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# 1-(4-*tert*-Butylbenzyl)-2-(4-*tert*-butylphenyl)-1*H*-benzimidazole

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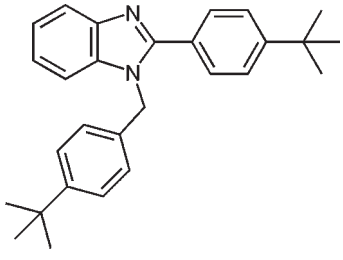
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; disorder in main residue; $R$ factor = 0.061; $wR$ factor = 0.135; data-to-parameter ratio = 17.3.

In the molecule of the title compound, $C_{28}H_{32}N_2$, the benzimidazole ring system is almost planar [maximum deviation = 0.0221 (15) Å] and forms dihedral angles of 85.86 (4) and 32.09 (6)° with the benzene rings. In the crystal structure, molecules are linked into chains running parallel to the *a* axis by intermolecular C—H···N hydrogen bonds. The methyl groups of a *tert*-butyl group are rotationally disordered over two positions with refined site-occupancy factors of 0.636 (4) and 0.364 (4).

## Related literature

For the biological and pharmaceutical properties of benzimidazole derivatives, see: Matsuno *et al.* (2000). Garuti *et al.* (1999). For reference structural data, see: Allen *et al.* (1987).



## Experimental

### Crystal data

$C_{28}H_{32}N_2$
$M_r$ = 396.56
Monoclinic, $P2_1/c$
$a$ = 6.2142 (5) Å
$b$ = 21.1112 (13) Å
$c$ = 17.4624 (12) Å
$\beta$ = 92.869 (6)°
$V$ = 2288.0 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 293 K
0.20 × 0.20 × 0.10 mm

### Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.987, $T_{max}$ = 0.993
24819 measured reflections
5239 independent reflections
4315 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.047

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.135
$S$ = 1.09
5239 reflections
302 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C18—H18$A$···N2$^{i}$ | 0.97 | 2.59 | 3.553 (2) | 174 |

Symmetry code: (i) $x-1, y, z$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2378).

## References

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# supplementary materials

*Acta Cryst.* (2009). E**65**, o3019 [ **doi:10.1107/S1600536809045668** ]

# 1-(4-*tert*-Butylbenzyl)-2-(4-*tert*-butylphenyl)-1*H*-benzimidazole

**J.-C. Zhou, Z.-Y. Zhang, N.-X. Li and C.-M. Zhang**

## Comment

Imidazole and benzimidazole derivatives are important heteroaromatic compounds which have attracted great attention due to their biological and pharmaceutical activities (Matsuno *et al.*, 2000; Garuti *et al.*, 1999). These compounds have also played an important role in the development of coordination chemistry. In this paper, we report the crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The benzimidazole ring system is substantially planar, with a maximum displacement of 0.0221 (15) Å for atom C1. The dihedral angle it forms with the C8—C13 and C19—C24 benzene rings are 32.09 (6) and 85.86 (4) Å, respectively. The benzene rings are oriented perpendicularly to each other, forming a dihedral angle of 89.58 (5) °. In the crystal packing, the molecule are linked into chains running parallel to the *a* axis by intermolecular C—H···N hydrogen bonds (Table 1). The methyl groups of a *tert*-butyl group exhibits rotational disorder over two orientations with site occupation factors of 0.636 (4) and 0.364 (4) for the major and minor components of disorder, respectively.

## Experimental

To a solution of *o*-phenylenediamine (0.432 g, 4 mmol) in ethanol(20 ml), 4-*tert*-butylbenzaldehyde (1.297 g, 8 mmol) was added. The mixture was heated to reflux with stirring for four hour, then cooled to room temperature. The resultant solution was filtered and allowed to evaporate slowly at room temperature. Colourless single crystals of the title compound suitable for X-ray diffraction study were obtained after several weeks.

## Refinement

The C15, C16 and C17 methyl carbon atoms of a *tert*-butyl group are rotationally disordered over two position with refined site occupancy factors of 0.636 (4) and 0.364 (4). All H atoms were located geometrically and treated as riding atoms, with C—H = 0.93–0.97 Å, and with $U_{iso}$(H) = 1.2 $U_{eq}$(C) or 1.5 $U_{eq}$(C) for methyl H atoms.

