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3-(Benzotriazol-1-yl)-2,2-dibromo-1-(2-chlorophenyl)propan-1-one

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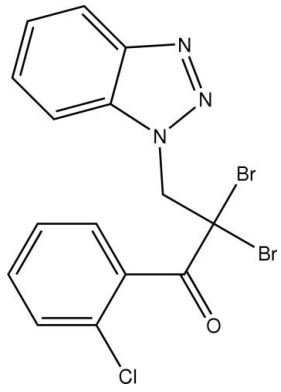
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.027; wR factor = 0.071; data-to-parameter ratio = 14.9.

In the title compound, $C_{15}H_{10}Br_2ClN_3O$, the benzotriazole mean plane makes a dihedral angle of 57.09 (1)° with the other benzene ring. In the crystal structure, the packing is stabilized by C—H···π interactions, together with close Br···N and Br···Br interactions [3.292 (3), 3.054 (3), 3.279 (3) and 3.571 (1) Å].

Related literature

For a related structure, see: Wan *et al.* (2006); for reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{15}H_{10}Br_2ClN_3O$
M_r = 443.53
Triclinic, $P\overline{1}$
a = 7.7509 (18) Å
b = 9.182 (2) Å
c = 12.563 (3) Å
α = 73.058 (3)°
β = 76.442 (3)°
γ = 71.700 (3)°
V = 801.9 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 5.22 mm^{-1}
T = 293 (2) K
0.25 × 0.23 × 0.06 mm

Data collection

Siemens SMART 1000 CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.361, T_{max} = 0.738
4374 measured reflections
2964 independent reflections
2528 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.071
S = 1.04
2964 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the N1–N3/C1/C2 triazole ring and the C1–C6 benzene ring, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···$Cg2^{i}$	0.97	2.87	3.523	126
C7—H7B···$Cg1^{i}$	0.97	2.88	3.484	122

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

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: SJ2399).

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  doi:10.1107/S1600536807054700

supplementary materials

Acta Cryst. (2007). E**63**, o4548 [**doi:10.1107/S1600536807054700**]

3-(Benzotriazol-1-yl)-2,2-dibromo-1-(2-chlorophenyl)propan-1-one

Y.-J. Zhu, M. Wang, J.-L. Bi and F. Li

Comment

Recently we reported the structure of 2-(1*H*-1,2,3-benzotriazol-1-yl)-1-benzoylethyl 2-chlorobenzoate (II) (Wan *et al.*, 2006). As part of our ongoing investigation of triazole derivatives with greater pharmacological activity, the title compound, (I), was synthesized and its structure is presented here, Fig. 1.

In the title compound (I), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable to those in the related compound, (II). The whole molecule is non-planar with a dihedral angle of 57.09 (1)° between the C10—C15 benzene ring and N1—N3/C1—C6 benzotriazole ring. The benzotriazole system is essentially planar with a dihedral angle of 3.27 (2)° between the N1—N3/C1/C6 triazole ring and C1—C6 benzene ring.

In the crystal structure, the packing is stabilized by C—H···π interactions (Table 1) and weak Br···N and Br···Br van der Waals forces with the distances Br1···N2, Br1···N3, Br2—N2 and Br2—Br2 of 3.292 (3), 3.054 (3), 3.279 (3) and 3.571 (1) Å, respectively.

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 six days.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C) for aromatic and 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2 atoms.

Figures

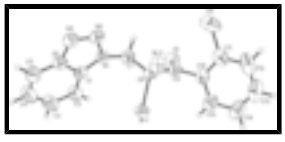

Fig. 1. The structure of the compound (I) showing 50% probability displacement ellipsoids and the atom numbering scheme.

