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3-(1*H*-Benzotriazol-1-yl)-2-bromo-1-*o*-tolylpropan-1-one

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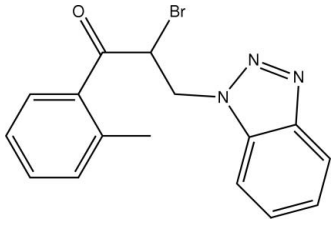
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.090; data-to-parameter ratio = 15.2.

In the molecule of the title compound, $C_{16}H_{14}BrN_3O$, the benzotriazole ring system makes a dihedral angle of 62.1 (1)° with the benzene ring of the tolyl group. Weak π–π stacking interactions are observed between the triazole rings of inversion-related molecules, with a centroid–centroid distance of 3.726 (1) Å.

Related literature

For a related structure, see: Wan *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{16}H_{14}BrN_3O$
M_r = 344.21
Monoclinic, $P2_1/n$
a = 7.3996 (6) Å
b = 13.1784 (11) Å
c = 15.4245 (13) Å
β = 100.664 (1)°
V = 1478.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.78 mm^{-1}
T = 293 (2) K
0.31 × 0.17 × 0.12 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.479, T_{max} = 0.731
8136 measured reflections
2900 independent reflections
2281 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 1.01
2900 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2503).

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  doi:10.1107/S1600536807055286

supplementary materials

Acta Cryst. (2007). E**63**, o4610 [**doi:10.1107/S1600536807055286**]

3-(1*H*-Benzotriazol-1-yl)-2-bromo-1-*o*-tolylpropan-1-one

J.-L. Bi, F. Li and S. Bi

Comment

We have recently reported the crystal structure of 2-(1*H*-1,2,3-benzotriazol-1-yl)-1-benzoylethyl 2-chlorobenzoate (Wan *et al.*, 2006). As part of our ongoing studies on triazole derivatives, the title compound was synthesized and its structure is reported here.

In the molecule of the title compound, the bond lengths and angles are within normal ranges (Allen *et al.*, 1987), and are comparable with those in the related structure (Wan *et al.*, 2006). The benzotriazole ring system is essentially planar, with a dihedral angle of 0.8 (1)° between the triazole (N1—N3/C10/C11) and benzene (C10—C15) rings. The molecule as a whole is non-planar. The dihedral angle between the benzotriazole system (N1—N3/C10—C15) and the benzene ring (C1—C6) is 62.1 (1)°.

The crystal structure is stabilized by weak π-π stacking interactions between the triazole rings of the molecules at (*x*, *y*, *z*) and (1 − *x*, −*y*, 1 − *z*), with a centroid-centroid distance of 3.726 (1) Å.

Experimental

The title compound was prepared according to the literature method of Wan *et al.* (2006). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution at room temperature over a period of 5 d.

Refinement

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(C_{methyl}).

Figures

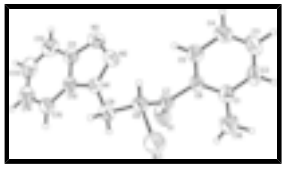

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom numbering scheme.

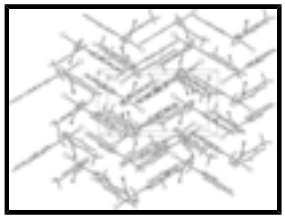

Fig. 2. The crystal packing of the title compound, viewed down the *c* axis.