## Figures

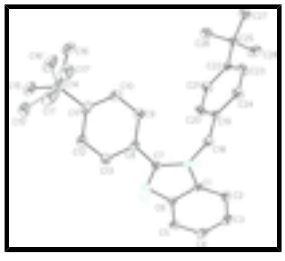


Fig. 1. The molecular structure of the title compound, showing the atomic numbering scheme. The displacement ellipsoids are drawn at the 30% probability level.

## 1-(4-*tert*-Butylbenzyl)-2-(4-*tert*-butylphenyl)-1*H*- benzimidazole

*Crystal data*

| | |
|---|---|
| $C_{28}H_{32}N_2$ | $F_{000}$ = 856 |
| $M_r$ = 396.56 | $D_x$ = 1.151 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 3426 reflections |
| $a$ = 6.2142 (5) Å | θ = 2.3–27.5º |
| $b$ = 21.1112 (13) Å | μ = 0.07 mm$^{-1}$ |
| $c$ = 17.4624 (12) Å | $T$ = 293 K |
| β = 92.869 (6)º | Block, colourless |
| $V$ = 2288.0 (3) Å$^3$ | 0.20 × 0.20 × 0.10 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Rigaku SCXmini diffractometer | 5239 independent reflections |
| Radiation source: fine-focus sealed tube | 4315 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.047 |
| Detector resolution: 13.6612 pixels mm$^{-1}$ | $\theta_{max}$ = 27.5º |
| $T$ = 293 K | $\theta_{min}$ = 3.3º |
| ω scans | $h$ = −8→8 |
| Absorption correction: Multi-scan (CrystalClear; Rigaku, 2005) | $k$ = −27→27 |
| $T_{min}$ = 0.987, $T_{max}$ = 0.993 | $l$ = −22→22 |
| 24819 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.061 | H-atom parameters constrained |
| $wR(F^2)$ = 0.135 | $w = 1/[\sigma^2(F_o^2) + (0.0431P)^2 + 0.936P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.09 | $(\Delta/\sigma)_{max} < 0.001$ |
| 5239 reflections | $\Delta\rho_{max}$ = 0.22 e Å$^{-3}$ |
| 302 parameters | $\Delta\rho_{min}$ = −0.18 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| N1 | 0.7010 (2) | 0.17678 (6) | 0.27399 (7) | 0.0256 (3) | |
| N2 | 1.0343 (2) | 0.14275 (6) | 0.31033 (7) | 0.0298 (3) | |
| C1 | 0.7112 (3) | 0.17535 (7) | 0.35346 (9) | 0.0270 (3) | |
| C2 | 0.5570 (3) | 0.18846 (8) | 0.40650 (10) | 0.0346 (4) | |
| H2B | 0.4192 | 0.2021 | 0.3913 | 0.041* | |
| C3 | 0.6195 (3) | 0.18016 (9) | 0.48290 (10) | 0.0392 (4) | |
| H3A | 0.5214 | 0.1884 | 0.5201 | 0.047* | |
| C4 | 0.8268 (3) | 0.15961 (9) | 0.50544 (10) | 0.0382 (4) | |
| H4A | 0.8632 | 0.1547 | 0.5574 | 0.046* | |
| C5 | 0.9793 (3) | 0.14633 (8) | 0.45281 (10) | 0.0344 (4) | |
| H5A | 1.1170 | 0.1328 | 0.4684 | 0.041* | |
| C6 | 0.9185 (3) | 0.15411 (7) | 0.37498 (9) | 0.0282 (3) | |
| C7 | 0.8992 (2) | 0.15635 (7) | 0.25137 (9) | 0.0258 (3) | |
| C8 | 0.9583 (2) | 0.14654 (7) | 0.17169 (9) | 0.0272 (3) | |
| C9 | 0.8876 (3) | 0.18418 (8) | 0.10959 (9) | 0.0310 (4) | |
| H9A | 0.7887 | 0.2164 | 0.1168 | 0.037* | |
| C10 | 0.9638 (3) | 0.17391 (9) | 0.03713 (10) | 0.0355 (4) | |
| H10A | 0.9141 | 0.1995 | −0.0033 | 0.043* | |
| C11 | 1.1119 (3) | 0.12648 (8) | 0.02342 (10) | 0.0344 (4) | |
| C12 | 1.1810 (3) | 0.08896 (8) | 0.08579 (10) | 0.0370 (4) | |
| H12A | 1.2802 | 0.0568 | 0.0785 | 0.044* | |
| C13 | 1.1055 (3) | 0.09845 (8) | 0.15806 (10) | 0.0335 (4) | |
| H13A | 1.1537 | 0.0723 | 0.1982 | 0.040* | |
| C14 | 1.1974 (3) | 0.11519 (9) | −0.05650 (10) | 0.0424 (5) | |
| C15 | 1.4372 (5) | 0.1228 (2) | −0.0550 (2) | 0.0569 (10) | 0.636 (4) |
| H15A | 1.4726 | 0.1670 | −0.0576 | 0.085* | 0.636 (4) |
| H15B | 1.4930 | 0.1011 | −0.0980 | 0.085* | 0.636 (4) |
| H15C | 1.4996 | 0.1051 | −0.0083 | 0.085* | 0.636 (4) |
| C16 | 1.1017 (6) | 0.16598 (17) | −0.11722 (17) | 0.0508 (9) | 0.636 (4) |
| H16A | 0.9475 | 0.1625 | −0.1212 | 0.076* | 0.636 (4) |
| H16B | 1.1587 | 0.1580 | −0.1664 | 0.076* | 0.636 (4) |
| H16C | 1.1414 | 0.2079 | −0.1004 | 0.076* | 0.636 (4) |
| C17 | 1.1189 (8) | 0.0513 (2) | −0.0846 (2) | 0.0687 (14) | 0.636 (4) |

