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: _138472_1

```
Bond precision:   C-C = 0.0063 A          Wavelength=1.54187

Cell:             a=6.2318(4)     b=16.9732(9)         c=11.3789(7)
                  alpha=90        beta=100.264(4)      gamma=90
Temperature:      293 K

                 Calculated                Reported
Volume           1184.33(12)               1184.33(12)
Space group      P 21                      P 1 21 1
Hall group       P 2yb                     P 2yb
Moiety formula   C19 H24 N O, C8 H7 O3     C27 H31 N O4
Sum formula      C27 H31 N O4              C27 H31 N O4
Mr               433.53                    433.55
Dx,g cm-3        1.216                     1.216
Z                2                         2
Mu (mm-1)        0.648                     0.649
F000             464.0                     464.0
F000'            465.37
h,k,lmax         7,20,14                   7,20,14
Nref             4631[ 2398]               4116
Tmin,Tmax        0.869,0.937               0.697,0.937
Tmin'            0.845

Correction method= # Reported T Limits: Tmin=0.697 Tmax=0.937
AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.89        Theta(max)= 71.750

R(reflections)= 0.0455( 6616)                wR2(reflections)=
                                             0.0668( 6669)
S = 1.058                 Npar= 325
```

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 = -1.770
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.

PLAT097_ALERT_2_A Large Reported Max. (Positive) Residual Density 1.90 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 -1.77 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 = 4116
Number of reflections greater than sigma threshold = 6616
PLAT230_ALERT_2_B Hirshfeld Test Diff for C9 --C23 . 7.7 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C19 --C30 . 7.9 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C19 --C32 . 10.2 s.u.
PLAT353_ALERT_3_B Long N-H (N0.87,N1.01A) N1 - H1 . 1.17 Ang.
PLAT703_ALERT_1_B Torsion Calc -3.3(7), Rep -4.8(11), Dev.. 2.14 Sigma
C(13-C(22-C(32-C(19 1_555 1_555 1_555 1_555 # 58 Check

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.
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ..... 7.38 Note
PLAT166_ALERT_4_C S.U's Given on Coordinates for Calc-flagged .... H1 Note
PLAT230_ALERT_2_C Hirshfeld Test Diff for C7 --C9 . 7.0 s.u.