3-(1*H*-Benzotriazol-1-yl)-2-bromo-1-*o*-tolylpropan-1-one

Crystal data

$C_{16}H_{14}BrN_3O$	F_{000} = 696
M_r = 344.21	D_x = 1.547 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2872 reflections
a = 7.3996 (6) Å	θ = 2.7–24.1º
b = 13.1784 (11) Å	μ = 2.78 mm^{-1}
c = 15.4245 (13) Å	T = 293 (2) K
β = 100.664 (1)º	Column, colourless
V = 1478.1 (2) Å^3	0.31 × 0.17 × 0.12 mm
Z = 4	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2900 independent reflections
Radiation source: fine-focus sealed tube	2281 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.018
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 26.0º
T = 293(2) K	θ_{min} = 2.1º
ω scans	h = −7→9
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	k = −10→16
T_{min} = 0.479, T_{max} = 0.731	l = −19→19
8136 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
$R[F^2 > 2\sigma(F^2)]$ = 0.035	H-atom parameters constrained
$wR(F^2)$ = 0.090	$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 0.5426P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
2900 reflections	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
191 parameters	$\Delta\rho_{min}$ = −0.45 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br1	0.62383 (5)	0.35726 (2)	0.51118 (2)	0.07057 (15)
O1	0.1695 (3)	0.29617 (17)	0.50821 (11)	0.0638 (5)
N1	0.3281 (3)	0.09442 (15)	0.43516 (12)	0.0420 (5)
N2	0.3079 (3)	0.05452 (17)	0.51348 (13)	0.0509 (5)
N3	0.2174 (3)	−0.03102 (17)	0.49977 (14)	0.0530 (5)
C1	0.2527 (3)	0.37181 (18)	0.69145 (16)	0.0442 (6)
C2	0.2812 (4)	0.3790 (2)	0.78361 (17)	0.0527 (7)
H2	0.2321	0.4340	0.8090	0.063*
C3	0.3792 (4)	0.3074 (2)	0.83770 (16)	0.0546 (7)
H3	0.3943	0.3140	0.8986	0.066*
C4	0.4548 (4)	0.2263 (2)	0.80183 (16)	0.0509 (6)
H4	0.5202	0.1773	0.8382	0.061*
C5	0.4333 (3)	0.21767 (19)	0.71118 (15)	0.0461 (6)
H5	0.4868	0.1633	0.6870	0.055*
C6	0.3330 (3)	0.28894 (17)	0.65560 (14)	0.0385 (5)
C7	0.3106 (3)	0.27566 (18)	0.55829 (15)	0.0413 (5)
C8	0.4743 (3)	0.23722 (18)	0.52122 (14)	0.0432 (5)
H8	0.5447	0.1887	0.5623	0.052*
C9	0.4245 (3)	0.18998 (19)	0.43053 (15)	0.0451 (6)
H9A	0.3468	0.2362	0.3912	0.054*
H9B	0.5353	0.1781	0.4069	0.054*
C10	0.2508 (3)	0.03255 (17)	0.36834 (15)	0.0409 (5)
C11	0.1782 (3)	−0.04722 (18)	0.40969 (16)	0.0460 (6)
C12	0.0827 (4)	−0.1259 (2)	0.3607 (2)	0.0582 (7)
H12	0.0329	−0.1795	0.3878	0.070*
C13	0.0659 (4)	−0.1206 (2)	0.2715 (2)	0.0654 (8)
H13	0.0025	−0.1718	0.2370	0.078*
C14	0.1407 (4)	−0.0407 (2)	0.22958 (19)	0.0623 (7)
H14	0.1268	−0.0409	0.1684	0.075*
C15	0.2337 (4)	0.0377 (2)	0.27630 (16)	0.0505 (6)
H15	0.2827	0.0911	0.2487	0.061*
C16	0.1467 (4)	0.4537 (2)	0.6365 (2)	0.0653 (8)
H16A	0.1440	0.5135	0.6718	0.098*

H16B	0.0233	0.4308	0.6151	0.098*
H16C	0.2051	0.4691	0.5874	0.098*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0782 (2)	0.0677 (2)	0.0682 (2)	−0.02565 (16)	0.01984 (16)	−0.00776 (15)
O1	0.0553 (11)	0.0908 (15)	0.0412 (10)	0.0213 (10)	−0.0016 (9)	−0.0095 (9)
N1	0.0486 (12)	0.0437 (11)	0.0354 (10)	0.0023 (9)	0.0121 (9)	−0.0012 (8)
N2	0.0599 (13)	0.0571 (13)	0.0371 (10)	−0.0003 (11)	0.0126 (10)	0.0017 (9)
N3	0.0589 (14)	0.0539 (13)	0.0482 (12)	−0.0028 (11)	0.0149 (10)	0.0058 (10)
C1	0.0396 (13)	0.0474 (14)	0.0477 (13)	−0.0048 (10)	0.0130 (11)	−0.0054 (11)
C2	0.0535 (15)	0.0589 (16)	0.0506 (14)	−0.0108 (13)	0.0224 (12)	−0.0199 (13)
C3	0.0554 (16)	0.0745 (19)	0.0353 (13)	−0.0196 (14)	0.0119 (12)	−0.0076 (13)
C4	0.0555 (15)	0.0566 (16)	0.0381 (13)	−0.0099 (13)	0.0021 (11)	0.0032 (12)
C5	0.0477 (14)	0.0475 (14)	0.0417 (13)	−0.0013 (11)	0.0051 (11)	−0.0037 (11)
C6	0.0377 (12)	0.0418 (13)	0.0359 (11)	−0.0049 (10)	0.0065 (10)	−0.0051 (10)
C7	0.0435 (13)	0.0435 (13)	0.0360 (12)	0.0040 (10)	0.0051 (11)	−0.0024 (10)
C8	0.0457 (14)	0.0461 (13)	0.0377 (12)	−0.0011 (11)	0.0077 (10)	−0.0009 (10)
C9	0.0521 (14)	0.0479 (14)	0.0383 (12)	0.0001 (11)	0.0160 (11)	−0.0013 (10)
C10	0.0375 (12)	0.0447 (13)	0.0405 (12)	0.0084 (10)	0.0076 (10)	−0.0027 (10)
C11	0.0397 (13)	0.0487 (14)	0.0499 (14)	0.0052 (11)	0.0092 (11)	−0.0006 (11)
C12	0.0495 (16)	0.0524 (17)	0.0736 (19)	−0.0038 (12)	0.0136 (14)	−0.0045 (14)
C13	0.0546 (17)	0.0663 (19)	0.072 (2)	−0.0022 (14)	0.0026 (15)	−0.0244 (16)
C14	0.0628 (18)	0.074 (2)	0.0473 (15)	0.0079 (15)	0.0034 (13)	−0.0142 (14)
C15	0.0572 (16)	0.0540 (16)	0.0412 (13)	0.0067 (12)	0.0121 (12)	−0.0003 (11)
C16	0.0717 (19)	0.0544 (17)	0.0706 (19)	0.0143 (14)	0.0156 (15)	−0.0045 (14)