| | | | | | |
|---|---|---|---|---|---|
| H17A | 0.9695 | 0.0541 | −0.1011 | 0.103* | 0.636 (4) |
| H17B | 1.1360 | 0.0209 | −0.0438 | 0.103* | 0.636 (4) |
| H17C | 1.2014 | 0.0381 | −0.1268 | 0.103* | 0.636 (4) |
| C16' | 1.3128 (12) | 0.1723 (4) | −0.0785 (4) | 0.073 (2) | 0.364 (4) |
| H16D | 1.2128 | 0.2068 | −0.0851 | 0.109* | 0.364 (4) |
| H16E | 1.3811 | 0.1648 | −0.1258 | 0.109* | 0.364 (4) |
| H16F | 1.4201 | 0.1828 | −0.0391 | 0.109* | 0.364 (4) |
| C15' | 1.3773 (13) | 0.0576 (4) | −0.0524 (3) | 0.077 (3) | 0.364 (4) |
| H15D | 1.3107 | 0.0193 | −0.0360 | 0.116* | 0.364 (4) |
| H15E | 1.4934 | 0.0688 | −0.0166 | 0.116* | 0.364 (4) |
| H15F | 1.4323 | 0.0514 | −0.1023 | 0.116* | 0.364 (4) |
| C17' | 1.0230 (11) | 0.0946 (4) | −0.1102 (3) | 0.0593 (19) | 0.364 (4) |
| H17D | 0.9132 | 0.1266 | −0.1137 | 0.089* | 0.364 (4) |
| H17E | 0.9627 | 0.0558 | −0.0922 | 0.089* | 0.364 (4) |
| H17F | 1.0787 | 0.0879 | −0.1598 | 0.089* | 0.364 (4) |
| C18 | 0.5117 (2) | 0.19700 (7) | 0.22771 (9) | 0.0276 (3) | |
| H18A | 0.3834 | 0.1845 | 0.2533 | 0.033* | |
| H18B | 0.5100 | 0.1753 | 0.1787 | 0.033* | |
| C19 | 0.5039 (2) | 0.26793 (7) | 0.21354 (8) | 0.0244 (3) | |
| C20 | 0.6751 (3) | 0.30771 (8) | 0.23238 (10) | 0.0345 (4) | |
| H20A | 0.7992 | 0.2912 | 0.2568 | 0.041* | |
| C21 | 0.6647 (3) | 0.37210 (8) | 0.21545 (10) | 0.0354 (4) | |
| H21A | 0.7823 | 0.3976 | 0.2292 | 0.042* | |
| C22 | 0.4846 (2) | 0.39941 (7) | 0.17869 (9) | 0.0255 (3) | |
| C23 | 0.3127 (3) | 0.35908 (8) | 0.16148 (11) | 0.0380 (4) | |
| H23A | 0.1875 | 0.3756 | 0.1379 | 0.046* | |
| C24 | 0.3214 (3) | 0.29478 (8) | 0.17827 (11) | 0.0370 (4) | |
| H24A | 0.2026 | 0.2694 | 0.1656 | 0.044* | |
| C25 | 0.4755 (3) | 0.47028 (7) | 0.15925 (10) | 0.0314 (4) | |
| C26 | 0.6985 (3) | 0.49533 (9) | 0.14043 (12) | 0.0454 (5) | |
| H26A | 0.7489 | 0.4729 | 0.0970 | 0.068* | |
| H26B | 0.7974 | 0.4891 | 0.1838 | 0.068* | |
| H26C | 0.6887 | 0.5397 | 0.1287 | 0.068* | |
| C27 | 0.3234 (3) | 0.48367 (9) | 0.08955 (12) | 0.0474 (5) | |
