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# 1-[2-(1*H*-Benzimidazol-2-yl)ethyl]-1*H*-1,2,3-benzotriazole

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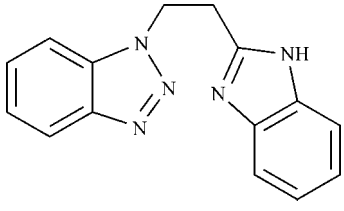
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.063; $wR$ factor = 0.125; data-to-parameter ratio = 12.7.

In the title compound, $C_{15}H_{13}N_5$, the N-containing heterocycles are linked by an ethylene spacer in a *gauche* conformation, the N—C—C—C torsion angle along the linker being 60.1 (3)°. The dihedral angle between the terminal benzotriazole and benzimidazole rings is 39.02 (6)°. In the crystal, adjacent molecules are connected by N—H···N hydrogen bonds, forming an infinite chain along the *c* axis. $\pi$–$\pi$ stacking interactions [centroid–centroid distance = 3.8772 (7) Å] between the benzotriazole rings of neighbouring chains extend these chains into a supramolecular sheet in the *bc* plane. Weak intermolecular C—H···N interactions further stabilize the crystal structure.

## Related literature

For the synthesis and antiviral activity of bis-heterocyclcic compounds containing both benzotriazole and benzimidazole, see: Pagani & Sparatore (1965); Paglietti *et al.* (1975); Katritzky *et al.* (1996); Yu *et al.* (2003); Tonelli *et al.* (2008). For the crystal structure of 1-(benzimidazol-2-ylmethyl)-1*H*-benzotriazole, see: Liu *et al.* (2007).




## Experimental

### Crystal data

$C_{15}H_{13}N_5$
$M_r$ = 263.30
Monoclinic, $P2_1/c$
$a$ = 6.3510 (13) Å
$b$ = 20.830 (4) Å
$c$ = 9.901 (2) Å
$\beta$ = 96.78 (3)°
$V$ = 1300.7 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 294 K
0.37 × 0.32 × 0.26 mm

### Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.969, $T_{max}$ = 0.978
10985 measured reflections
2290 independent reflections
1608 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.071

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.125
$S$ = 1.01
2290 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N4—H14···N5$^{i}$ | 0.84 | 2.04 | 2.855 (3) | 162 |
| C1—H1···N3$^{ii}$ | 0.93 | 2.54 | 3.456 (3) | 167 |

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $x-1, y, z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2029).

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# supplementary materials

*Acta Cryst.* (2011). E**67**, o3167 [ **doi:10.1107/S1600536811045442** ]

# 1-[2-(1*H*-Benzimidazol-2-yl)ethyl]-1*H*-1,2,3-benzotriazole

**Z. Zhang, W. Lu and D. Wu**

## Comment

A family of asymmetric bis-heterocycle compounds comprising both benzotriazole and benzimidazole entities have been prepared (Pagani *et al.* 1965; Paglietti *et al.* 1975; Katritzky *et al.* 1996) and some of them exhibit potent antiviral activity (Yu *et al.* 2003; Tonelli *et al.* 2008), but the structure-function relationship of these novel potential drugs is still a research focus. The structural determination of 1-(Benzimidazol-2-ylmethyl)-1*H*-benzotriazole has been fulfilled (Liu *et al.* 2007). In this paper, the crystal structure of its analogue 1-(2-(1*H*-Benzimidazol-2-yl)ethyl)-1*H*-benzotriazole was reported. The molecular structure of the title compound, (I), is depicted in Fig. 1. In the molecule, benzotriazole and benzimidazole rings are arranged in a *gauche* conformation about the ethylidene linkage, as described by the N1—C7—C8—C9 torsion angle of 60.1 (3) °. Both heterocyclic rings are planar and the dihedral angle between them is 39.02 (6) °. In the crystal packing, adjacent molecules are self-assembled through intermolecular N4—H14···N5$^{i}$ hydrogen bonds (Table 1) between benzimidazole groups into an infinite one-dimensional non-linear chain along the *c* axis (Fig. 2), which is further held together *via* face-to-face π—π stacking [centriod-centriod distance = 3.8772 (7) Å, symmetry code: -*x*, 1 - *y*,2 - *z*] between the benzotriazole groups coming from neighbouring non-linear chains resulting in a two-dimensional supramolecular layer parallel to the *bc* plane (Fig. 3). Weak C1—H1···N3$^{ii}$ hydrogen bonds (Table 1) exist between the layers contributing to the construction of the three-dimensional network.