Geometric parameters (Å, °)

Br1—C8	1.953 (2)	C7—C8	1.519 (3)
O1—C7	1.209 (3)	C8—C9	1.513 (3)
N1—N2	1.351 (3)	C8—H8	0.98
N1—C10	1.355 (3)	C9—H9A	0.97
N1—C9	1.456 (3)	C9—H9B	0.97
N2—N3	1.308 (3)	C10—C11	1.388 (3)
N3—C11	1.382 (3)	C10—C15	1.403 (3)
C1—C2	1.401 (4)	C11—C12	1.396 (4)
C1—C6	1.404 (3)	C12—C13	1.361 (4)
C1—C16	1.500 (4)	C12—H12	0.93
C2—C3	1.374 (4)	C13—C14	1.402 (4)
C2—H2	0.93	C13—H13	0.93
C3—C4	1.370 (4)	C14—C15	1.370 (4)
C3—H3	0.93	C14—H14	0.93
C4—C5	1.382 (3)	C15—H15	0.93
C4—H4	0.93	C16—H16A	0.96
C5—C6	1.390 (3)	C16—H16B	0.96
C5—H5	0.93	C16—H16C	0.96
C6—C7	1.490 (3)		

N2—N1—C10	110.18 (19)	Br1—C8—H8	109.8
N2—N1—C9	121.12 (19)	N1—C9—C8	110.40 (18)
C10—N1—C9	128.68 (18)	N1—C9—H9A	109.6
N3—N2—N1	109.20 (19)	C8—C9—H9A	109.6
N2—N3—C11	107.5 (2)	N1—C9—H9B	109.6
C2—C1—C6	117.2 (2)	C8—C9—H9B	109.6
C2—C1—C16	119.3 (2)	H9A—C9—H9B	108.1
C6—C1—C16	123.5 (2)	N1—C10—C11	104.53 (19)
C3—C2—C1	122.2 (2)	N1—C10—C15	133.4 (2)
C3—C2—H2	118.9	C11—C10—C15	122.1 (2)
C1—C2—H2	118.9	N3—C11—C10	108.5 (2)
C4—C3—C2	120.0 (2)	N3—C11—C12	130.5 (2)
C4—C3—H3	120.0	C10—C11—C12	120.9 (2)
C2—C3—H3	120.0	C13—C12—C11	116.9 (3)
C3—C4—C5	119.5 (2)	C13—C12—H12	121.6
C3—C4—H4	120.2	C11—C12—H12	121.6
C5—C4—H4	120.2	C12—C13—C14	122.3 (3)
C4—C5—C6	121.1 (2)	C12—C13—H13	118.8
C4—C5—H5	119.4	C14—C13—H13	118.8
C6—C5—H5	119.4	C15—C14—C13	121.8 (3)
C5—C6—C1	119.9 (2)	C15—C14—H14	119.1
C5—C6—C7	119.3 (2)	C13—C14—H14	119.1
C1—C6—C7	120.8 (2)	C14—C15—C10	116.0 (3)
