checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SQ1820, SQDH2020

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: SQ1820

```
Bond precision:  C-C = 0.0004 A          Wavelength=0.71073

Cell:              a=15.072(2)      b=7.9873(9)      c=6.8410(9)
                   alpha=90         beta=90          gamma=90
Temperature:       18 K

                 Calculated                Reported
Volume           823.55(18)                823.55(18)
Space group      P b c n                   P b c n
Hall group       -P 2n 2ab                 -P 2n 2ab
Moiety formula   C8 H12 N2 O2              C8 H12 N2 O2
Sum formula      C8 H12 N2 O2              C8 H12 N2 O2
Mr               168.20                    168.20
Dx,g cm-3        1.357                     1.357
Z                4                         4
Mu (mm-1)        0.099                     0.099
F000             360.0                     360.0
F000'            360.16
h,k,lmax         34,18,15                  34,18,15
Nref             5162                      5163
Tmin,Tmax        0.963,0.976               0.970,0.979
Tmin'            0.963

Correction method= # Reported T Limits: Tmin=0.970 Tmax=0.979
AbsCorr = NONE

Data completeness= 1.000          Theta(max)= 54.394

R(reflections)= 0.0314( 4340)     wR2(reflections)= 0.0989( 5163)

S = 1.113                 Npar= 56
```

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

CELLK01_ALERT_1_C Check that the cell measurement temperature is in Kelvin.
Value of measurement temperature given = 18.000

Author Response: That's correct. The data collection was performed at 18(1) K.

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

Author Response: The maximum Fourier difference is located near the C1 atom. It depends on the anisotropic features of its charge density distribution. The latter are neatly detectable with the Independent Atom Model, as this dataset was collected at 18(1) K.

PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 0.61 eA-3

Author Response: The maximum Fourier difference is located near the C1 atom. It depends on the anisotropic features of its charge density distribution. The latter are neatly detectable with the Independent Atom Model, as this dataset was collected at 18(1) K.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H4A . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H4B . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H4C . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H3A . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H3B . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

```
PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H3C        .          6 Check
```

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

```
PLAT351_ALERT_3_C Long   C-H (X0.96,N1.08A)  C4       - H4C      .       1.11 Ang.
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.08000, Rep   1.0793(3) ......  Senseless s.u.
              C3       -H3A            1.555   1.555 ........     #    7 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.09000, Rep   1.0873(3) ......  Senseless s.u.
              C3       -H3B            1.555   1.555 ........     #    8 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.06000, Rep   1.0624(3) ......  Senseless s.u.
              C3       -H3C            1.555   1.555 ........     #    9 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.06000, Rep   1.0624(3) ......  Senseless s.u.
              C4       -H4A            1.555   1.555 ........     #   11 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.07000, Rep   1.0728(3) ......  Senseless s.u.
              C4       -H4B            1.555   1.555 ........     #   12 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.11000, Rep   1.1144(3) ......  Senseless s.u.
              C4       -H4C            1.555   1.555 ........     #   13 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   109.60(3) ......  Senseless s.u.
             N6      -C3      -H3A        1.555  1.555  1.555     #    7 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep   109.39(3) ......  Senseless s.u.
             N6      -C3      -H3B        1.555  1.555  1.555     #    8 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   110.11(3) ......  Senseless s.u.
             H3A     -C3      -H3B        1.555  1.555  1.555     #    9 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      108.00, Rep   107.77(2) ......  Senseless s.u.
             N6      -C3      -H3C        1.555  1.555  1.555     #   10 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   109.57(3) ......  Senseless s.u.
             H3A     -C3      -H3C        1.555  1.555  1.555     #   11 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   110.36(3) ......  Senseless s.u.
             H3B     -C3      -H3C        1.555  1.555  1.555     #   12 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep   109.40(2) ......  Senseless s.u.
             N6      -C4      -H4A        1.555  1.555  1.555     #   13 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   110.08(3) ......  Senseless s.u.
             N6      -C4      -H4B        1.555  1.555  1.555     #   14 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   109.53(3) ......  Senseless s.u.
             H4A     -C4      -H4B        1.555  1.555  1.555     #   15 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep   109.00(2) ......  Senseless s.u.
             N6      -C4      -H4C        1.555  1.555  1.555     #   16 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   109.86(3) ......  Senseless s.u.
             H4A     -C4      -H4C        1.555  1.555  1.555     #   17 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep   108.97(2) ......  Senseless s.u.
             H4B     -C4      -H4C        1.555  1.555  1.555     #   18 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -0.209 Report
```

Author Response: This is a high-resolution dataset collected at 18(1) K. The problem is due to weak high-order data and is solved by applying a multipole model for the charge density analysis.

Alert level G

```
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C1              3.17 Ang.
                                          1-x,y,1/2-z  =      2_655 Check
PLAT760_ALERT_1_G CIF Contains no Torsion Angles .................          ? Info
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.17 Ratio
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          4 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  29 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

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
  19 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: SQDH2020

Bond precision: C-C = 0.0008 A Wavelength=0.71073

Cell: a=7.959(1) b=7.154(1) c=17.799(2)
alpha=90 beta=91.68(1) gamma=90
Temperature: 20 K

	Calculated	Reported
Volume	1013.0(2)	1013.0(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C8 H12 N2 O2, 2(H2 O)	C8 H12 N2 O2, 2(H2 O)
Sum formula	C8 H16 N2 O4	C8 H16 N2 O4
Mr	204.23	204.23
Dx,g cm-3	1.339	1.339
Z	4	4
Mu (mm-1)	0.107	0.107
F000	440.0	440.0
F000’	440.24	
h,k,lmax	18,16,40	18,15,38
Nref	12822	5535
Tmin,Tmax	0.968,0.984	0.968,0.984
Tmin’	0.948	

Correction method= # Reported T Limits: Tmin=0.968 Tmax=0.984
AbsCorr = NONE

Data completeness= 0.432 Theta(max)= 54.629

R(reflections)= 0.0305(4873) wR2(reflections)= 0.0867(5535)

S = 1.052 Npar= 127

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
CELLK01_ALERT_1_C Check that the cell measurement temperature is in Kelvin.
Value of measurement temperature given = 20.000

Author Response: That’s correct. The data collection was performed at 20(1) K.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H1 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H2 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H3 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H4 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H5 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H6 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H7 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H8 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H9 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H10 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H11 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H12 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H13 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H14 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H15 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT218_ALERT_3_C Constrained U(ij) Components(s) for H16 . 6 Check

Author Response: Anisotropic U(ij) components were estimated by ADPH (Roversi & Destro, 2004) and never refined.

PLAT230_ALERT_2_C Hirshfeld Test Diff for O2 --C5 . 5.5 s.u.

Author Response: This minor failure of the Hirshfeld rigid bond test is likely due to the rigid body librational motion of the C~4~ ring, but it does not hamper the accurate determination of the overall molecular charge density features.

PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C8 - H10 . 1.11 Ang.

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.07000, Rep   1.0735(6) ......  Senseless s.u.
             C3       -H1             1.555   1.555 ........     #    8 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.10000, Rep   1.0989(6) ......  Senseless s.u.
             C3       -H2             1.555   1.555 ........     #    9 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.09000, Rep   1.0911(6) ......  Senseless s.u.
             C3       -H3             1.555   1.555 ........     #   10 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.06000, Rep   1.0614(6) ......  Senseless s.u.
             C4       -H4             1.555   1.555 ........     #   11 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.09000, Rep   1.0885(6) ......  Senseless s.u.
             C4       -H5             1.555   1.555 ........     #   12 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.08000, Rep   1.0757(6) ......  Senseless s.u.
             C4       -H6             1.555   1.555 ........     #   13 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.09000, Rep   1.0869(6) ......  Senseless s.u.
             C7       -H7             1.555   1.555 ........     #   21 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.08000, Rep   1.0785(6) ......  Senseless s.u.
             C7       -H8             1.555   1.555 ........     #   22 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.09000, Rep   1.0886(6) ......  Senseless s.u.
              C7       -H9             1.555   1.555 ........     #   23 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.11000, Rep   1.1059(7) ......  Senseless s.u.
              C8       -H10            1.555   1.555 ........     #   24 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.08000, Rep   1.0780(6) ......  Senseless s.u.
              C8       -H11            1.555   1.555 ........     #   25 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     1.09000, Rep   1.0908(6) ......  Senseless s.u.
              C8       -H12            1.555   1.555 ........     #   26 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     0.96000, Rep   0.9622(5) ......  Senseless s.u.
              O3       -H13            1.555   1.555 ........     #   27 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     0.96000, Rep   0.9625(5) ......  Senseless s.u.
              O3       -H14            1.555   1.555 ........     #   28 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     0.96000, Rep   0.9628(5) ......  Senseless s.u.
              O4       -H15            1.555   1.555 ........     #   29 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT751_ALERT_4_C Bond    Calc     0.96000, Rep   0.9621(5) ......  Senseless s.u.
              O4       -H16            1.555   1.555 ........     #   30 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep   108.59(5) ......  Senseless s.u.
             N1      -C3      -H1         1.555  1.555  1.555     #   10 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      109.00, Rep   108.79(5) ......  Senseless s.u.
             N1      -C3      -H2         1.555  1.555  1.555     #   11 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      111.00, Rep   110.60(5) ......  Senseless s.u.
             H1      -C3      -H2         1.555  1.555  1.555     #   12 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      108.00, Rep   108.14(5) ......  Senseless s.u.
             N1      -C3      -H3         1.555  1.555  1.555     #   13 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   110.44(6) ......  Senseless s.u.
             H1      -C3      -H3         1.555  1.555  1.555     #   14 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   110.22(5) ......  Senseless s.u.
             H2      -C3      -H3         1.555  1.555  1.555     #   15 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      108.00, Rep   107.99(5) ......  Senseless s.u.
             N1      -C4      -H4         1.555  1.555  1.555     #   16 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      110.00, Rep   109.52(5) ......  Senseless s.u.
             N1      -C4      -H5         1.555  1.555  1.555     #   17 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 109.00, Rep 109.12(6) ..... Senseless s.u.
H4 -C4 -H5 1.555 1.555 1.555 # 18 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 109.00, Rep 108.77(5) ..... Senseless s.u.
N1 -C4 -H6 1.555 1.555 1.555 # 19 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 111.00, Rep 110.59(5) ..... Senseless s.u.
H4 -C4 -H6 1.555 1.555 1.555 # 20 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 111.00, Rep 110.81(5) ..... Senseless s.u.
H5 -C4 -H6 1.555 1.555 1.555 # 21 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 109.00, Rep 109.00(5) ..... Senseless s.u.
N2 -C7 -H7 1.555 1.555 1.555 # 31 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 109.00, Rep 109.48(5) ..... Senseless s.u.
N2 -C7 -H8 1.555 1.555 1.555 # 32 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 110.00, Rep 110.33(5) ..... Senseless s.u.
H7 -C7 -H8 1.555 1.555 1.555 # 33 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 109.00, Rep 109.35(5) ..... Senseless s.u.
N2 -C7 -H9 1.555 1.555 1.555 # 34 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 108.00, Rep 107.65(5) ..... Senseless s.u.
H7 -C7 -H9 1.555 1.555 1.555 # 35 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 111.00, Rep 110.98(5) ..... Senseless s.u.
H8 -C7 -H9 1.555 1.555 1.555 # 36 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 109.00, Rep 108.99(5) ..... Senseless s.u.
N2 -C8 -H10 1.555 1.555 1.555 # 37 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 109.00, Rep 108.53(5) ..... Senseless s.u.
N2 -C8 -H11 1.555 1.555 1.555 # 38 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 111.00, Rep 111.01(5) ..... Senseless s.u.
H10 -C8 -H11 1.555 1.555 1.555 # 39 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 109.00, Rep 109.17(5) ..... Senseless s.u.
N2 -C8 -H12 1.555 1.555 1.555 # 40 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 110.00, Rep 110.08(5) ..... Senseless s.u.
H10 -C8 -H12 1.555 1.555 1.555 # 41 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

PLAT752_ALERT_4_C Angle Calc 109.00, Rep 109.03(5) ..... Senseless s.u.
H11 -C8 -H12 1.555 1.555 1.555 # 42 Check

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      104.00, Rep   103.66(5) ......  Senseless s.u.
             H13     -O3      -H14        1.555  1.555  1.555     #   43 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

```
PLAT752_ALERT_4_C Angle   Calc      108.00, Rep   108.13(5) ......  Senseless s.u.
             H15     -O4      -H16        1.555  1.555  1.555     #   44 Check
```

Author Response: Positions of H atoms were estimated from multipole refinements with polarized basis.

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          4 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical         ? Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C1       ..C5             3.20 Ang.
                                                    x,y,z  =      1_555 Check
PLAT760_ALERT_1_G CIF Contains no Torsion Angles .................         ? Info
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.17 Ratio
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
             H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          4 Note
             H2 O
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       7169 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.0 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ           2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ           2 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          4 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  61 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

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
  18 ALERT type 3 Indicator that the structure quality may be low
  46 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

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checkCIF publication errors

Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

```
   0 ALERT level A = Data missing that is essential or data in wrong format
   1 ALERT level G = General alerts. Data that may be required is missing
```

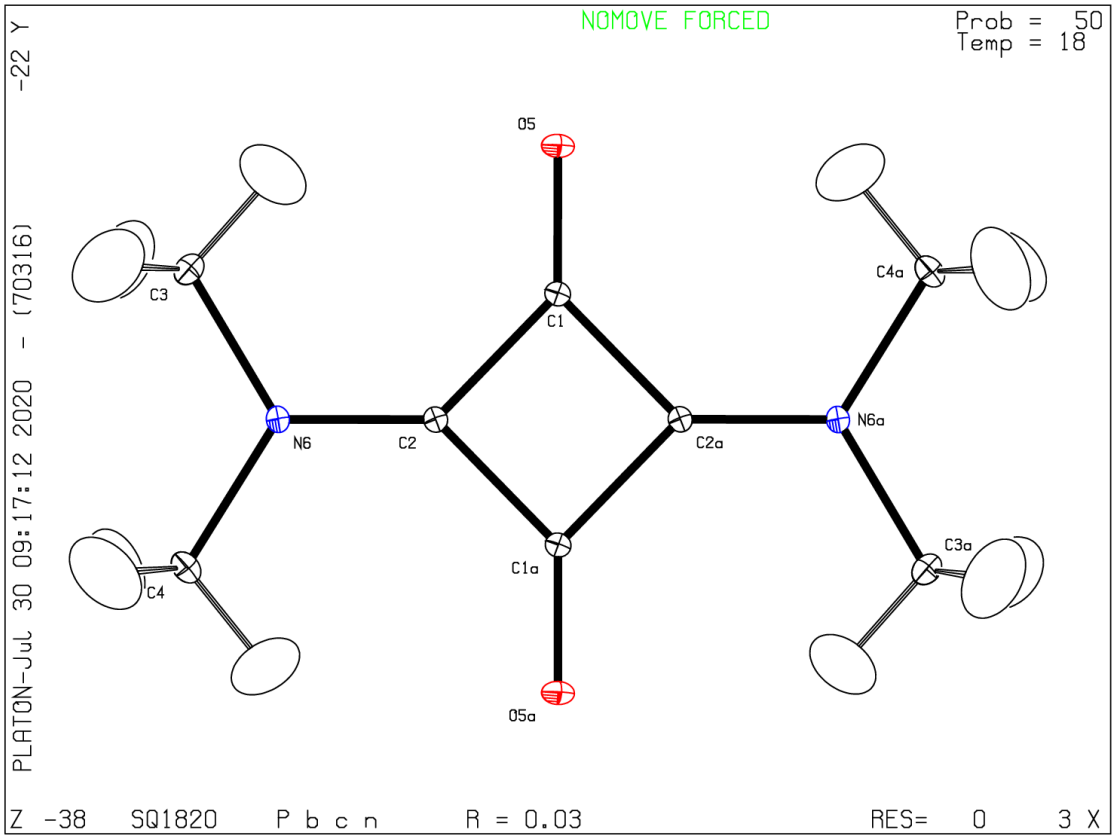
Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 16/07/2020; check.def file version of 12/07/2020

Datablock SQ1820 - ellipsoid plot



Datablock SQDH2020 - ellipsoid plot