H27 N O S              C18 H27 N O S
Sum formula       C18 H27 N O S              C18 H27 N O S
Mr                305.48                     305.47
Dx,g cm-3         1.121                      1.121
Z                 2                          2
Mu (mm-1)         0.178                      0.178
F000              332.0                      332.0
F000'             332.36
h,k,lmax          14,7,15                    14,7,15
Nref              1767[ 3205]                3206
Tmin,Tmax         0.958,0.984                0.913,0.984
Tmin'             0.921

Correction method= MULTI-SCAN

Data completeness= 1.81/1.00       Theta(max)= 25.050

R(reflections)= 0.0384( 2776)      wR2(reflections)= 0.0833( 3206)

S = 1.003                 Npar= 198
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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 C**
PLAT420_ALERT_2_C D-H Without Acceptor        N1     -   H1N    ...        ?

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⚪ **Alert level G**

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF        ?
PLAT791_ALERT_4_G Note: The Model has Chirality at C1     (Verify)        R
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and su ..      0.08
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still        70 Perc.
PLAT916_ALERT_2_G Hooft y and Flack x Parameter values differ by .      0.23
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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
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   5 ALERT level G = General information/check it is not something unexpected

   0 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
   1 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
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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.
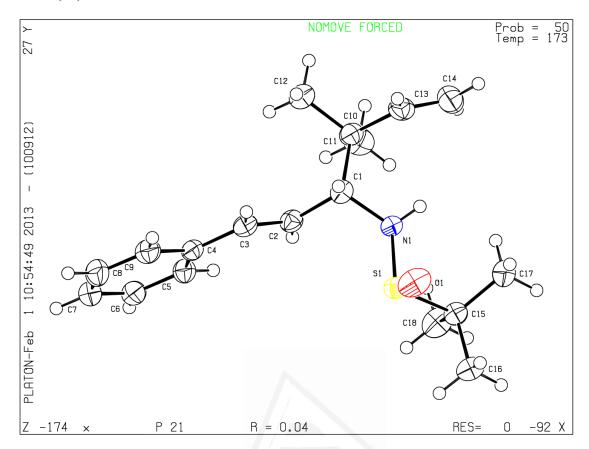
**Publication of your CIF in IUCr journals**

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 05/11/2012; check.def file version of 05/11/2012**