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Ethyl 2-(1*H*-1,2,3-benzotriazol-1-yl)-acetate

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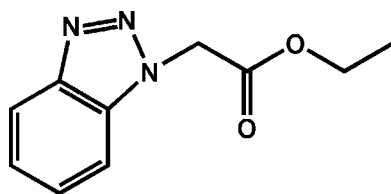
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å;
 R factor = 0.067; wR factor = 0.231; data-to-parameter ratio = 18.6.

The title compound, $\text{C}_{10}\text{H}_{11}\text{N}_3\text{O}_2$, was synthesized by the reaction of 1*H*-benzotriazole with ethyl 2-chloroacetate in ethanol. The non-H atoms, excluding the benzotriazol-1-yl group, are almost coplanar (r.m.s. deviation of the non-H atoms = 0.0409 Å). The dihedral angle formed between this plane and the benzotriazole ring is 79.12 (5)°. In the crystal, weak intermolecular C—H...N and C—H...O interactions help to consolidate the three-dimensional network.

Related literature

For related structures, see: Shi *et al.* (2007*a,b*); Ji *et al.* (2008); Zhang *et al.* (2009).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{11}\text{N}_3\text{O}_2$
 $M_r = 205.22$

Monoclinic, $C2/c$
 $a = 20.6734$ (9) Å

$b = 11.9284$ (5) Å
 $c = 9.3420$ (4) Å
 $\beta = 111.770$ (3)°
 $V = 2139.44$ (16) Å³
 $Z = 8$

Mo $K\alpha$ radiation $\mu = 0.09$ mm⁻¹ $T = 296$ K $0.23 \times 0.18 \times 0.16$ mm

Data collection

Bruker SMART APEX CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2007)
 $T_{\min} = 0.980$, $T_{\max} = 0.985$

9605 measured reflections
2551 independent reflections
1360 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.231$
 $S = 1.07$
2551 reflections
137 parameters

1 restraint

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.50$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C2-H2A\cdots N2^i$	0.93	2.57	3.457 (3)	159
$C7-H7A\cdots N3^i$	0.97	2.51	3.387 (3)	150
$C7-H7B\cdots O1^{ii}$	0.97	2.49	3.451 (3)	173

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; 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: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2062).

References

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supporting information

Acta Cryst. (2011). E67, o140 [https://doi.org/10.1107/S160053681005138X]

Ethyl 2-(1*H*-1,2,3-benzotriazol-1-yl)acetate

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S1. Comment

The Schiff-bases derived from benzotriazol-1-yl-acetic acid hydrazide with a relevant aldehyde or ketone have been widely investigated in recent years (Shi *et al.*, 2007*a*; Shi *et al.*, 2007*b*; Ji *et al.*, 2008). As an important intermediate in the synthesis procedure of benzotriazol-1-yl-acetic acid hydrazide (Zhang *et al.*, 2009), the title compound, (I), was synthesized and characterized by X-ray diffraction. The asymmetric unit of (I) comprises one independent molecule (Fig. 1). All the bond lengths are comparable with those observed in benzotriazol-1-yl-acetic acid hydrazide. In the crystal, weak intermolecular C—H \cdots N and C—H \cdots O interactions are helpful to consolidate the three-dimensional network (Fig. 2, Table 1).

S2. Experimental

1*H*-benzotriazole (1 mmol) and sodium hydroxide (1 mmol) were dissolved in ethanol (10 ml), and an ethanol (5 ml) solution of ethyl 2-chloroacetate (1 mmol) was added dropwise. After stirring for 4 h at room temperature, the mixture was filtered and set aside to crystallize at room temperature for several days, giving colourless block crystals.

S3. Refinement

The C7—C8 bond length was restrained to a reasonable distance: C7—C8 = 1.501 (4) Å (command *DFIX*). All H atoms were situated at idealized positions with the carrier atom-H distances = 0.93 Å for aryl, 0.97 for methylene, 0.96 Å for the methyl. The U_{iso} values were constrained to be $1.5U_{\text{eq}}$ of the carrier atom for the methyl H atoms and $1.2U_{\text{eq}}$ for the remaining H.

