

# checkCIF/PLATON (full publication check)

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.  
Please wait while processing ....

[CIF dictionary](#)  
[Interpreting this report](#)

## Datablock: I

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Bond precision: C-C = 0.0028 A Wavelength=1.54187  
Cell: a=10.217(2) b=11.676(3) c=10.273(2)  
alpha=90 beta=114.186(13) gamma=90  
Temperature: 123 K

	Calculated	Reported
Volume	1117.9(4)	1117.9(4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C11 H17 N O4	C11 H17 N O4
Sum formula	C11 H17 N O4	C11 H17 N O4
Mr	227.26	227.26
Dx, g cm <sup>-3</sup>	1.350	1.350
Z	4	4
Mu (mm <sup>-1</sup> )	0.855	0.857
F000	488.0	488.0
F000'	489.64	
h, k, lmax	12, 14, 12	12, 14, 12
Nref	2046	2042
Tmin, Tmax	0.773, 0.918	0.721, 0.918
Tmin'	0.773	

Correction method= EMPIRICAL  
Data completeness= 0.998 Theta (max)= 68.190  
R(reflections)= 0.0428( 1845) wR2(reflections)= 0.1266( 2042)  
S = 1.195 Npar= Npar = 148

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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.

### Alert level G

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<a href="#">PLAT005_ALERT_5_G</a>	No iucr_refine_instructions details in the CIF	Please Do !
<a href="#">PLAT793_ALERT_4_G</a>	The Model has Chirality at C2 .....	S Verify
<a href="#">PLAT793_ALERT_4_G</a>	The Model has Chirality at C4 .....	S Verify

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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
- 0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 3 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

- 0 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 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

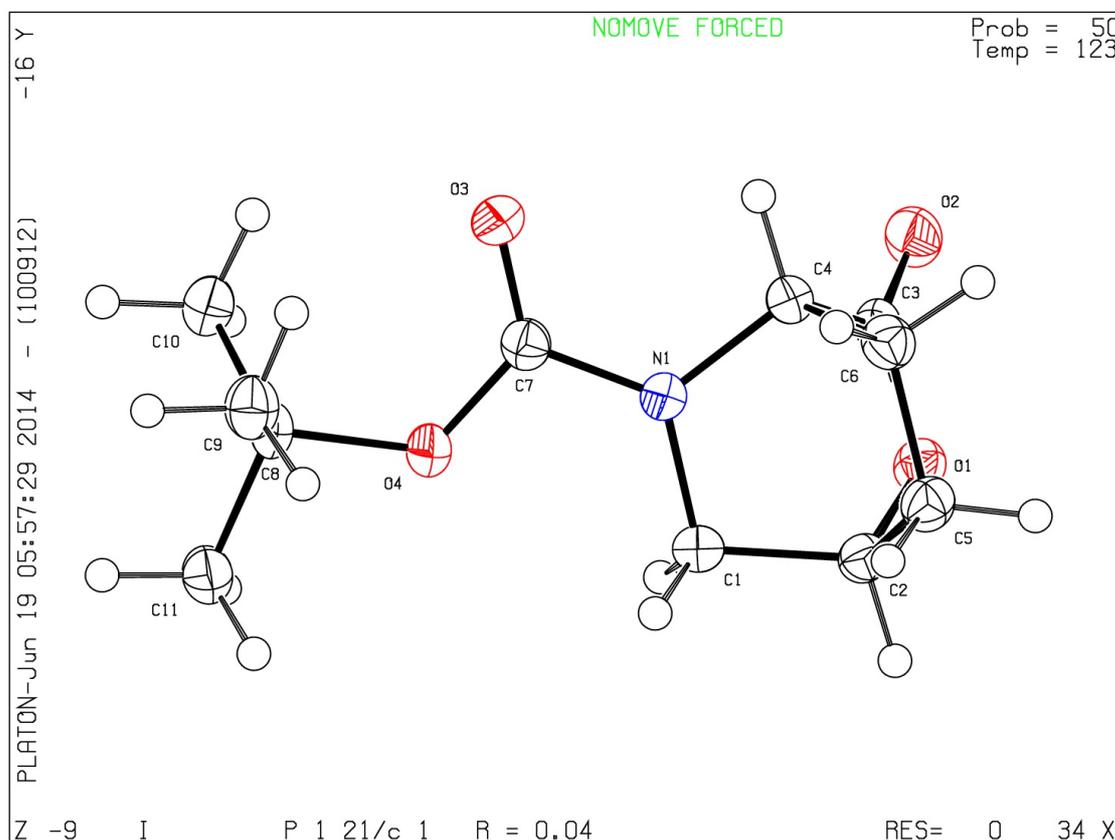
### Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via [the web](#). If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic [submission](#) or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 05/02/2014; check.def file version of 05/02/2014

### Datablock I – ellipsoid plot



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