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[2-(Benzotriazol-1-yl)ethyl][2-(benzotriazol-2-yl)-ethyl]amine

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Key indicators

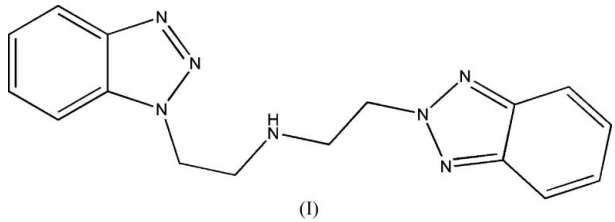
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.059
wR factor = 0.167
Data-to-parameter ratio = 15.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{16}H_{17}N_7$, the dihedral angle between the two benzotriazole ring systems is 73.97 (4)°. N—H···N and C—H···N hydrogen bonds link the molecules into a chain along the *a* axis. The packing is further stabilized by π–π stacking interactions involving two benzotriazole ring systems.

Comment

Benzotriazole and its derivatives have good anti-wear properties, and they are well established corrosion inhibitors for copper and its alloys (Ren *et al.*, 1994; Dugdale & Cotton, 1963). In view of these properties, the title compound, (I), was synthesized according to the literature procedure (Liao *et al.*, 1998), and its crystal stucture is reported here.



(I)

The structural investigation of (I) indicates that the geometry around atom N4 is pyramidal (Fig. 1). The Csp^3—N bond distances range from 1.455 (3) to 1.460 (2) Å (Table 1). The dihedral angle between the two benzotriazole ring systems is 73.97 (4)°. The N—Csp^3—Csp^3—N torsion angles [179.4 (2) and 58.6 (2)°] define the conformation of the central linkage.

In the crystal packing of (I), molecules translated one unit cell along the *a* direction are linked to form a chain *via* N—H···N and C—H···N hydrogen bonds (Table 2 and Fig. 2). The packing is further stabilized by π–π stacking interactions between the N1-benzotriazole ring system at (x, y, z) and the N5-benzotriazole ring system at the symmetry position ($x-1$, $\frac{1}{2}-y$, $z-\frac{1}{2}$) [centroid···centroid distance 3.718 (2) Å].

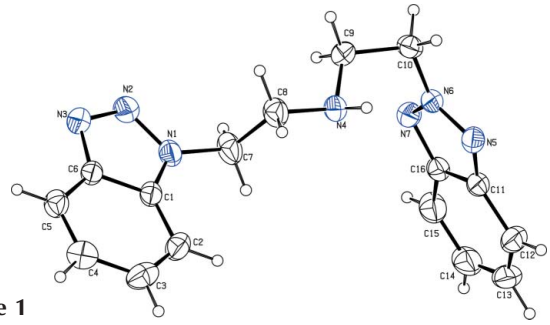


Figure 1
The structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

Experimental

Compound (I) was synthesized according to the literature procedure of Liao *et al.* (1998). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{16}H_{17}N_7$
M_r = 307.37
Monoclinic, $P2_1/c$
a = 6.2180 (16) Å
b = 24.893 (6) Å
c = 10.020 (3) Å
β = 100.650 (4)°
V = 1524.2 (7) Å^3
Z = 4
D_x = 1.339 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5137 reflections
θ = 2.2–26.6°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.966, T_{max} = 0.983
12667 measured reflections
3313 independent reflections
2647 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.0°
$h = -7 \rightarrow 7$
$k = -31 \rightarrow 31$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.167
S = 1.04
3313 reflections
212 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0783P)^2 + 0.5802P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.363 (3)	C10—N6	1.459 (2)
C6—N3	1.369 (3)	C11—N5	1.352 (3)
C7—N1	1.460 (2)	C16—N7	1.353 (2)
C7—C8	1.470 (3)	N1—N2	1.345 (3)
C8—N4	1.458 (3)	N2—N3	1.302 (2)
C9—N4	1.455 (3)	N5—N6	1.321 (2)
C9—C10	1.503 (3)	N6—N7	1.317 (2)
N1—C7—C8—N4	179.4 (2)	C10—C9—N4—C8	167.99 (17)
N4—C9—C10—N6	58.6 (2)	C7—C8—N4—C9	92.9 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8B···N3^{i}	0.97	2.59	3.495 (3)	156
N4—H4A···N2^{i}	0.92 (3)	2.60 (3)	3.254 (3)	128 (2)

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

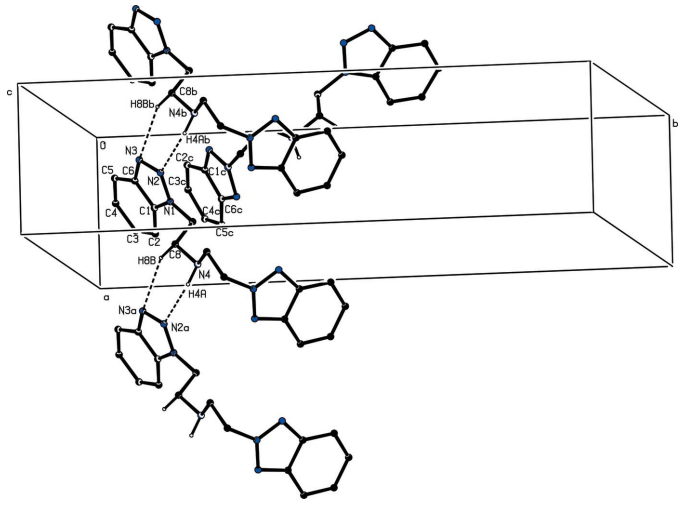


Figure 2
Part of the crystal packing of (I), showing a hydrogen-bonded (dashed lines) chain along the a axis and π–π interactions. For clarity, only H atoms involved in the hydrogen bonding are shown. Atoms labelled with the suffixes a, b and c are generated by the symmetry operations $(1 + x, y, z)$, $(x - 1, y, z)$ and $(x - 1, \frac{1}{2} - y, z - \frac{1}{2})$, respectively.

Atom H4*A* was located in a difference Fourier map and refined isotropically. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H$_{methylene}$ = 0.97 Å and C—H$_{aromatic}$ = 0.93 Å, and with U_{iso}(H) = 1.2U_{eq}(C). The three highest peaks in the final difference map indicated disorder for the C7–C8–N4 chain segment. However, refinement based on a disordered chain segment model led to very high displacement parameters.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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