## Experimental

The mixture of 3-(1*H*-benzotriazole-1-yl)-propionic acid (3.8 g, 0.02 mol) and o-phenylenediamine (3.2 g, 0.03 mol) were dissolved in 2 mol/*L* HCl (10 ml) and refluxed for 10 h to yield a brown solution. After cooling, the solution was filtered to remove the unreacted o-phenylenediamine. Concentrated $NH_3.H_2O$ was added to the resulting filtrate continuously until the gray solid was precipitated completely. The gray solid was redissolved in a small amount of $CH_3OH$ at room temperature. Two weeks ago, colorless block-like crystals of (I) suitable for X-ray diffraction analysis were obtained. (yield 47%) Elemental analysis found: C 68.69; H 5.32; N 26.64%; calculated for $C_{15}H_{13}N_5$: C 68.42; H 4.98; N 26.60%.

## Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å and N—H = 0.84 Å) and refined as riding atoms, with $U_{iso}$(H) = 1.2 times $U_{eq}$(C) or 1.5 times $U_{eq}$(N).

## Figures

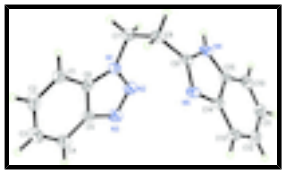

Fig. 1. The molecular structure of the title compound (I), showing the atom labeling scheme and 30% displacement ellipsoids.

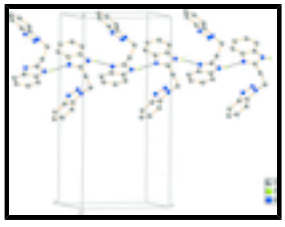

Fig. 2. The crystal packing of the title compound (I), showing the one-dimensional hydrogen-bonding chain. Hydrogen bonds are shown as black dashed lines.

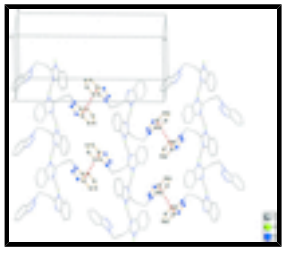

Fig. 3. A view of the two-dimensional supramolecular sheet constructed from one-dimensional chains *via* π—π stacking of heterocyclic rings. π—π stacking interactions are represented by red dashed lines.

## 1-[2-(1*H*-Benzimidazol-2-yl)ethyl]-1*H*-1,2,3-benzotriazole

*Crystal data*

| | |
|---|---|
| $C_{15}H_{13}N_5$ | $F(000) = 552$ |
| $M_r = 263.30$ | $D_x = 1.345$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 10162 reflections |
| $a = 6.3510$ (13) Å | $\theta = 3.2$–$27.8°$ |
| $b = 20.830$ (4) Å | $\mu = 0.09$ mm$^{-1}$ |
| $c = 9.901$ (2) Å | $T = 294$ K |
| $\beta = 96.78$ (3)° | Block, colourless |
| $V = 1300.7$ (5) Å$^3$ | 0.37 × 0.32 × 0.26 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker APEX CCD area-detector diffractometer | 2290 independent reflections |
| Radiation source: fine-focus sealed tube | 1608 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.071$ |
| phi and ω scans | $\theta_{max} = 25.0°$, $\theta_{min} = 3.2°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2001) | $h = -7 \rightarrow 7$ |
| $T_{min} = 0.969$, $T_{max} = 0.978$ | $k = -24 \rightarrow 24$ |
| 10985 measured reflections | $l = -11 \rightarrow 11$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.063$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.125$ | H-atom parameters constrained |
| $S = 1.01$ | $w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.8P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2290 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 181 parameters | $\Delta\rho_{max} = 0.18$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.21$ e Å$^{-3}$ |