| H27A | 0.3723 | 0.4612 | 0.0459 | 0.071* | |
| H27B | 0.3218 | 0.5283 | 0.0791 | 0.071* | |
| H27C | 0.1806 | 0.4699 | 0.1000 | 0.071* | |
| C28 | 0.3968 (4) | 0.50619 (9) | 0.22849 (12) | 0.0586 (6) | |
| H28A | 0.2570 | 0.4909 | 0.2404 | 0.088* | |
| H28B | 0.3882 | 0.5506 | 0.2168 | 0.088* | |
| H28C | 0.4959 | 0.4997 | 0.2717 | 0.088* | |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0275 (7) | 0.0240 (6) | 0.0255 (7) | 0.0003 (5) | 0.0032 (5) | 0.0028 (5) |
| N2 | 0.0303 (7) | 0.0312 (7) | 0.0280 (7) | 0.0019 (5) | 0.0030 (6) | 0.0021 (6) |
| C1 | 0.0328 (8) | 0.0225 (7) | 0.0259 (8) | −0.0023 (6) | 0.0048 (6) | 0.0025 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0335 (9) | 0.0364 (9) | 0.0344 (9) | 0.0014 (7) | 0.0075 (7) | 0.0009 (7) |
| C3 | 0.0449 (11) | 0.0425 (10) | 0.0311 (9) | −0.0027 (8) | 0.0118 (8) | −0.0010 (8) |
| C4 | 0.0482 (11) | 0.0403 (10) | 0.0263 (9) | −0.0046 (8) | 0.0030 (7) | 0.0035 (7) |
| C5 | 0.0375 (9) | 0.0350 (9) | 0.0306 (9) | −0.0009 (7) | 0.0007 (7) | 0.0044 (7) |
| C6 | 0.0321 (8) | 0.0255 (8) | 0.0271 (8) | −0.0018 (6) | 0.0038 (6) | 0.0023 (6) |
| C7 | 0.0281 (8) | 0.0217 (7) | 0.0277 (8) | −0.0012 (6) | 0.0038 (6) | 0.0016 (6) |
| C8 | 0.0281 (8) | 0.0261 (8) | 0.0276 (8) | −0.0049 (6) | 0.0029 (6) | −0.0006 (6) |
| C9 | 0.0323 (9) | 0.0304 (8) | 0.0303 (9) | −0.0015 (7) | 0.0032 (7) | 0.0001 (7) |
| C10 | 0.0395 (10) | 0.0388 (9) | 0.0282 (9) | −0.0057 (7) | 0.0023 (7) | 0.0015 (7) |
| C11 | 0.0351 (9) | 0.0387 (9) | 0.0300 (9) | −0.0102 (7) | 0.0067 (7) | −0.0082 (7) |
| C12 | 0.0371 (10) | 0.0354 (9) | 0.0391 (10) | 0.0023 (7) | 0.0076 (8) | −0.0077 (8) |
| C13 | 0.0353 (9) | 0.0323 (9) | 0.0330 (9) | 0.0015 (7) | 0.0034 (7) | −0.0003 (7) |
| C14 | 0.0468 (11) | 0.0484 (11) | 0.0333 (10) | −0.0098 (9) | 0.0136 (8) | −0.0078 (8) |
| C15 | 0.048 (2) | 0.078 (3) | 0.047 (2) | 0.0041 (18) | 0.0199 (15) | 0.0108 (18) |
| C16 | 0.056 (2) | 0.070 (2) | 0.0278 (15) | −0.0027 (17) | 0.0097 (14) | 0.0037 (15) |