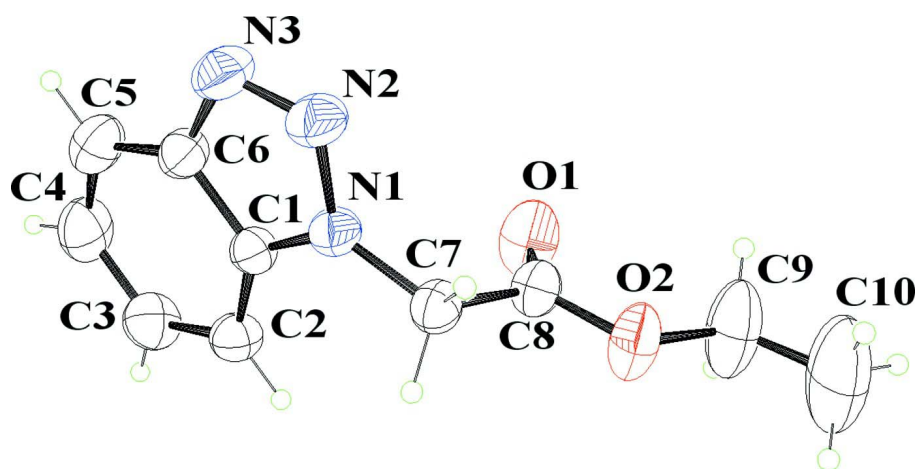


Figure 1

The title molecule with the displacement ellipsoids shown at the 30% probability level.

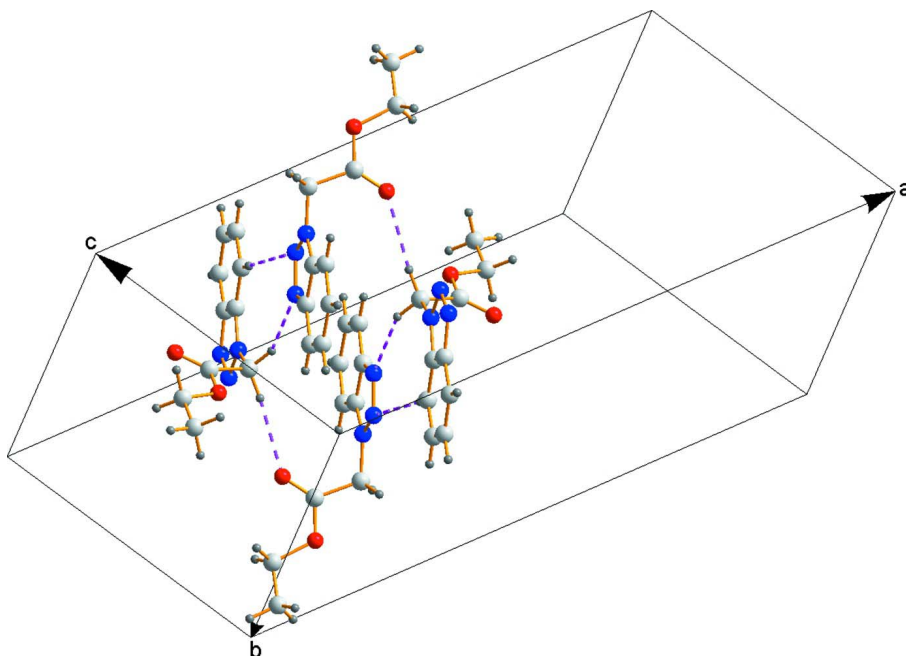


Figure 2

The crystal packing for the title compound *via* C—H···O and C—H···N weak interactions shown as dashed lines.

Ethyl 2-(1*H*-1,2,3-benzotriazol-1-yl)acetate

Crystal data

$C_{10}H_{11}N_3O_2$

$M_r = 205.22$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 20.6734\ (9)\ \text{\AA}$

$b = 11.9284\ (5)\ \text{\AA}$

$c = 9.3420\ (4)\ \text{\AA}$

$\beta = 111.770\ (3)^\circ$

$V = 2139.44\ (16)\ \text{\AA}^3$

$Z = 8$

$F(000) = 864$

$D_x = 1.274\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1764 reflections

$\theta = 2.8\text{--}21.8^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Block, colourless

$0.23 \times 0.18 \times 0.16\ \text{mm}$

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2007)

$T_{\min} = 0.980$, $T_{\max} = 0.985$

9605 measured reflections

2551 independent reflections

1360 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 27.9^\circ$, $\theta_{\min} = 2.0^\circ$

$h = -24 \rightarrow 27$

$k = -15 \rightarrow 13$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.067$