*Special details*

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | −0.2105 (4) | 0.96993 (13) | 0.3185 (3) | 0.0476 (7) |
| H1 | −0.3426 | 0.9620 | 0.3468 | 0.057* |
| C2 | −0.1838 (5) | 1.01290 (14) | 0.2171 (3) | 0.0573 (8) |
| H2 | −0.3016 | 1.0346 | 0.1748 | 0.069* |
| C3 | 0.0144 (5) | 1.02507 (15) | 0.1755 (3) | 0.0567 (8) |
| H3 | 0.0252 | 1.0549 | 0.1068 | 0.068* |
| C4 | 0.1916 (5) | 0.99482 (14) | 0.2323 (3) | 0.0539 (8) |
| H4 | 0.3230 | 1.0028 | 0.2029 | 0.065* |
| C5 | 0.1695 (4) | 0.95122 (13) | 0.3364 (3) | 0.0414 (7) |
| C6 | −0.0285 (4) | 0.93888 (12) | 0.3764 (3) | 0.0367 (6) |
| C7 | −0.1427 (4) | 0.85935 (13) | 0.5476 (3) | 0.0448 (7) |
| H7A | −0.2662 | 0.8860 | 0.5547 | 0.054* |
| H7B | −0.0790 | 0.8493 | 0.6391 | 0.054* |
| C8 | −0.2120 (4) | 0.79717 (13) | 0.4733 (3) | 0.0435 (7) |
| H8A | −0.3149 | 0.7754 | 0.5220 | 0.052* |
| H8B | −0.2801 | 0.8074 | 0.3830 | 0.052* |
| C9 | −0.0301 (4) | 0.75382 (12) | 0.4618 (2) | 0.0344 (6) |
| C10 | 0.4117 (5) | 0.65844 (13) | 0.5972 (3) | 0.0482 (7) |
| H10 | 0.4180 | 0.6501 | 0.6899 | 0.058* |
| C11 | 0.5649 (5) | 0.63636 (13) | 0.5222 (3) | 0.0526 (8) |
| H11 | 0.6778 | 0.6127 | 0.5648 | 0.063* |
| C12 | 0.5546 (5) | 0.64870 (13) | 0.3839 (3) | 0.0498 (8) |