| C17 | 0.105 (4) | 0.059 (2) | 0.045 (2) | −0.023 (2) | 0.032 (2) | −0.0254 (19) |
| C16' | 0.081 (6) | 0.077 (5) | 0.063 (4) | −0.019 (4) | 0.041 (4) | −0.001 (4) |
| C15' | 0.095 (6) | 0.103 (6) | 0.036 (3) | 0.056 (5) | 0.024 (3) | 0.003 (4) |
| C17' | 0.069 (4) | 0.073 (5) | 0.036 (3) | 0.006 (3) | 0.002 (3) | −0.015 (3) |
| C18 | 0.0254 (8) | 0.0258 (8) | 0.0316 (8) | −0.0026 (6) | −0.0001 (6) | 0.0012 (6) |
| C19 | 0.0251 (8) | 0.0247 (7) | 0.0236 (7) | −0.0008 (6) | 0.0039 (6) | −0.0004 (6) |
| C20 | 0.0289 (9) | 0.0296 (8) | 0.0437 (10) | −0.0010 (6) | −0.0107 (7) | 0.0043 (7) |
| C21 | 0.0303 (9) | 0.0272 (8) | 0.0476 (11) | −0.0054 (6) | −0.0080 (7) | 0.0018 (7) |
| C22 | 0.0273 (8) | 0.0250 (7) | 0.0243 (8) | 0.0017 (6) | 0.0041 (6) | −0.0007 (6) |
| C23 | 0.0271 (9) | 0.0309 (9) | 0.0548 (11) | 0.0012 (7) | −0.0097 (8) | 0.0059 (8) |
| C24 | 0.0260 (8) | 0.0303 (9) | 0.0538 (11) | −0.0057 (7) | −0.0074 (7) | 0.0032 (8) |
| C25 | 0.0382 (9) | 0.0248 (8) | 0.0316 (9) | 0.0022 (7) | 0.0056 (7) | 0.0022 (7) |
| C26 | 0.0454 (11) | 0.0331 (9) | 0.0576 (12) | −0.0072 (8) | 0.0028 (9) | 0.0099 (9) |
| C27 | 0.0487 (12) | 0.0408 (10) | 0.0525 (12) | 0.0016 (9) | −0.0011 (9) | 0.0176 (9) |
| C28 | 0.1005 (19) | 0.0285 (9) | 0.0493 (12) | 0.0113 (10) | 0.0287 (12) | 0.0019 (9) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C7 | 1.3816 (19) | C17—H17A | 0.9600 |
| N1—C1 | 1.386 (2) | C17—H17B | 0.9600 |
| N1—C18 | 1.4571 (19) | C17—H17C | 0.9600 |
| N2—C7 | 1.327 (2) | C16'—H16D | 0.9600 |
| N2—C6 | 1.390 (2) | C16'—H16E | 0.9600 |
| C1—C2 | 1.393 (2) | C16'—H16F | 0.9600 |
| C1—C6 | 1.398 (2) | C15'—H15D | 0.9600 |
| C2—C3 | 1.382 (2) | C15'—H15E | 0.9600 |
| C2—H2B | 0.9300 | C15'—H15F | 0.9600 |
| C3—C4 | 1.397 (3) | C17'—H17D | 0.9600 |
| C3—H3A | 0.9300 | C17'—H17E | 0.9600 |
| C4—C5 | 1.381 (2) | C17'—H17F | 0.9600 |
| C4—H4A | 0.9300 | C18—C19 | 1.518 (2) |
| C5—C6 | 1.402 (2) | C18—H18A | 0.9700 |
| C5—H5A | 0.9300 | C18—H18B | 0.9700 |
| C7—C8 | 1.471 (2) | C19—C20 | 1.382 (2) |