$wR(F^2) = 0.231$

$S = 1.07$

2551 reflections

137 parameters

1 restraint

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.1115P)^2 + 0.7271P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.50 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0044 (15)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.22410 (13)	-0.01039 (19)	0.6218 (3)	0.0558 (6)
C2	0.19757 (14)	-0.1116 (2)	0.5489 (3)	0.0682 (7)
H2A	0.2148	-0.1805	0.5934	0.082*
C3	0.14480 (17)	-0.1032 (3)	0.4084 (3)	0.0850 (9)
H3A	0.1254	-0.1685	0.3554	0.102*
C4	0.11878 (19)	0.0009 (3)	0.3412 (4)	0.0953 (11)
H4A	0.0829	0.0026	0.2448	0.114*
C5	0.14479 (17)	0.0994 (3)	0.4138 (3)	0.0847 (9)
H5A	0.1273	0.1683	0.3695	0.102*
C6	0.19825 (14)	0.0923 (2)	0.5557 (3)	0.0646 (7)
C7	0.31980 (13)	-0.0550 (2)	0.8782 (3)	0.0599 (7)
H7A	0.2938	-0.1200	0.8893	0.072*
H7B	0.3356	-0.0143	0.9751	0.072*
C8	0.38177 (14)	-0.0931 (2)	0.8442 (3)	0.0656 (7)
C9	0.4915 (2)	-0.1815 (5)	0.9535 (4)	0.1336 (18)
H9A	0.4811	-0.2436	0.8814	0.160*
H9B	0.5121	-0.1219	0.9141	0.160*
C10	0.5370 (3)	-0.2152 (7)	1.0919 (6)	0.193 (3)
H10A	0.5790	-0.2408	1.0814	0.289*
H10B	0.5168	-0.2753	1.1299	0.289*
H10C	0.5474	-0.1536	1.1630	0.289*
N1	0.27471 (10)	0.01616 (16)	0.7579 (2)	0.0587 (6)
N2	0.28073 (12)	0.12909 (18)	0.7742 (3)	0.0746 (7)
N3	0.23544 (14)	0.17555 (18)	0.6542 (3)	0.0791 (7)
O1	0.39013 (12)	-0.0827 (2)	0.7269 (2)	0.1030 (8)
O2	0.42674 (10)	-0.1412 (2)	0.9665 (2)	0.0926 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0550 (14)	0.0542 (14)	0.0614 (14)	0.0012 (11)	0.0252 (11)	0.0022 (11)
C2	0.0740 (18)	0.0594 (15)	0.0700 (16)	-0.0027 (13)	0.0252 (14)	-0.0003 (12)
C3	0.086 (2)	0.088 (2)	0.0721 (18)	-0.0117 (17)	0.0185 (16)	-0.0098 (16)
C4	0.079 (2)	0.122 (3)	0.0710 (19)	0.005 (2)	0.0117 (16)	0.0104 (19)
C5	0.086 (2)	0.085 (2)	0.0772 (19)	0.0188 (17)	0.0246 (17)	0.0170 (16)
C6	0.0655 (16)	0.0586 (15)	0.0730 (16)	0.0084 (12)	0.0295 (14)	0.0083 (12)
C7	0.0588 (15)	0.0603 (15)	0.0571 (13)	0.0023 (11)	0.0173 (11)	0.0007 (11)
C8	0.0630 (16)	0.0714 (17)	0.0584 (15)	0.0066 (13)	0.0179 (12)	0.0009 (12)
C9	0.088 (3)	0.212 (5)	0.099 (3)	0.066 (3)	0.032 (2)	0.013 (3)
C10	0.095 (3)	0.328 (8)	0.153 (4)	0.078 (4)	0.043 (3)	0.042 (5)
N1	0.0619 (13)	0.0470 (11)	0.0653 (12)	0.0005 (9)	0.0214 (10)	-0.0025 (9)
N2	0.0837 (16)	0.0490 (12)	0.0866 (16)	0.0008 (11)	0.0264 (13)	-0.0048 (11)
N3	0.0919 (18)	0.0531 (13)	0.0878 (16)	0.0087 (12)	0.0282 (14)	0.0035 (12)
O1	0.0971 (17)	0.151 (2)	0.0722 (13)	0.0321 (14)	0.0445 (12)	0.0153 (13)
O2	0.0721 (13)	0.1303 (19)	0.0729 (12)	0.0370 (13)	0.0240 (10)	0.0187 (12)

