checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . . . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) ma34

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

Structure factor report

Datablock: ma34

```
Bond precision:        C-C = 0.0142 A                  Wavelength=0.71073
Cell:        a=14.266(4)       b=16.785(4)       c=9.785(3)
             alpha=90          beta=97.40(2)     gamma=90
Temperature: 173 K
                     Calculated                          Reported
Volume               2323.6(11)                          2323.6(11)
Space group          P 21/c                              P 21/c
Hall group           -P 2ybc                             -P 2ybc
Moiety formula       C25 H24 N2 O4                       C25 H24 N2 O4
Sum formula          C25 H24 N2 O4                       C25 H24 N2 O4
Mr                   416.46                              416.46
Dx,g cm-3            1.191                               1.191
Z                    4                                   4
Mu (mm-1)            0.081                               0.081
F000                 880.0                               880.0
F000'                880.41
h,k,lmax             16,19,11                            16,19,11
Nref                 4105                                4096
Tmin,Tmax            0.998,0.999                         0.511,1.000
Tmin'                0.990
Correction method= # Reported T Limits: Tmin=0.511 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.998          Theta(max)= 25.025
R(reflections)= 0.0904( 997)          wR2(reflections)= 0.1816( 4096)
S = 0.811               Npar= 281
```

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 A

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.258

Author Response: The crystal was a weakly diffracting extremely thin needle.

PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 ..... 0.258 Report

Author Response: The crystal was a weakly diffracting extremely thin needle.

PLAT026_ALERT_3_A Ratio Observed / Unique Reflections (too) Low .. 24% Check

Author Response: The crystal was a weakly diffracting extremely thin needle.

Alert level B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01417 Ang.

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C21 --C26 . 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C11 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C14 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 117.169 Check
And 6 other PLAT906 Alerts
More ...
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 9 Note

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Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT793_ALERT_4_G Model has Chirality at C2 (Centro SPGR) R Verify
PLAT793_ALERT_4_G Model has Chirality at C3 (Centro SPGR) R Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT908_ALERT_2_G Max. Perc. Data with I > 2*s(I) per Res.Shell . 55.34% Note
PLAT963_ALERT_2_G Both SHELXL WEIGHT Parameter Values Zero ..... Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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3 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
12 ALERT type 3 Indicator that the structure quality may be low
3 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 worthwhi In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structu 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 C checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts th are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspe 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

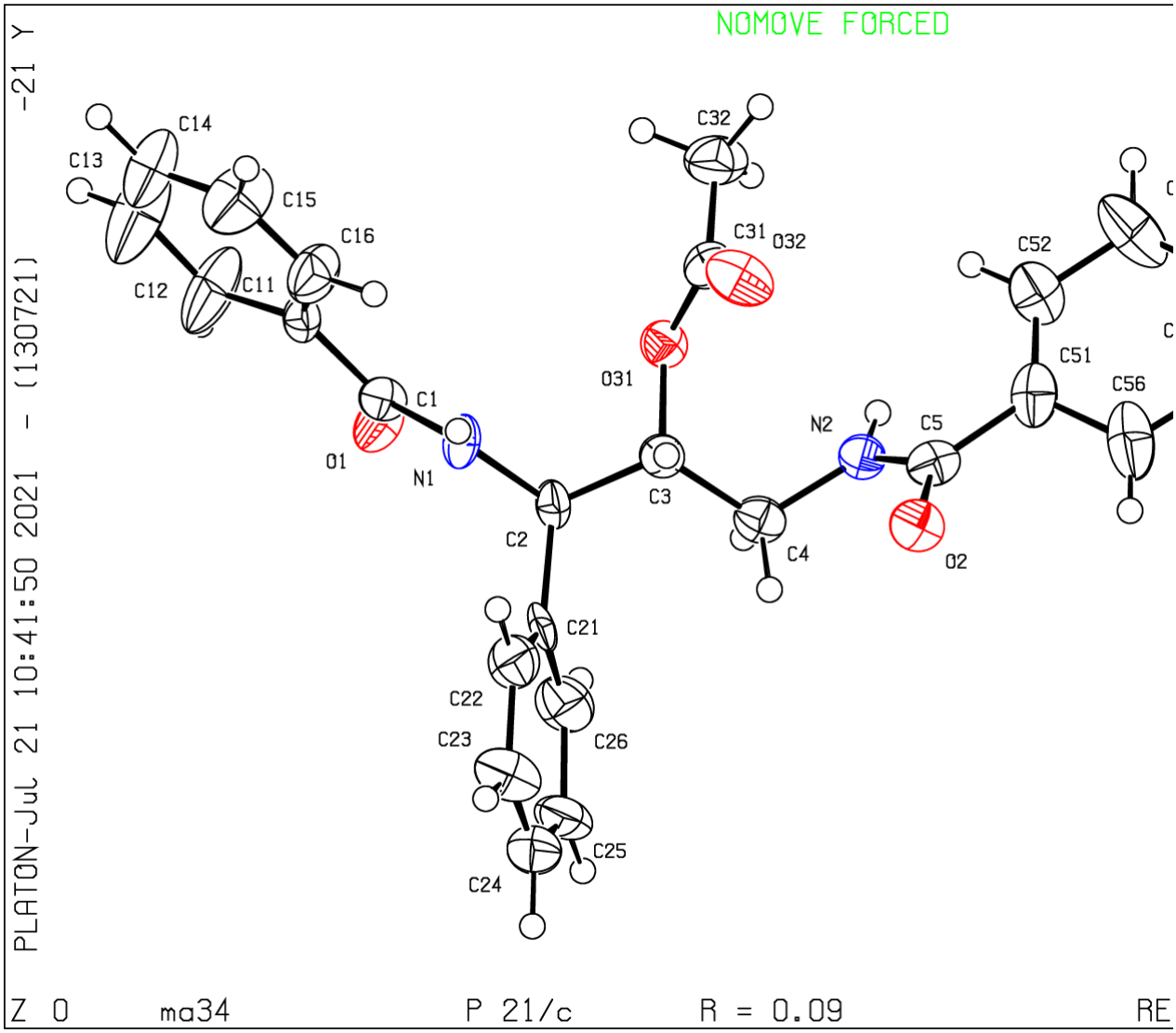
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if yo intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks ar 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 13/07/2021; check.def file version of 13/07/2021

Datablock ma34 - ellipsoid plot



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