| | | | |
|---|---|---|---|
| C8—C13 | 1.395 (2) | C19—C24 | 1.385 (2) |
| C8—C9 | 1.397 (2) | C20—C21 | 1.392 (2) |
| C9—C10 | 1.390 (2) | C20—H20A | 0.9300 |
| C9—H9A | 0.9300 | C21—C22 | 1.387 (2) |
| C10—C11 | 1.389 (2) | C21—H21A | 0.9300 |
| C10—H10A | 0.9300 | C22—C23 | 1.387 (2) |
| C11—C12 | 1.397 (3) | C22—C25 | 1.535 (2) |
| C11—C14 | 1.536 (2) | C23—C24 | 1.389 (2) |
| C12—C13 | 1.383 (2) | C23—H23A | 0.9300 |
| C12—H12A | 0.9300 | C24—H24A | 0.9300 |
| C13—H13A | 0.9300 | C25—C28 | 1.528 (2) |
| C14—C17' | 1.463 (6) | C25—C27 | 1.530 (2) |
| C14—C16' | 1.465 (7) | C25—C26 | 1.534 (2) |
| C14—C15 | 1.498 (4) | C26—H26A | 0.9600 |
| C14—C17 | 1.508 (4) | C26—H26B | 0.9600 |
| C14—C16 | 1.601 (4) | C26—H26C | 0.9600 |
| C14—C15' | 1.650 (6) | C27—H27A | 0.9600 |
| C15—H15A | 0.9600 | C27—H27B | 0.9600 |
| C15—H15B | 0.9600 | C27—H27C | 0.9600 |
| C15—H15C | 0.9600 | C28—H28A | 0.9600 |
| C16—H16A | 0.9600 | C28—H28B | 0.9600 |
| C16—H16B | 0.9600 | C28—H28C | 0.9600 |
| C16—H16C | 0.9600 | | |
| C7—N1—C1 | 106.40 (13) | C14—C17—H17A | 109.5 |
| C7—N1—C18 | 129.74 (13) | C14—C17—H17B | 109.5 |
| C1—N1—C18 | 123.86 (13) | H17A—C17—H17B | 109.5 |
| C7—N2—C6 | 105.05 (13) | C14—C17—H17C | 109.5 |
| N1—C1—C2 | 131.48 (15) | H17A—C17—H17C | 109.5 |
| N1—C1—C6 | 105.77 (13) | H17B—C17—H17C | 109.5 |
| C2—C1—C6 | 122.70 (15) | C14—C16'—H16D | 109.5 |
| C3—C2—C1 | 116.56 (16) | C14—C16'—H16E | 109.5 |
| C3—C2—H2B | 121.7 | H16D—C16'—H16E | 109.5 |
| C1—C2—H2B | 121.7 | C14—C16'—H16F | 109.5 |
| C2—C3—C4 | 121.47 (16) | H16D—C16'—H16F | 109.5 |
| C2—C3—H3A | 119.3 | H16E—C16'—H16F | 109.5 |
| C4—C3—H3A | 119.3 | C14—C15'—H15D | 109.5 |
| C5—C4—C3 | 121.94 (16) | C14—C15'—H15E | 109.5 |
| C5—C4—H4A | 119.0 | H15D—C15'—H15E | 109.5 |
| C3—C4—H4A | 119.0 | C14—C15'—H15F | 109.5 |
| C4—C5—C6 | 117.44 (16) | H15D—C15'—H15F | 109.5 |
| C4—C5—H5A | 121.3 | H15E—C15'—H15F | 109.5 |
| C6—C5—H5A | 121.3 | C14—C17'—H17D | 109.5 |
| N2—C6—C1 | 110.16 (13) | C14—C17'—H17E | 109.5 |
| N2—C6—C5 | 129.95 (15) | H17D—C17'—H17E | 109.5 |
| C1—C6—C5 | 119.88 (15) | C14—C17'—H17F | 109.5 |
| N2—C7—N1 | 112.61 (14) | H17D—C17'—H17F | 109.5 |
| N2—C7—C8 | 121.68 (14) | H17E—C17'—H17F | 109.5 |
| N1—C7—C8 | 125.63 (14) | N1—C18—C19 | 113.43 (12) |
| C13—C8—C9 | 117.69 (15) | N1—C18—H18A | 108.9 |