| | | | | |
|---|---|---|---|---|
| H12 | 0.6615 | 0.6333 | 0.3361 | 0.060* |
| C13 | 0.3915 (4) | 0.68287 (13) | 0.3161 (3) | 0.0438 (7) |
| H13 | 0.3856 | 0.6904 | 0.2232 | 0.053* |
| C14 | 0.2348 (4) | 0.70614 (12) | 0.3900 (2) | 0.0344 (6) |
| C15 | 0.2474 (4) | 0.69362 (12) | 0.5293 (2) | 0.0363 (6) |
| N1 | 0.0085 (3) | 0.89470 (10) | 0.4772 (2) | 0.0388 (6) |
| N2 | 0.2169 (4) | 0.87999 (11) | 0.4968 (2) | 0.0491 (6) |
| N3 | 0.3165 (3) | 0.91386 (12) | 0.4137 (3) | 0.0530 (7) |
| N4 | 0.0740 (3) | 0.72406 (10) | 0.5709 (2) | 0.0398 (6) |
| H14 | 0.0439 | 0.7286 | 0.6512 | 0.060* |
| N5 | 0.0578 (3) | 0.74388 (10) | 0.3498 (2) | 0.0379 (5) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0375 (16) | 0.0444 (17) | 0.0615 (19) | −0.0022 (14) | 0.0082 (14) | −0.0019 (15) |
| C2 | 0.0480 (19) | 0.0470 (19) | 0.074 (2) | 0.0052 (15) | −0.0048 (16) | 0.0073 (18) |
| C3 | 0.060 (2) | 0.0481 (18) | 0.061 (2) | −0.0064 (16) | 0.0035 (17) | 0.0156 (16) |
| C4 | 0.0446 (18) | 0.0541 (19) | 0.065 (2) | −0.0064 (15) | 0.0167 (16) | 0.0090 (17) |
| C5 | 0.0365 (15) | 0.0413 (16) | 0.0473 (17) | −0.0015 (13) | 0.0086 (13) | −0.0024 (14) |
| C6 | 0.0373 (16) | 0.0330 (15) | 0.0399 (16) | −0.0013 (12) | 0.0045 (13) | −0.0062 (13) |
| C7 | 0.0474 (17) | 0.0458 (17) | 0.0440 (17) | −0.0007 (14) | 0.0173 (14) | −0.0020 (14) |
| C8 | 0.0403 (16) | 0.0504 (17) | 0.0411 (16) | −0.0085 (14) | 0.0103 (13) | −0.0003 (14) |
| C9 | 0.0388 (15) | 0.0400 (15) | 0.0247 (14) | −0.0109 (12) | 0.0045 (12) | −0.0014 (12) |
| C10 | 0.0574 (19) | 0.0471 (17) | 0.0390 (16) | −0.0050 (15) | 0.0007 (15) | 0.0113 (14) |
| C11 | 0.0498 (19) | 0.0397 (17) | 0.067 (2) | 0.0042 (14) | 0.0008 (16) | 0.0082 (16) |
| C12 | 0.0539 (19) | 0.0389 (17) | 0.059 (2) | 0.0011 (15) | 0.0152 (16) | −0.0045 (15) |
| C13 | 0.0539 (18) | 0.0435 (17) | 0.0349 (15) | −0.0027 (14) | 0.0092 (14) | −0.0063 (13) |
| C14 | 0.0454 (16) | 0.0332 (14) | 0.0249 (13) | −0.0068 (13) | 0.0057 (12) | −0.0048 (12) |
| C15 | 0.0455 (16) | 0.0321 (15) | 0.0317 (14) | −0.0060 (13) | 0.0063 (13) | −0.0012 (12) |
| N1 | 0.0346 (13) | 0.0403 (13) | 0.0422 (13) | −0.0008 (10) | 0.0072 (10) | 0.0007 (11) |
| N2 | 0.0369 (14) | 0.0555 (16) | 0.0547 (15) | 0.0026 (12) | 0.0045 (12) | 0.0074 (13) |
| N3 | 0.0338 (13) | 0.0617 (16) | 0.0645 (17) | −0.0004 (12) | 0.0099 (12) | 0.0116 (14) |
| N4 | 0.0486 (14) | 0.0480 (14) | 0.0240 (12) | −0.0074 (11) | 0.0095 (10) | −0.0008 (10) |
| N5 | 0.0419 (13) | 0.0465 (13) | 0.0257 (11) | −0.0022 (11) | 0.0057 (10) | 0.0004 (10) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.370 (4) | C8—H8B | 0.9700 |
| C1—C6 | 1.388 (4) | C9—N5 | 1.316 (3) |
| C1—H1 | 0.9300 | C9—N4 | 1.348 (3) |
| C2—C3 | 1.393 (4) | C10—C11 | 1.372 (4) |
| C2—H2 | 0.9300 | C10—C15 | 1.383 (4) |
| C3—C4 | 1.353 (4) | C10—H10 | 0.9300 |
| C3—H3 | 0.9300 | C11—C12 | 1.387 (4) |
| C4—C5 | 1.394 (4) | C11—H11 | 0.9300 |
| C4—H4 | 0.9300 | C12—C13 | 1.366 (4) |
| C5—N3 | 1.376 (3) | C12—H12 | 0.9300 |
| C5—C6 | 1.386 (3) | C13—C14 | 1.391 (3) |

