

checkCIF/PLATON (standard)

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

No syntax errors found.
Please wait while processing

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

Datablock: 9APPHA

Bond precision:	C-C = 0.0030 A	Wavelength=0.71075
Cell:	a=8.784(2) b=20.520(5) c=29.114(7)	
	alpha=90 beta=90 gamma=90	
Temperature:	93 K	
	Calculated	Reported
Volume	5248(2)	5248(2)
Space group	P b c a	Pbca
Hall group	-P 2ac 2ab	?
Moiety formula	C38 H29 N	?
Sum formula	C38 H29 N	C38 H29 N
Mr	499.62	499.62
Dx, g cm ⁻³	1.265	1.265
Z	8	8
Mu (mm ⁻¹)	0.072	0.072
F000	2112.0	2112.0
F000'	2112.75	
h, k, lmax	10, 24, 34	10, 24, 34
Nref	4637	4631
Tmin, Tmax	0.987, 0.993	0.986, 0.993
Tmin'	0.986	
Correction method=	MULTI-SCAN	
Data completeness=	0.999	Theta(max)= 25.000
R(reflections)=	0.0592(3997)	wR2(reflections)= 0.1272(4631)
S =	1.143	Npar= 355

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

[PLAT230_ALERT_2_C](#) Hirshfeld Test Diff for C31 -- C32 .. 6.1 su

● Alert level G

[PLAT005_ALERT_5_G](#) No _iucr_refine_instructions_details in the CIF Please Do !

[PLAT066_ALERT_1_G](#) Predicted and Reported Tmin&Tmax Range Identical ? Check

- 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
- 2 **ALERT level G** = General information/check it is not something unexpected

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

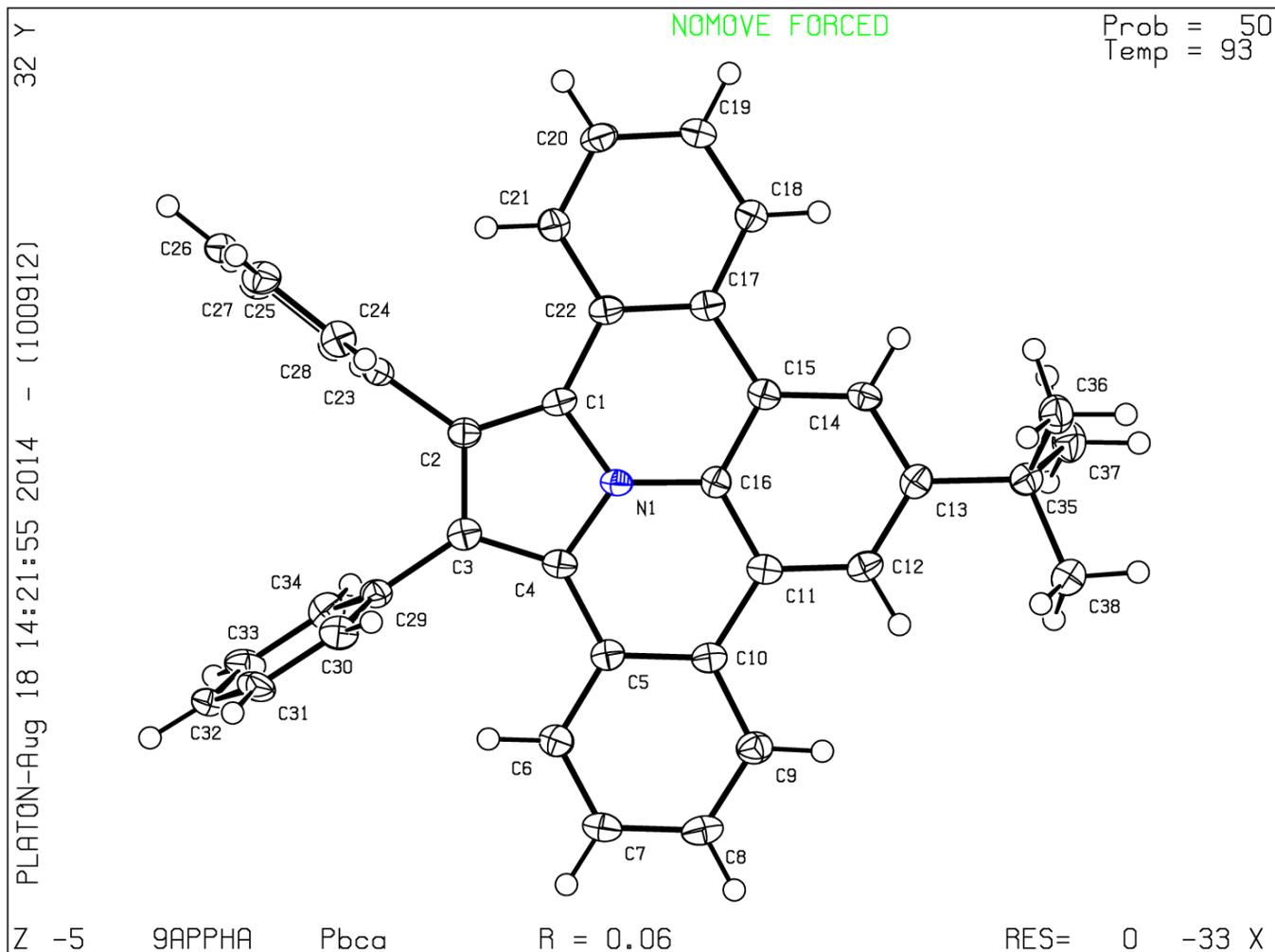
Crystallography, Journal of Synchrotron Radiation); however, if you intend to submit to Acta Crystallographica Section C or E, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

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 24/07/2014; check.def file version of 24/07/2014

Datablock 9APPHA - ellipsoid plot



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