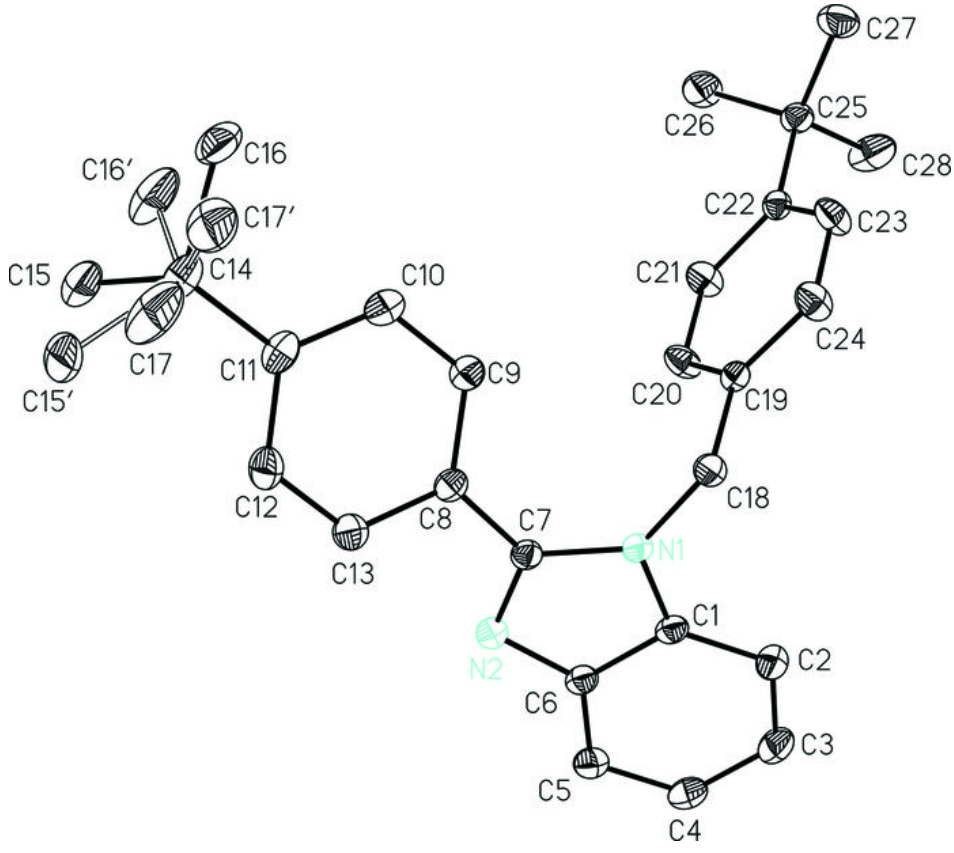
| | | | |
|---|---|---|---|
| C13—C8—C7 | 117.42 (14) | C19—C18—H18A | 108.9 |
| C9—C8—C7 | 124.78 (14) | N1—C18—H18B | 108.9 |
| C10—C9—C8 | 120.65 (16) | C19—C18—H18B | 108.9 |
| C10—C9—H9A | 119.7 | H18A—C18—H18B | 107.7 |
| C8—C9—H9A | 119.7 | C20—C19—C24 | 117.44 (14) |
| C11—C10—C9 | 121.88 (16) | C20—C19—C18 | 122.86 (14) |
| C11—C10—H10A | 119.1 | C24—C19—C18 | 119.67 (14) |
| C9—C10—H10A | 119.1 | C19—C20—C21 | 121.05 (15) |
| C10—C11—C12 | 117.05 (15) | C19—C20—H20A | 119.5 |
| C10—C11—C14 | 122.04 (17) | C21—C20—H20A | 119.5 |
| C12—C11—C14 | 120.91 (16) | C22—C21—C20 | 122.13 (15) |
| C13—C12—C11 | 121.63 (16) | C22—C21—H21A | 118.9 |
| C13—C12—H12A | 119.2 | C20—C21—H21A | 118.9 |
| C11—C12—H12A | 119.2 | C23—C22—C21 | 116.09 (14) |
| C12—C13—C8 | 121.10 (16) | C23—C22—C25 | 122.07 (14) |
| C12—C13—H13A | 119.5 | C21—C22—C25 | 121.83 (14) |
| C8—C13—H13A | 119.5 | C22—C23—C24 | 122.19 (15) |
| C17'—C14—C16' | 115.7 (5) | C22—C23—H23A | 118.9 |
| C17'—C14—C15 | 138.4 (3) | C24—C23—H23A | 118.9 |
| C16'—C14—C15 | 54.3 (4) | C19—C24—C23 | 121.07 (15) |
| C17'—C14—C17 | 46.3 (3) | C19—C24—H24A | 119.5 |
| C16'—C14—C17 | 143.7 (3) | C23—C24—H24A | 119.5 |
| C15—C14—C17 | 114.0 (3) | C28—C25—C27 | 109.18 (16) |
| C17'—C14—C11 | 110.5 (3) | C28—C25—C26 | 109.07 (16) |
| C16'—C14—C11 | 107.9 (3) | C27—C25—C26 | 107.14 (15) |