| | | | |
|---|---|---|---|
| C6—N1 | 1.357 (3) | C13—H13 | 0.9300 |
| C7—N1 | 1.453 (3) | C14—N5 | 1.391 (3) |
| C7—C8 | 1.529 (4) | C14—C15 | 1.397 (3) |
| C7—H7A | 0.9700 | C15—N4 | 1.375 (3) |
| C7—H7B | 0.9700 | N1—N2 | 1.350 (3) |
| C8—C9 | 1.481 (4) | N2—N3 | 1.303 (3) |
| C8—H8A | 0.9700 | N4—H14 | 0.8453 |
| C2—C1—C6 | 116.0 (3) | N5—C9—N4 | 112.7 (2) |
| C2—C1—H1 | 122.0 | N5—C9—C8 | 125.0 (2) |
| C6—C1—H1 | 122.0 | N4—C9—C8 | 122.1 (2) |
| C1—C2—C3 | 122.0 (3) | C11—C10—C15 | 117.2 (3) |
| C1—C2—H2 | 119.0 | C11—C10—H10 | 121.4 |
| C3—C2—H2 | 119.0 | C15—C10—H10 | 121.4 |
| C4—C3—C2 | 121.9 (3) | C10—C11—C12 | 121.3 (3) |
| C4—C3—H3 | 119.0 | C10—C11—H11 | 119.4 |
| C2—C3—H3 | 119.0 | C12—C11—H11 | 119.4 |
| C3—C4—C5 | 117.3 (3) | C13—C12—C11 | 121.8 (3) |
| C3—C4—H4 | 121.3 | C13—C12—H12 | 119.1 |
| C5—C4—H4 | 121.3 | C11—C12—H12 | 119.1 |
| N3—C5—C6 | 108.4 (2) | C12—C13—C14 | 118.1 (3) |
| N3—C5—C4 | 131.2 (3) | C12—C13—H13 | 120.9 |
| C6—C5—C4 | 120.4 (3) | C14—C13—H13 | 120.9 |
| N1—C6—C5 | 104.6 (2) | C13—C14—N5 | 130.6 (2) |
| N1—C6—C1 | 133.1 (2) | C13—C14—C15 | 119.6 (2) |
| C5—C6—C1 | 122.3 (3) | N5—C14—C15 | 109.8 (2) |
| N1—C7—C8 | 111.6 (2) | N4—C15—C10 | 133.1 (2) |
| N1—C7—H7A | 109.3 | N4—C15—C14 | 104.8 (2) |
| C8—C7—H7A | 109.3 | C10—C15—C14 | 122.1 (3) |
| N1—C7—H7B | 109.3 | N2—N1—C6 | 109.9 (2) |
| C8—C7—H7B | 109.3 | N2—N1—C7 | 120.6 (2) |
| H7A—C7—H7B | 108.0 | C6—N1—C7 | 129.0 (2) |
| C9—C8—C7 | 111.8 (2) | N3—N2—N1 | 109.1 (2) |
| C9—C8—H8A | 109.3 | N2—N3—C5 | 108.0 (2) |
| C7—C8—H8A | 109.3 | C9—N4—C15 | 107.9 (2) |
| C9—C8—H8B | 109.3 | C9—N4—H14 | 124.0 |
| C7—C8—H8B | 109.3 | C15—N4—H14 | 127.7 |
| H8A—C8—H8B | 107.9 | C9—N5—C14 | 104.9 (2) |
| C6—C1—C2—C3 | −0.5 (4) | N5—C14—C15—N4 | 0.5 (3) |
| C1—C2—C3—C4 | 0.5 (5) | C13—C14—C15—C10 | −0.1 (4) |
| C2—C3—C4—C5 | −0.9 (5) | N5—C14—C15—C10 | −178.3 (2) |
| C3—C4—C5—N3 | −179.5 (3) | C5—C6—N1—N2 | −0.8 (3) |
| C3—C4—C5—C6 | 1.5 (4) | C1—C6—N1—N2 | −179.3 (3) |
| N3—C5—C6—N1 | 0.4 (3) | C5—C6—N1—C7 | −173.1 (2) |
| C4—C5—C6—N1 | 179.6 (2) | C1—C6—N1—C7 | 8.4 (5) |
| N3—C5—C6—C1 | 179.1 (2) | C8—C7—N1—N2 | −83.6 (3) |
| C4—C5—C6—C1 | −1.7 (4) | C8—C7—N1—C6 | 88.0 (3) |
| C2—C1—C6—N1 | 179.4 (3) | C6—N1—N2—N3 | 1.0 (3) |
| C2—C1—C6—C5 | 1.2 (4) | C7—N1—N2—N3 | 174.1 (2) |

| | | | |
|---|---|---|---|
| N1—C7—C8—C9 | 60.1 (3) | N1—N2—N3—C5 | −0.7 (3) |
| C7—C8—C9—N5 | −105.2 (3) | C6—C5—N3—N2 | 0.2 (3) |
| C7—C8—C9—N4 | 69.2 (3) | C4—C5—N3—N2 | −178.9 (3) |
| C15—C10—C11—C12 | −0.2 (4) | N5—C9—N4—C15 | 1.9 (3) |
| C10—C11—C12—C13 | −0.4 (4) | C8—C9—N4—C15 | −173.2 (2) |
| C11—C12—C13—C14 | 0.8 (4) | C10—C15—N4—C9 | 177.2 (3) |
| C12—C13—C14—N5 | 177.2 (3) | C14—C15—N4—C9 | −1.4 (3) |
| C12—C13—C14—C15 | −0.5 (4) | N4—C9—N5—C14 | −1.5 (3) |
| C11—C10—C15—N4 | −177.9 (3) | C8—C9—N5—C14 | 173.4 (2) |
| C11—C10—C15—C14 | 0.5 (4) | C13—C14—N5—C9 | −177.3 (3) |
| C13—C14—C15—N4 | 178.7 (2) | C15—C14—N5—C9 | 0.6 (3) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N4—H14···N5$^{i}$ | 0.84 | 2.04 | 2.855 (3) | 162 |
| C1—H1···N3$^{ii}$ | 0.93 | 2.54 | 3.456 (3) | 167 |

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) *x*−1, *y*, *z*.