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PLAT230_ALERT_2_C Hirshfeld Test Diff for    C18      --C28      .        5.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C23      --C25      .        5.2 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22      --C32      .       0.16 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00627 Ang.
PLAT703_ALERT_1_C Torsion Calc     17.2(3), Rep     17.7(5), Dev..       1.67 Sigma
             C(6)-O(1)-C(25-C(23  1_555  1_555  1_555  1_555      #    1 Check
PLAT703_ALERT_1_C Torsion Calc     60.4(4), Rep     59.9(5), Dev..       1.25 Sigma
             C(12-N(1)-C(7)-C(9)  1_555  1_555  1_555  1_555      #    5 Check
PLAT703_ALERT_1_C Torsion Calc     17.6(4), Rep     17.1(6), Dev..       1.25 Sigma
             O(2)-C(1)-C(31-O(5)  1_555  1_555  1_555  1_555      #    7 Check
PLAT703_ALERT_1_C Torsion Calc   -157.7(3), Rep   -157.3(5), Dev..       1.33 Sigma
             O(1)-C(6)-C(8)-C(15  1_555  1_555  1_555  1_555      #   11 Check
PLAT703_ALERT_1_C Torsion Calc   -179.7(3), Rep    179.9(3), Dev..       1.33 Sigma
             O(1)-C(6)-C(11-C(17  1_555  1_555  1_555  1_555      #   15 Check
PLAT703_ALERT_1_C Torsion Calc      2.8(5), Rep      2.2(8), Dev..       1.20 Sigma
             C(15-C(8)-C(24-C(29  1_555  1_555  1_555  1_555      #   33 Check
PLAT703_ALERT_1_C Torsion Calc     -1.1(7), Rep      0.0(10), Dev..      1.57 Sigma
             C(20-C(13-C(22-C(32  1_555  1_555  1_555  1_555      #   41 Check
PLAT703_ALERT_1_C Torsion Calc      3.4(6), Rep     2.6(10), Dev..       1.33 Sigma
             C(22-C(13-C(20-C(30  1_555  1_555  1_555  1_555      #   42 Check
PLAT703_ALERT_1_C Torsion Calc   -175.8(4), Rep   -175.3(6), Dev..       1.25 Sigma
             C(31-C(13-C(22-C(32  1_555  1_555  1_555  1_555      #   48 Check
PLAT703_ALERT_1_C Torsion Calc      5.2(8), Rep     6.7(12), Dev..       1.88 Sigma
             C(30-C(19-C(32-C(22  1_555  1_555  1_555  1_555      #   55 Check
PLAT703_ALERT_1_C Torsion Calc     -3.0(9), Rep    -4.3(13), Dev..       1.44 Sigma
             C(32-C(19-C(30-C(20  1_555  1_555  1_555  1_555      #   56 Check
PLAT703_ALERT_1_C Torsion Calc     -1.3(8), Rep    -0.4(11), Dev..       1.12 Sigma
             C(13-C(20-C(30-C(19  1_555  1_555  1_555  1_555      #   57 Check
PLAT703_ALERT_1_C Torsion Calc     11.8(3), Rep     11.4(4), Dev..       1.33 Sigma
             C(9)-C(23-C(25-O(1)  1_555  1_555  1_555  1_555      #   59 Check
PLAT751_ALERT_4_C Bond    Calc     0.95000, Rep    0.950(4) ......  Senseless s.u.
             C(9)     -H(17)           1_555   1_555 ........     #   21 Check
PLAT752_ALERT_4_C Angle   Calc      111.00, Rep    111.2(3) ......  Senseless s.u.
             C(6)    -C(9)    -H(17)      1_555  1_555  1_555     #   29 Check
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep    110.4(3) ......  Senseless s.u.
             C(7)    -C(9)    -H(17)      1_555  1_555  1_555     #   31 Check
PLAT752_ALERT_4_C Angle   Calc      112.00, Rep    112.4(3) ......  Senseless s.u.
             C(23)   -C(9)    -H(17)      1_555  1_555  1_555     #   32 Check
PLAT754_ALERT_4_C Contact Calc     3.19000, Rep    3.189(4) ......  Senseless s.u.
             O(1)     -H(17)           1_555   1_655 ........     #   65 Check
PLAT754_ALERT_4_C Contact Calc     3.55000, Rep    3.552(5) ......  Senseless s.u.
             C(27)    -H(17)           1_555   1_655 ........     #   65 Check
PLAT754_ALERT_4_C Contact Calc     3.19000, Rep    3.189(4) ......  Senseless s.u.
             H(17)    -O(1)            1_555   1_455 ........     #   65 Check
PLAT754_ALERT_4_C Contact Calc     3.55000, Rep    3.552(5) ......  Senseless s.u.
             H(17)    -C(27)           1_555   1_455 ........     #   65 Check
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Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
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       .      106.6 Degree
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PLAT791_ALERT_4_G Model has Chirality at C9          (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C31         (Sohnke SpGr)          R Verify
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 with s.u.       0.20 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 !
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   3 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  34 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

  22 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
  13 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__138472_1
;
PROBLEM: The number of reflections greater than the sigma threshold
RESPONSE: ...
;
_vrf_DIFMN03__138472_1
;
PROBLEM: The minimum difference density is < -0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_DIFMX02__138472_1
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT230__138472_1
;
PROBLEM: Hirshfeld Test Diff for    C9       --C23      .        7.7 s.u.
RESPONSE: ...
;
_vrf_PLAT353__138472_1
;
PROBLEM: Long   N-H (N0.87,N1.01A)  N1       - H1       .       1.17 Ang.
RESPONSE: ...
;
_vrf_PLAT703__138472_1
;
PROBLEM: Torsion Calc     -3.3(7), Rep    -4.8(11), Dev..       2.14 Sigma
RESPONSE: ...
;
_vrf_PLAT042__138472_1
;
PROBLEM: Calc. and Reported MoietyFormula Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT089__138472_1
;
PROBLEM: Poor Data / Parameter Ratio (Zmax < 18) ........       7.38 Note
RESPONSE: ...
;
_vrf_PLAT166__138472_1
;
PROBLEM: S.U's Given on Coordinates for Calc-flagged ....         H1 Note
RESPONSE: ...
;
_vrf_PLAT234__138472_1
;
PROBLEM: Large Hirshfeld Difference C22      --C32      .       0.16 Ang.
RESPONSE: ...
;
_vrf_PLAT242__138472_1
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of         N1 Check
RESPONSE: ...
;
_vrf_PLAT340__138472_1
```

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;
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.00627 Ang.
RESPONSE: ...
;
_vrf_PLAT751__138472_1
;
PROBLEM: Bond    Calc     0.95000, Rep    0.950(4) ......  Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT752__138472_1
;
PROBLEM: Angle   Calc      111.00, Rep    111.2(3) ......  Senseless s.u.
RESPONSE: ...
;
_vrf_PLAT754__138472_1
;
PROBLEM: Contact Calc     3.19000, Rep    3.189(4) ......  Senseless s.u.
RESPONSE: ...
;
# end Validation Reply Form
```

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

Datablock _138472_1 - ellipsoid plot