checkCIF/PLATON report

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. CIF dictionary Interpreting this report

Datablock: _138468_1

```
Bond precision:   C-C = 0.0065 A          Wavelength=1.54187

Cell:             a=29.229(5)     b=6.0958(10)         c=9.3517(15)
                  alpha=90        beta=102.518(6)      gamma=90
Temperature:      293 K

                 Calculated                Reported
Volume           1626.6(5)                 1626.6(5)
Space group      C 2                       C 1 2 1
Hall group       C 2y                      C 2y
Moiety formula   C19 H23 N O               C19 H23 N O
Sum formula      C19 H23 N O               C19 H23 N O
Mr               281.38                    281.40
Dx,g cm-3        1.149                     1.149
Z                4                         4
Mu (mm-1)        0.541                     0.542
F000             608.0                     608.0
F000'            609.61
h,k,lmax         35,7,11                   33,7,11
Nref             3170[ 1743]               2829
Tmin,Tmax        0.895,0.917               0.741,0.919
Tmin'            0.604

Correction method= # Reported T Limits: Tmin=0.741 Tmax=0.919
AbsCorr = MULTI-SCAN

Data completeness= 1.62/0.89        Theta(max)= 71.500

R(reflections)= 0.0563( 4770)                wR2(reflections)=
                                             0.0967( 4829)
S = 0.940                 Npar= 217
```

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

DIFMN02_ALERT_2_A The minimum difference density is < -0.1*ZMAX*2.00
_refine_diff_density_min given = -1.780
Test value = -1.600

Author Response: Altough the residual density is out of border but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.921 Why?

Author Response: 180 images were collected with an IP instrument.

PLAT097_ALERT_2_A Large Reported Max. (Positive) Residual Density 1.66 eA-3

Author Response: Altough the residual density is out of border but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

PLAT098_ALERT_2_A Large Reported Min. (Negative) Residual Density -1.78 eA-3

Author Response: Altough the residual density is out of border but there is no doubt about the chemical structure taking into account other evidences, e.g. NMR. The error maybe due to crystal imperfections.

Alert level B

REFLT02_ALERT_1_B The number of reflections greater than the sigma threshold
cannot exceed the number of symmetry-independent reflections
Number of symmetry-independent reflections = 2829
Number of reflections greater than sigma threshold = 4770
PLAT230_ALERT_2_B Hirshfeld Test Diff for N2 --C18 . 9.4 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C8 --C12 . 9.2 s.u.

Alert level C

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged .... H3 Note
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C4 --C7 . 6.8 s.u.

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PLAT230_ALERT_2_C Hirshfeld Test Diff for    C6       --C10      .        6.2 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C19 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N2 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0065 Ang.
PLAT703_ALERT_1_C Torsion Calc     38.5(5), Rep     37.9(6), Dev..       1.20 Sigma
             C(10-C(6)-C(13-C(7)  1_555  1_555  1_555  1_555      #   14 Check
PLAT703_ALERT_1_C Torsion Calc     41.8(4), Rep     42.3(5), Dev..       1.25 Sigma
             C(15-C(6)-C(13-O(1)  1_555  1_555  1_555  1_555      #   20 Check
PLAT703_ALERT_1_C Torsion Calc    -52.3(5), Rep    -52.9(6), Dev..       1.20 Sigma
             C(4)-C(7)-C(13-C(8)  1_555  1_555  1_555  1_555      #   25 Check
PLAT703_ALERT_1_C Torsion Calc     -1.6(6), Rep     -0.9(7), Dev..       1.17 Sigma
             C(4)-C(7)-C(14-C(17  1_555  1_555  1_555  1_555      #   26 Check
PLAT703_ALERT_1_C Torsion Calc   -107.4(4), Rep   -106.6(5), Dev..       2.00 Sigma
             C(14-C(7)-C(13-C(6)  1_555  1_555  1_555  1_555      #   29 Check
PLAT703_ALERT_1_C Torsion Calc     80.3(5), Rep     81.0(6), Dev..       1.40 Sigma
             C(11-C(8)-C(13-C(7)  1_555  1_555  1_555  1_555      #   35 Check
```

Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      0.500 Report
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..       0.93 mm
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  C2             I2 Note
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O1       .      108.7 Degree
PLAT791_ALERT_4_G Model has Chirality at C6          (Sohnke SpGr)          R Verify
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ           2 Units
```

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

  13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   3 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* or *IUCrData*, 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