**Fig. 1**

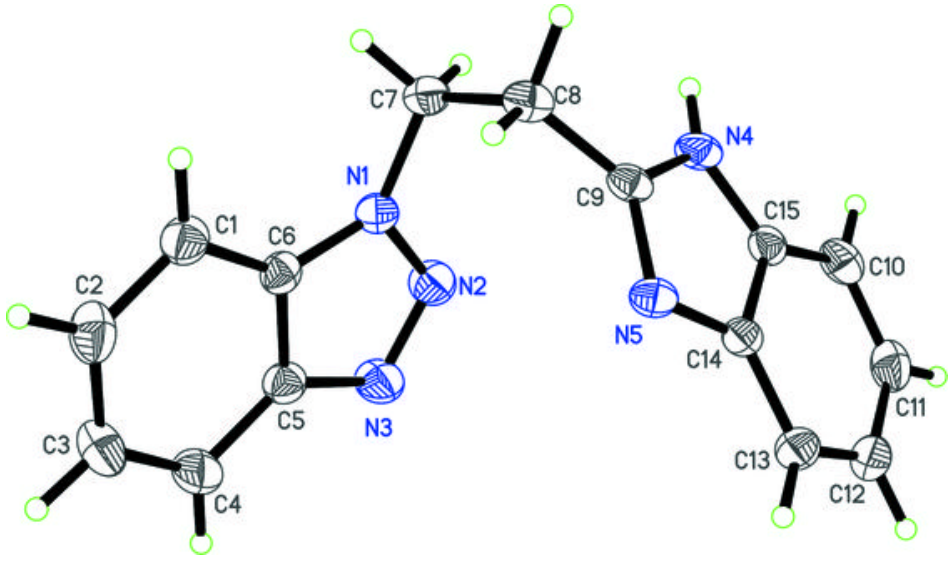

**Fig. 2**

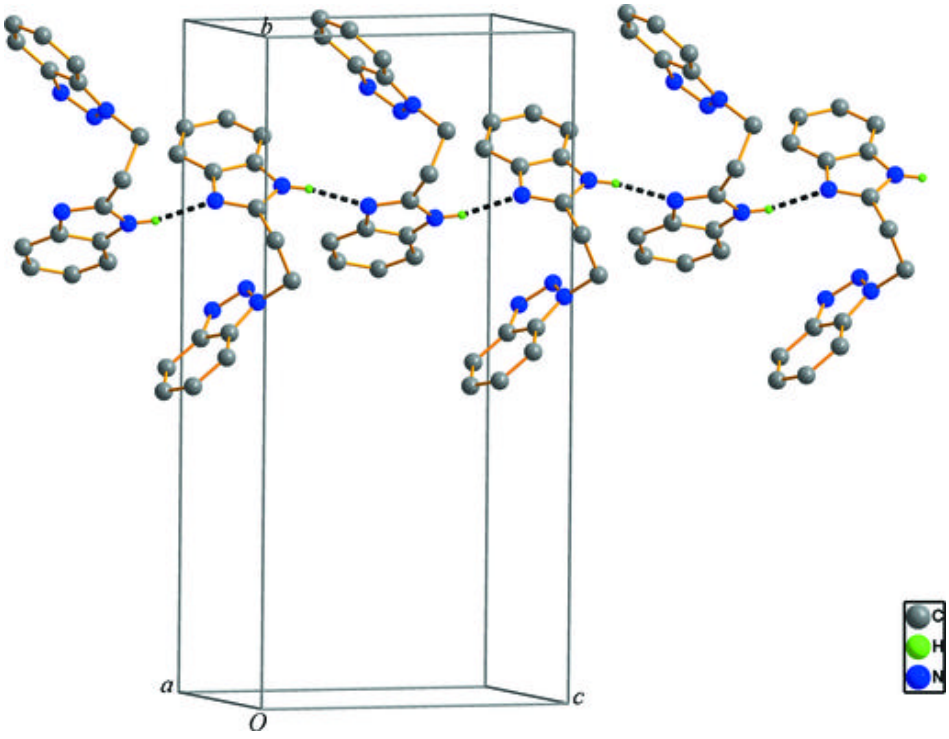

**Fig. 3**