O1—C7—C6	122.6 (2)	C14—C15—H15	122.0
O1—C7—C8	119.2 (2)	C10—C15—H15	122.0
C6—C7—C8	118.10 (19)	C1—C16—H16A	109.5
C9—C8—C7	114.2 (2)	C1—C16—H16B	109.5
C9—C8—Br1	107.75 (15)	H16A—C16—H16B	109.5
C7—C8—Br1	105.22 (16)	C1—C16—H16C	109.5
C9—C8—H8	109.8	H16A—C16—H16C	109.5
C7—C8—H8	109.8	H16B—C16—H16C	109.5
C10—N1—N2—N3	−0.9 (3)	N2—N1—C9—C8	−5.8 (3)
C9—N1—N2—N3	−179.9 (2)	C10—N1—C9—C8	175.4 (2)
N1—N2—N3—C11	0.2 (3)	C7—C8—C9—N1	−69.1 (3)
C6—C1—C2—C3	−1.6 (4)	Br1—C8—C9—N1	174.40 (16)
C16—C1—C2—C3	−179.1 (2)	N2—N1—C10—C11	1.1 (2)
C1—C2—C3—C4	0.8 (4)	C9—N1—C10—C11	−180.0 (2)
C2—C3—C4—C5	0.7 (4)	N2—N1—C10—C15	−179.8 (3)
C3—C4—C5—C6	−1.3 (4)	C9—N1—C10—C15	−0.9 (4)
C4—C5—C6—C1	0.5 (4)	N2—N3—C11—C10	0.5 (3)
C4—C5—C6—C7	−179.0 (2)	N2—N3—C11—C12	−178.9 (3)
C2—C1—C6—C5	0.9 (3)	N1—C10—C11—N3	−1.0 (2)
C16—C1—C6—C5	178.3 (2)	C15—C10—C11—N3	179.8 (2)
C2—C1—C6—C7	−179.6 (2)	N1—C10—C11—C12	178.5 (2)
C16—C1—C6—C7	−2.3 (4)	C15—C10—C11—C12	−0.7 (4)
C5—C6—C7—O1	142.3 (3)	N3—C11—C12—C13	179.8 (3)
C1—C6—C7—O1	−37.2 (4)	C10—C11—C12—C13	0.4 (4)
C5—C6—C7—C8	−39.3 (3)	C11—C12—C13—C14	0.3 (4)

C1—C6—C7—C8	141.3 (2)	C12—C13—C14—C15	−0.8 (5)
O1—C7—C8—C9	−22.9 (3)	C13—C14—C15—C10	0.5 (4)
C6—C7—C8—C9	158.6 (2)	N1—C10—C15—C14	−178.7 (3)
O1—C7—C8—Br1	95.1 (2)	C11—C10—C15—C14	0.2 (4)
C6—C7—C8—Br1	−83.4 (2)		

Fig. 1

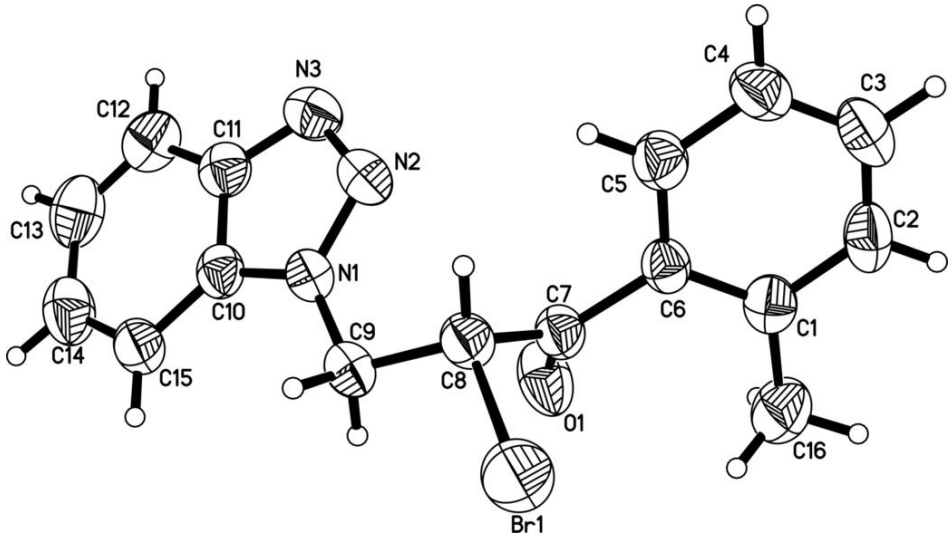
C4
C3
N3
C12
C11
N2
C5
C2
C13
N1
C7
C6
C10
C1
C9
C14
C15
C8
O1
C16
Br1

Fig. 2