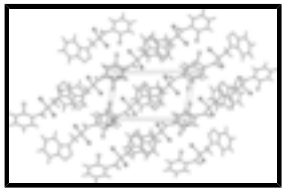

Fig. 2. A packing diagram of (I), viewed down the *a* axis

3-(Benzotriazol-1-yl)-2,2-dibromo-1-(2-chlorophenyl)propan-1-one

Crystal data

$C_{15}H_{10}Br_2ClN_3O$	$Z = 2$
$M_r = 443.53$	$F_{000} = 432$
Triclinic, $P\overline{1}$	$D_x = 1.837$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.7509$ (18) Å	Cell parameters from 2538 reflections
$b = 9.182$ (2) Å	$\theta = 2.4$–25.6º
$c = 12.563$ (3) Å	$\mu = 5.22$ mm^{-1}
$\alpha = 73.058$ (3)º	$T = 293$ (2) K
$\beta = 76.442$ (3)º	Plate, colourless
$\gamma = 71.700$ (3)º	0.25 × 0.23 × 0.06 mm
$V = 801.9$ (3) Å^3	

Data collection

Siemens SMART 1000 CCD area detector diffractometer	2964 independent reflections
Radiation source: fine-focus sealed tube	2528 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.012$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 25.7$º
$T = 293(2)$ K	$\theta_{min} = 1.7$º
ω scans	$h = -6 \rightarrow 9$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$k = -11 \rightarrow 11$
$T_{min} = 0.361$, $T_{max} = 0.738$	$l = -15 \rightarrow 14$
4374 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
$R[F^2 > 2\sigma(F^2)] = 0.027$	H-atom parameters constrained
$wR(F^2) = 0.071$	$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2 + 0.2687P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = <0.001$
2964 reflections	$\Delta\rho_{max} = 0.69$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.59$ 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	0.10429 (4)	0.39211 (3)	0.34085 (2)	0.04875 (11)
Br2	0.44143 (4)	0.43973 (3)	0.14942 (2)	0.05179 (11)
Cl1	0.34216 (14)	0.86655 (11)	0.01049 (10)	0.0815 (3)
N1	0.5040 (3)	0.4005 (3)	0.39885 (19)	0.0444 (5)
N2	0.6829 (3)	0.3765 (3)	0.3484 (2)	0.0556 (6)
N3	0.7793 (3)	0.2462 (3)	0.4054 (2)	0.0594 (7)
O1	0.0957 (3)	0.7883 (3)	0.2727 (2)	0.0677 (6)
C1	0.4867 (4)	0.2817 (3)	0.4925 (2)	0.0414 (6)
C2	0.3399 (4)	0.2528 (4)	0.5773 (3)	0.0541 (7)
H2	0.2212	0.3188	0.5761	0.065*
C3	0.3822 (5)	0.1211 (4)	0.6622 (3)	0.0712 (10)
H3	0.2884	0.0968	0.7200	0.085*
C4	0.5594 (5)	0.0216 (4)	0.6660 (3)	0.0731 (10)
H4	0.5804	−0.0659	0.7263	0.088*
C5	0.7018 (5)	0.0493 (4)	0.5840 (3)	0.0634 (9)
H5	0.8198	−0.0176	0.5864	0.076*
C6	0.6638 (4)	0.1829 (3)	0.4955 (3)	0.0474 (7)
C7	0.3712 (4)	0.5435 (3)	0.3528 (2)	0.0443 (6)
