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.   CIF dictionary
Please wait while processing ....   Interpreting this report

Datablock: 9APDMCPA

```
Bond precision:          C-C = 0.0041 A                  Wavelength=0.71075

Cell:         a=9.666(3)        b=22.449(6)      c=29.445(8)
              alpha=90          beta=90          gamma=90

Temperature: 93 K

                       Calculated                    Reported
Volume                 6389(3)                       6389(3)
Space group            P b c a                       Pbca
Hall group             -P 2ac 2ab                    ?
Moiety formula         C42 H33 N O4                  ?
Sum formula            C42 H33 N O4                  C42 H33 N O4
Mr                     615.69                        615.69
Dx,g cm-3              1.280                         1.280
Z                      8                             8
Mu (mm-1)              0.082                         0.082
F000                   2592.0                        2592.0
F000'                  2593.15
h,k,lmax               11,26,35                      11,26,35
Nref                   5629                          5622
Tmin,Tmax              0.985,0.992                   0.976,0.992
Tmin'                  0.976

Correction method= MULTI-SCAN

Data completeness= 0.999        Theta(max)= 25.000

R(reflections)= 0.0799( 5262)       wR2(reflections)= 0.1455( 5622)

S = 1.301               Npar= 429
```

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
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.0041 Ang.

⚪ 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
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.   8.01 Report

  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
  3 **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
  1 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
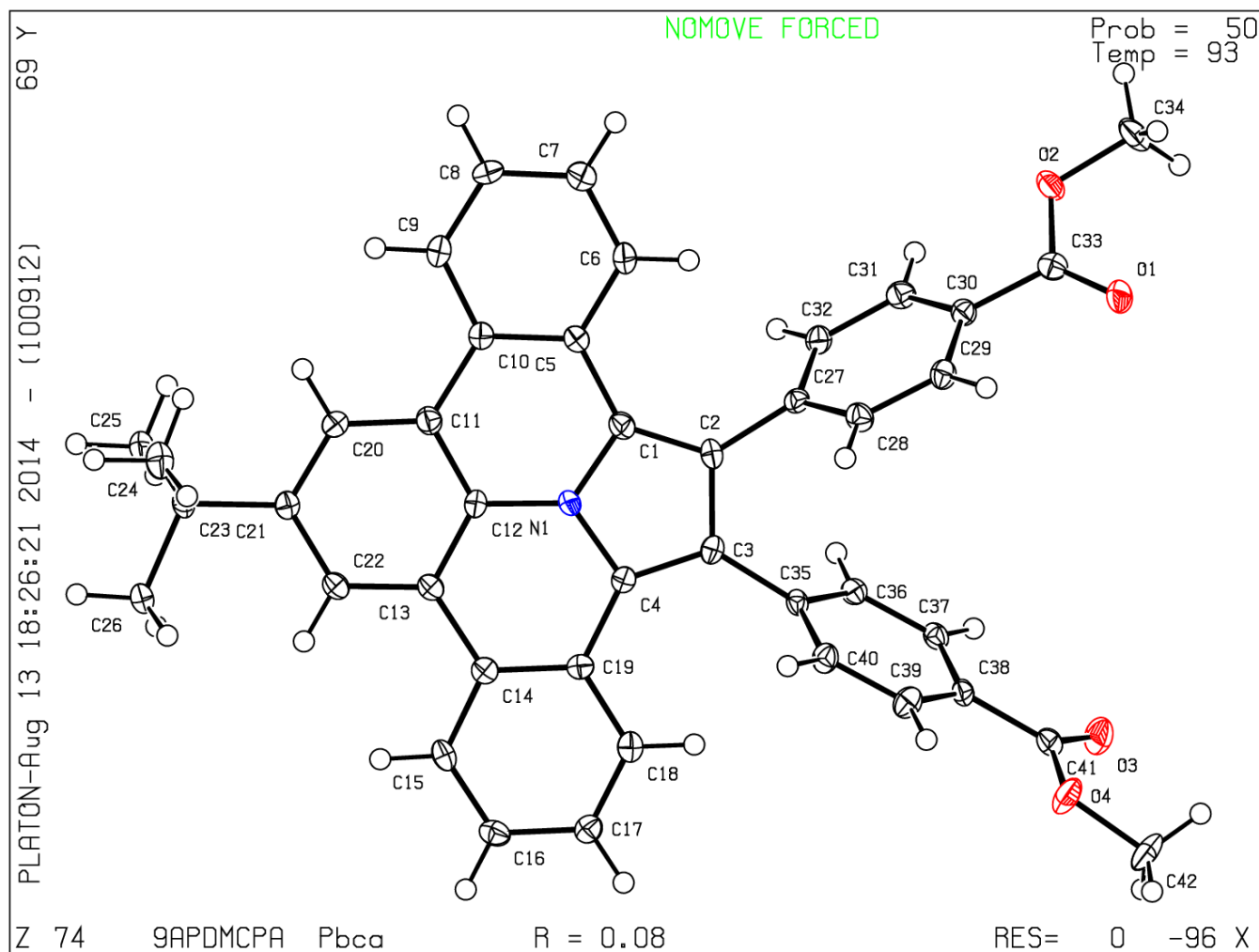
PLATON version of 24/07/2014; check.def file version of 24/07/2014

Datablock 9APDMCPA - ellipsoid plot

Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry