checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: subTAPOH

Bond precision: C-C = 0.0083 A Wavelength=0.71070

Cell: a=12.859(4) b=10.915(4) c=16.933(6)
alpha=90 beta=93.780(6) gamma=90

	Calculated	Reported
Volume	2371.5(14)	2371.0(10)
Space group	P c	P 1 c 1
Hall group	P -2yc	?
Moiety formula	C24 H31 B N6 O	C48 H62 B2 N12 O2
Sum formula	C24 H31 B N6 O	C48 H62 B2 N12 O2
Mr	430.36	860.72
Dx,g cm-3	1.205	1.205
Z	4	2
Mu (mm-1)	0.076	0.076
F000	920.0	0.0
F000'	920.29	
h,k,lmax	15,13,20	15,13,20
Nref	4670(9327)	8427
Tmin,Tmax	0.981,0.992	0.904,0.992
Tmin'	0.981	

Correction method= 'MULTI-SCAN'

Data completeness= 1.80(0.90) Theta(max)= 26.00

R(reflections)= 0.0460(5761) wR2(reflections)= wR= 0.0498(5761)

S = 1.139 Npar= 577

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

```
WEIGH01_ALERT_1_A  Unit weights are not acceptable for submissions to Acta
            Crystallographica Section C.
            n.b. unit is however a legal CIF keyword.
PLAT220_ALERT_2_A Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       4.53 Ratio
PLAT351_ALERT_3_A Long    C-H Bond (0.96A)   C17    -   H12    ...       1.29 Ang.
PLAT390_ALERT_3_A Deviating Methyl C40     X-C-H Bond Angle ......      93.31 Deg.
```

```
PLAT390_ALERT_3_A Deviating Methyl C44     X-C-H Bond Angle ......     126.59 Deg.
PLAT390_ALERT_3_A Deviating Methyl C46     X-C-H Bond Angle ......     134.37 Deg.
PLAT391_ALERT_3_A Deviating Methyl C24     H-C-H Bond Angle ......     124.31 Deg.
PLAT391_ALERT_3_A Deviating Methyl C24     H-C-H Bond Angle ......      77.53 Deg.
PLAT391_ALERT_3_A Deviating Methyl C44     H-C-H Bond Angle ......      85.49 Deg.
```

Alert level B

```
PLAT024_ALERT_4_B Merging of Friedel pairs is STRONGLY indicated .          !
PLAT220_ALERT_2_B Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       4.21 Ratio
PLAT351_ALERT_3_B Long    C-H Bond (0.96A)   C44    -   H49    ...       1.20 Ang.
PLAT390_ALERT_3_B Deviating Methyl C18     X-C-H Bond Angle ......      95.63 Deg.
PLAT390_ALERT_3_B Deviating Methyl C38     X-C-H Bond Angle ......      96.67 Deg.
PLAT390_ALERT_3_B Deviating Methyl C40     X-C-H Bond Angle ......     122.19 Deg.
PLAT413_ALERT_2_B Short Inter XH3 .. XHn     H20    ..  H47     ..       1.98 Ang.
```

Alert level C

```
REFLE01_ALERT_3_C  The _reflns_threshold_multiplier given is >= 4
            Premultiplier =    4.00
REFLE01_ALERT_3_C  The _reflns_threshold_multiplier given is >= 4
            Premultiplier =    4.00
SHFSU01_ALERT_2_C  The absolute value of parameter shift to su ratio > 0.05
            Absolute value of the parameter shift to su ratio given   0.065
            Additional refinement cycles may be required.
PLAT041_ALERT_1_C Calc. and Rep. SumFormula Strings    Differ ....          ?
PLAT042_ALERT_1_C Calc. and Rep. MoietyFormula Strings Differ ....          ?
PLAT045_ALERT_1_C Calculated and Reported Z Differ by ............       2.00 Ratio
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...          ?
PLAT080_ALERT_2_C Maximum Shift/Error ............................       0.06
PLAT150_ALERT_1_C Volume as Calculated Differs from that Given ...    2371.00 Ang-3
PLAT152_ALERT_1_C Supplied and Calc Volume s.u. Inconsistent .....          ?
PLAT213_ALERT_2_C Atom C19     has ADP max/min Ratio ............       3.70 prolat
PLAT222_ALERT_3_C Large Non-Solvent    H     Ueq(max)/Ueq(min) ...       3.17 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C15    -   C16     ..       5.18 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C37    -   C38     ..       5.05 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C45    -   C46     ..       5.01 su
PLAT242_ALERT_2_C Check Low    U(eq) as Compared to Neighbors  for        C45
PLAT320_ALERT_2_C Check Hybridisation of  C19    in Main Residue .          ?
PLAT320_ALERT_2_C Check Hybridisation of  C44    in Main Residue .          ?
PLAT320_ALERT_2_C Check Hybridisation of  C46    in Main Residue .          ?
PLAT340_ALERT_3_C Low Bond Precision on C-C bonds (x 1000) Ang ...          8
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C15    -   H6     ...       1.14 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C17    -   H11    ...       1.15 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C19    -   H17    ...       1.12 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C37    -   H33    ...       1.14 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C39    -   H38    ...       1.13 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C40    -   H39    ...       1.14 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C40    -   H40    ...       1.13 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C47    -   H57    ...       1.14 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C47    -   H58    ...       1.11 Ang.
PLAT351_ALERT_3_C Long    C-H Bond (0.96A)   C48    -   H60    ...       1.11 Ang.
PLAT355_ALERT_3_C Long    O-H Bond (0.82A)   O1     -   H31    ...       1.06 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C19    -   C20    ...       1.37 Ang.
PLAT390_ALERT_3_C Deviating Methyl C24     X-C-H Bond Angle ......     118.54 Deg.
PLAT390_ALERT_3_C Deviating Methyl C24     X-C-H Bond Angle ......     117.70 Deg.
PLAT390_ALERT_3_C Deviating Methyl C42     X-C-H Bond Angle ......     101.76 Deg.
PLAT390_ALERT_3_C Deviating Methyl C44     X-C-H Bond Angle ......     116.75 Deg.
PLAT390_ALERT_3_C Deviating Methyl C46     X-C-H Bond Angle ......     101.73 Deg.
PLAT391_ALERT_3_C Deviating Methyl C16     H-C-H Bond Angle ......     101.29 Deg.
PLAT391_ALERT_3_C Deviating Methyl C46     H-C-H Bond Angle ......     101.53 Deg.
```

```
PLAT391_ALERT_3_C Deviating Methyl C46     H-C-H Bond Angle ......     100.88 Deg.
PLAT411_ALERT_2_C Short Inter H...H Contact  H2     ..  H22     ..       2.15 Ang.
PLAT432_ALERT_2_C Short Inter X...Y Contact  C12    ..  C28     ..       3.16 Ang.
PLAT731_ALERT_1_C Bond    Calc    1.380(9), Rep    1.379(4) ......       2.25 su-Rat
              N(1) -C(1)    1.555   1.555
PLAT731_ALERT_1_C Bond    Calc    1.349(9), Rep    1.349(4) ......       2.25 su-Rat
              N(4) -C(4)    1.555   1.555
PLAT731_ALERT_1_C Bond    Calc    1.347(9), Rep    1.347(4) ......       2.25 su-Rat
              N(5) -C(9)    1.555   1.555
PLAT731_ALERT_1_C Bond    Calc    1.345(9), Rep    1.345(4) ......       2.25 su-Rat
              N(7) -C(28)   1.555   1.555
PLAT731_ALERT_1_C Bond    Calc    1.369(9), Rep    1.369(4) ......       2.25 su-Rat
              N(8) -C(29)   1.555   1.555
PLAT731_ALERT_1_C Bond    Calc    1.350(9), Rep    1.350(4) ......       2.25 su-Rat
              N(12)-C(25)   1.555   1.555
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          2
              C24 H31 B N6 O
```

Alert level G

```
REFLT03_ALERT_4_G  ALERT: MoKa measured Friedel data cannot be used to
                   determine absolute structure in a light-atom
                   study EXCEPT under VERY special conditions.
                   It is preferred that Friedel data is merged in such cases.
           From the CIF: _diffrn_reflns_theta_max           26.00
           From the CIF: _reflns_number_total               8427
           Count of symmetry unique reflns         4670
           Completeness (_total/calc)            180.45%
           TEST3: Check Friedels for noncentro structure
           Estimate of Friedel pairs measured      3757
           Fraction of Friedel pairs measured     0.804
           Are heavy atom types Z>Si present         no
```

---

9 **ALERT level A** = In general: serious problem
7 **ALERT level B** = Potentially serious problem
49 **ALERT level C** = Check and explain
1 **ALERT level G** = General alerts; check

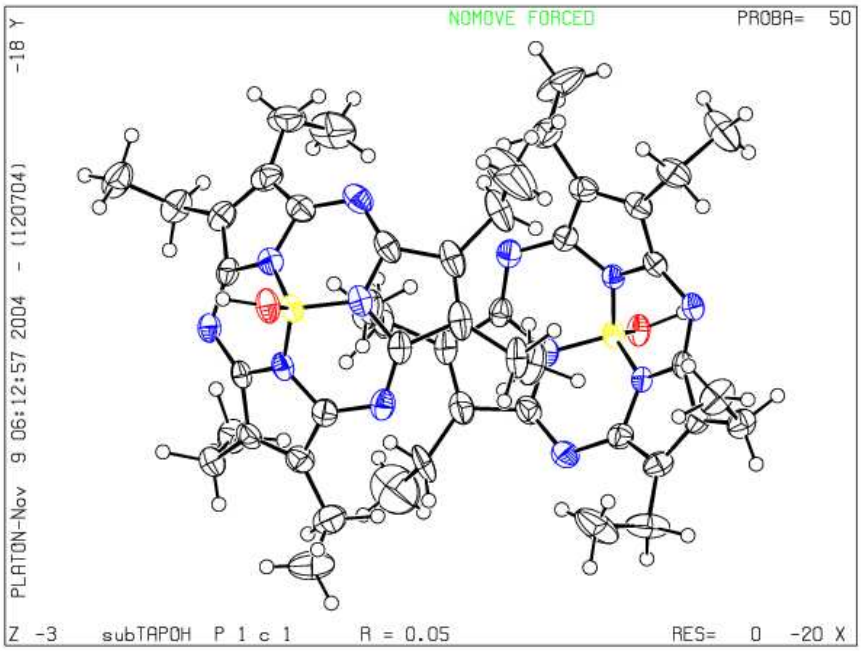
13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 ALERT type 2 Indicator that the structure model may be wrong or deficient
34 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion

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*, 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.

PLATON version of 12/07/2004; check.def file version of 12/07/2004

Datablock subTAPOH - ellipsoid plot