| C15—C14—C11 | 110.84 (19) | C28—C25—C22 | 108.57 (14) |
| C17—C14—C11 | 108.26 (19) | C27—C25—C22 | 111.76 (14) |
| C17'—C14—C16 | 62.4 (3) | C26—C25—C22 | 111.08 (14) |
| C16'—C14—C16 | 56.3 (4) | C25—C26—H26A | 109.5 |
| C15—C14—C16 | 106.1 (2) | C25—C26—H26B | 109.5 |
| C17—C14—C16 | 106.3 (3) | H26A—C26—H26B | 109.5 |
| C11—C14—C16 | 111.34 (18) | C25—C26—H26C | 109.5 |
| C17'—C14—C15' | 106.7 (4) | H26A—C26—H26C | 109.5 |
| C16'—C14—C15' | 106.2 (5) | H26B—C26—H26C | 109.5 |
| C15—C14—C15' | 53.6 (4) | C25—C27—H27A | 109.5 |
| C17—C14—C15' | 64.1 (4) | C25—C27—H27B | 109.5 |
| C11—C14—C15' | 109.8 (2) | H27A—C27—H27B | 109.5 |
| C16—C14—C15' | 138.6 (3) | C25—C27—H27C | 109.5 |
| C14—C15—H15A | 109.5 | H27A—C27—H27C | 109.5 |
| C14—C15—H15B | 109.5 | H27B—C27—H27C | 109.5 |
| H15A—C15—H15B | 109.5 | C25—C28—H28A | 109.5 |
| C14—C15—H15C | 109.5 | C25—C28—H28B | 109.5 |
| H15A—C15—H15C | 109.5 | H28A—C28—H28B | 109.5 |
| H15B—C15—H15C | 109.5 | C25—C28—H28C | 109.5 |
| C14—C16—H16A | 109.5 | H28A—C28—H28C | 109.5 |
| C14—C16—H16B | 109.5 | H28B—C28—H28C | 109.5 |
| C14—C16—H16C | 109.5 | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C18—H18A···N2$^{i}$ | 0.97 | 2.59 | 3.553 (2) | 174 |

Symmetry codes: (i) *x*−1, *y*, *z*.

**Fig. 1**


C27
C26
C25
C28
C22
C23
C21
C24
C20
C19
C18
C16
C16′
C17′
C15
C14
C10
C17
C11
C9
C15′
C12
C8
C7
N1
C13
C1
N2
C2
C6
C3
C5
C4