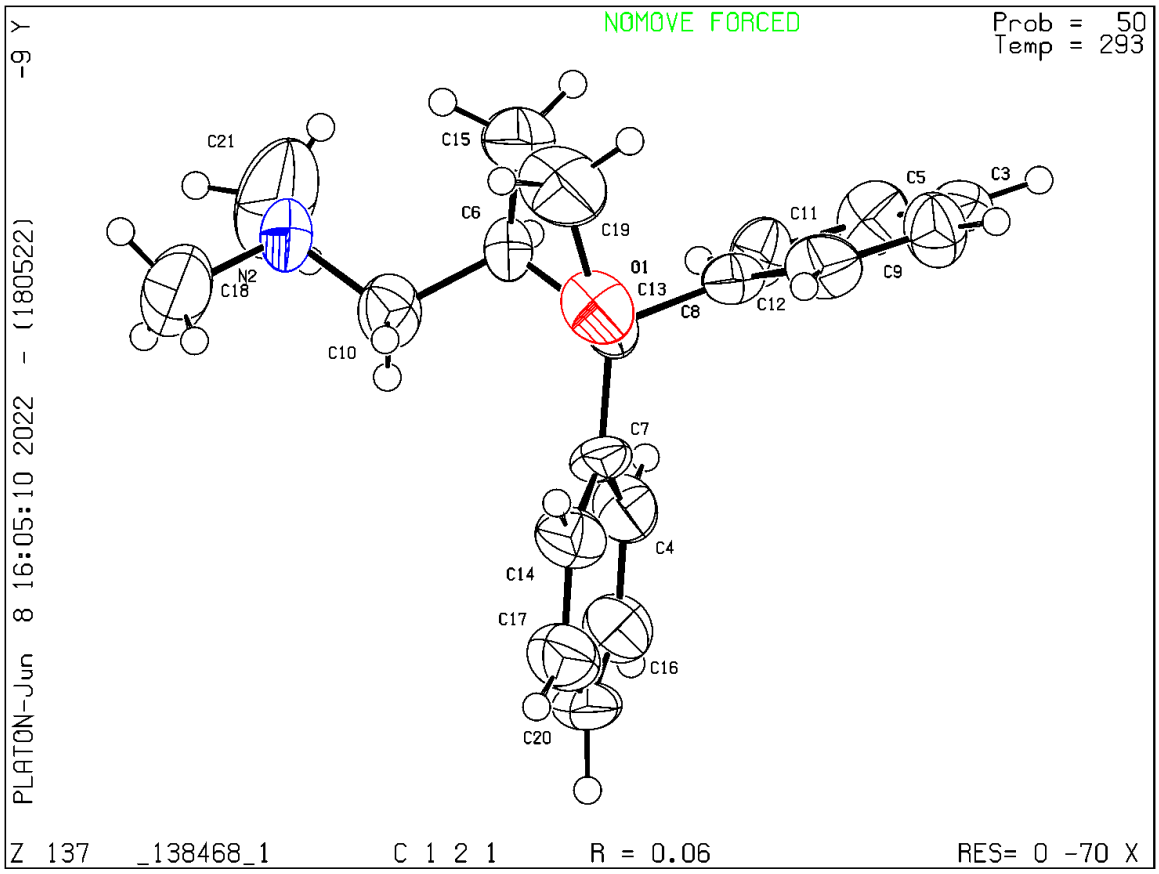
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_REFLT02__138468_1
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__138468_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMX02__138468_1
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT230__138468_1
;
PROBLEM: Hirshfeld Test Diff for    N2       --C18      .        9.4 s.u.
RESPONSE: ...
;
_vrf_PLAT166__138468_1
```

```
;
PROBLEM: S.U's Given on Coordinates for Calc-flagged ....         H3 Note
RESPONSE: ...
;
_vrf_PLAT220__138468_1
;
PROBLEM: NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.3 Ratio
RESPONSE: ...
;
_vrf_PLAT241__138468_1
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of        C19 Check
RESPONSE: ...
;
_vrf_PLAT242__138468_1
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of         N2 Check
RESPONSE: ...
;
_vrf_PLAT340__138468_1
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............     0.0065 Ang.
RESPONSE: ...
;
_vrf_PLAT703__138468_1
;
PROBLEM: Torsion Calc     38.5(5), Rep     37.9(6), Dev..       1.20 Sigma
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock _138468_1 - ellipsoid plot