H7A	0.4347	0.6252	0.3163	0.053*
H7B	0.2812	0.5782	0.4146	0.053*
C8	0.2698 (3)	0.5274 (3)	0.2683 (2)	0.0396 (6)
C9	0.1419 (4)	0.6891 (3)	0.2196 (2)	0.0443 (6)
C10	0.0762 (4)	0.7164 (3)	0.1099 (2)	0.0465 (7)
C11	0.1573 (4)	0.7987 (3)	0.0101 (3)	0.0574 (8)
C12	0.0944 (6)	0.8256 (4)	−0.0910 (3)	0.0786 (12)
H12	0.1506	0.8800	−0.1578	0.094*
C13	−0.0504 (7)	0.7714 (5)	−0.0909 (4)	0.0878 (13)
H13	−0.0920	0.7881	−0.1582	0.105*
C14	−0.1343 (6)	0.6934 (5)	0.0063 (4)	0.0781 (11)
H14	−0.2346	0.6593	0.0050	0.094*
C15	−0.0727 (4)	0.6640 (4)	0.1074 (3)	0.0589 (8)
H15	−0.1306	0.6095	0.1735	0.071*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04169 (17)	0.04869 (18)	0.05735 (19)	−0.01748 (12)	−0.00454 (13)	−0.01130 (13)
Br2	0.04431 (17)	0.05571 (19)	0.04718 (18)	−0.00010 (13)	0.00003 (12)	−0.01991 (13)
Cl1	0.0693 (6)	0.0616 (5)	0.1009 (7)	−0.0246 (4)	0.0143 (5)	−0.0143 (5)
N1	0.0339 (12)	0.0526 (14)	0.0472 (13)	−0.0139 (10)	−0.0044 (10)	−0.0116 (11)
N2	0.0350 (13)	0.0698 (17)	0.0593 (16)	−0.0190 (12)	−0.0050 (11)	−0.0073 (13)
N3	0.0387 (13)	0.0676 (17)	0.0655 (17)	−0.0140 (12)	−0.0068 (12)	−0.0069 (14)
O1	0.0695 (15)	0.0545 (13)	0.0823 (17)	0.0054 (11)	−0.0242 (13)	−0.0349 (12)
C1	0.0414 (15)	0.0452 (15)	0.0423 (14)	−0.0140 (12)	−0.0050 (12)	−0.0158 (12)
C2	0.0463 (17)	0.0572 (18)	0.0503 (17)	−0.0078 (14)	0.0013 (13)	−0.0132 (14)
C3	0.065 (2)	0.069 (2)	0.062 (2)	−0.0191 (18)	0.0106 (17)	−0.0047 (18)
C4	0.073 (2)	0.053 (2)	0.072 (2)	−0.0104 (17)	−0.0037 (19)	0.0046 (17)
C5	0.0552 (19)	0.0501 (18)	0.077 (2)	−0.0038 (15)	−0.0121 (17)	−0.0122 (16)
C6	0.0411 (15)	0.0466 (16)	0.0565 (17)	−0.0120 (12)	−0.0048 (13)	−0.0169 (13)
C7	0.0434 (15)	0.0438 (15)	0.0499 (16)	−0.0140 (12)	−0.0075 (12)	−0.0145 (12)
C8	0.0338 (13)	0.0414 (14)	0.0434 (14)	−0.0110 (11)	0.0020 (11)	−0.0148 (11)
C9	0.0343 (14)	0.0457 (15)	0.0518 (16)	−0.0098 (11)	−0.0011 (12)	−0.0152 (13)
C10	0.0427 (15)	0.0410 (15)	0.0500 (16)	0.0001 (12)	−0.0076 (13)	−0.0139 (12)
C11	0.0537 (18)	0.0425 (16)	0.062 (2)	0.0004 (13)	−0.0004 (15)	−0.0129 (14)
C12	0.103 (3)	0.057 (2)	0.050 (2)	0.009 (2)	−0.012 (2)	−0.0064 (16)
C13	0.106 (4)	0.080 (3)	0.072 (3)	0.010 (2)	−0.043 (3)	−0.024 (2)
C14	0.070 (2)	0.073 (2)	0.098 (3)	0.0038 (19)	−0.043 (2)	−0.031 (2)
C15	0.0494 (18)	0.0570 (19)	0.070 (2)	−0.0050 (14)	−0.0172 (15)	−0.0174 (16)