Geometric parameters (\AA , $^\circ$)

C1—N1	1.351 (3)	C7—H7A	0.9700
C1—C6	1.387 (3)	C7—H7B	0.9700
C1—C2	1.395 (3)	C8—O1	1.177 (3)
C2—C3	1.364 (4)	C8—O2	1.309 (3)
C2—H2A	0.9300	C9—C10	1.348 (5)
C3—C4	1.405 (5)	C9—O2	1.468 (4)
C3—H3A	0.9300	C9—H9A	0.9700
C4—C5	1.364 (5)	C9—H9B	0.9700
C4—H4A	0.9300	C10—H10A	0.9600
C5—C6	1.378 (4)	C10—H10B	0.9600
C5—H5A	0.9300	C10—H10C	0.9600
C6—N3	1.378 (3)	N1—N2	1.356 (3)
C7—N1	1.441 (3)	N2—N3	1.289 (3)
C7—C8	1.501 (4)		
N1—C1—C6	104.3 (2)	H7A—C7—H7B	107.9
N1—C1—C2	133.6 (2)	O1—C8—O2	123.9 (3)
C6—C1—C2	122.1 (2)	O1—C8—C7	126.7 (3)
C3—C2—C1	115.8 (3)	O2—C8—C7	109.5 (2)
C3—C2—H2A	122.1	C10—C9—O2	110.6 (3)
C1—C2—H2A	122.1	C10—C9—H9A	109.5
C2—C3—C4	122.1 (3)	O2—C9—H9A	109.5
C2—C3—H3A	118.9	C10—C9—H9B	109.5
C4—C3—H3A	118.9	O2—C9—H9B	109.5
C5—C4—C3	121.6 (3)	H9A—C9—H9B	108.1
C5—C4—H4A	119.2	C9—C10—H10A	109.5
C3—C4—H4A	119.2	C9—C10—H10B	109.5

C4—C5—C6	116.9 (3)	H10A—C10—H10B	109.5
C4—C5—H5A	121.5	C9—C10—H10C	109.5
C6—C5—H5A	121.5	H10A—C10—H10C	109.5
N3—C6—C5	130.4 (3)	H10B—C10—H10C	109.5
N3—C6—C1	108.2 (2)	C1—N1—N2	110.22 (19)
C5—C6—C1	121.4 (3)	C1—N1—C7	130.4 (2)
N1—C7—C8	111.7 (2)	N2—N1—C7	119.4 (2)
N1—C7—H7A	109.3	N3—N2—N1	108.8 (2)
C8—C7—H7A	109.3	N2—N3—C6	108.5 (2)
N1—C7—H7B	109.3	C8—O2—C9	116.4 (2)
C8—C7—H7B	109.3		
N1—C1—C2—C3	179.7 (3)	C2—C1—N1—N2	179.5 (3)
C6—C1—C2—C3	0.3 (4)	C6—C1—N1—C7	179.3 (2)
C1—C2—C3—C4	0.0 (5)	C2—C1—N1—C7	-0.2 (5)
C2—C3—C4—C5	-0.4 (5)	C8—C7—N1—C1	83.0 (3)
C3—C4—C5—C6	0.5 (5)	C8—C7—N1—N2	-96.6 (3)
C4—C5—C6—N3	178.7 (3)	C1—N1—N2—N3	0.6 (3)
C4—C5—C6—C1	-0.3 (4)	C7—N1—N2—N3	-179.7 (2)
N1—C1—C6—N3	1.1 (3)	N1—N2—N3—C6	0.1 (3)
C2—C1—C6—N3	-179.3 (2)	C5—C6—N3—N2	-179.9 (3)
N1—C1—C6—C5	-179.7 (2)	C1—C6—N3—N2	-0.8 (3)
C2—C1—C6—C5	-0.1 (4)	O1—C8—O2—C9	1.3 (5)
N1—C7—C8—O1	-10.6 (4)	C7—C8—O2—C9	-178.8 (3)
N1—C7—C8—O2	169.5 (2)	C10—C9—O2—C8	171.7 (5)
C6—C1—N1—N2	-1.0 (3)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2 <i>A</i> ...N2 ⁱ	0.93	2.57	3.457 (3)	159
C7—H7 <i>A</i> ...N3 ⁱ	0.97	2.51	3.387 (3)	150
C7—H7 <i>B</i> ...O1 ⁱⁱ	0.97	2.49	3.451 (3)	173

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