Geometric parameters (Å, °)

Br1—C8	1.952 (3)	C5—C6	1.400 (4)
Br2—C8	1.935 (3)	C5—H5	0.9300
Cl1—C11	1.734 (4)	C7—C8	1.524 (4)
N1—N2	1.360 (3)	C7—H7A	0.9700
N1—C1	1.364 (4)	C7—H7B	0.9700
N1—C7	1.451 (3)	C8—C9	1.547 (4)
N2—N3	1.301 (4)	C9—C10	1.507 (4)
N3—C6	1.374 (4)	C10—C11	1.384 (4)
O1—C9	1.200 (3)	C10—C15	1.392 (4)
C1—C6	1.390 (4)	C11—C12	1.394 (5)
C1—C2	1.399 (4)	C12—C13	1.362 (6)
C2—C3	1.368 (5)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.355 (6)
C3—C4	1.393 (5)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.385 (5)
C4—C5	1.355 (5)	C14—H14	0.9300
C4—H4	0.9300	C15—H15	0.9300
N2—N1—C1	109.8 (2)	H7A—C7—H7B	107.5
N2—N1—C7	118.7 (2)	C7—C8—C9	110.2 (2)

C1—N1—C7	131.4 (2)	C7—C8—Br2	110.90 (17)
N3—N2—N1	108.8 (2)	C9—C8—Br2	111.06 (19)
N2—N3—C6	108.5 (2)	C7—C8—Br1	111.43 (18)
N1—C1—C6	104.4 (2)	C9—C8—Br1	104.46 (17)
N1—C1—C2	133.8 (3)	Br2—C8—Br1	108.57 (13)
C6—C1—C2	121.8 (3)	O1—C9—C10	122.2 (3)
C3—C2—C1	115.7 (3)	O1—C9—C8	118.0 (3)
C3—C2—H2	122.2	C10—C9—C8	119.8 (2)
C1—C2—H2	122.2	C11—C10—C15	118.4 (3)
C2—C3—C4	123.0 (3)	C11—C10—C9	121.1 (3)
C2—C3—H3	118.5	C15—C10—C9	120.4 (3)
C4—C3—H3	118.5	C10—C11—C12	120.9 (4)
C5—C4—C3	121.5 (3)	C10—C11—Cl1	119.5 (3)
C5—C4—H4	119.3	C12—C11—Cl1	119.6 (3)
C3—C4—H4	119.3	C13—C12—C11	119.3 (4)
C4—C5—C6	117.2 (3)	C13—C12—H12	120.3
C4—C5—H5	121.4	C11—C12—H12	120.3
C6—C5—H5	121.4	C14—C13—C12	120.7 (4)
N3—C6—C1	108.5 (3)	C14—C13—H13	119.6
N3—C6—C5	130.6 (3)	C12—C13—H13	119.6
C1—C6—C5	120.9 (3)	C13—C14—C15	120.9 (4)
N1—C7—C8	115.0 (2)	C13—C14—H14	119.6
N1—C7—H7A	108.5	C15—C14—H14	119.6
C8—C7—H7A	108.5	C14—C15—C10	119.7 (4)
N1—C7—H7B	108.5	C14—C15—H15	120.1
C8—C7—H7B	108.5	C10—C15—H15	120.1

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7A···Cg2^{i}	0.97	2.87	3.523	126
C7—H7B···Cg1^{i}	0.97	2.88	3.484	122

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1

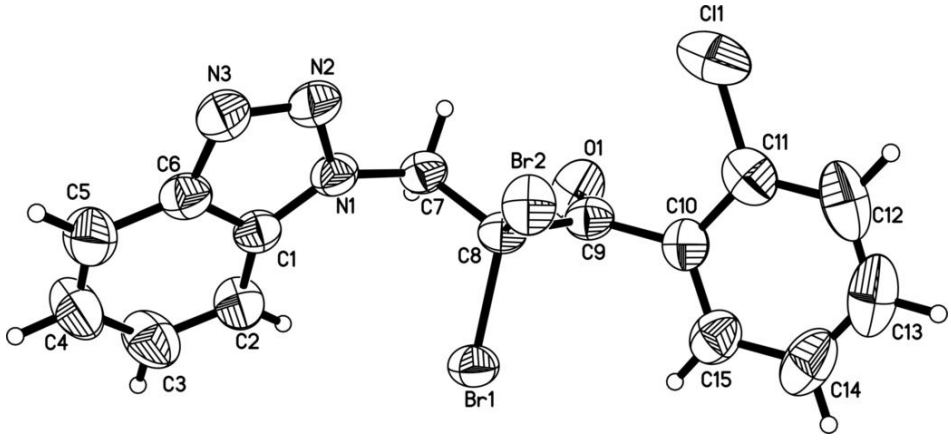
Cl1
N3
N2
C6
C5
N1
C7
Br2
O1
C11
C10
C12
C1
C8
C9
C4
C2
C13
C3
Br1
C15
C14

Fig. 2