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5-(4-Nitrobenzyl)-1*H*-1,2,3,4-tetrazole

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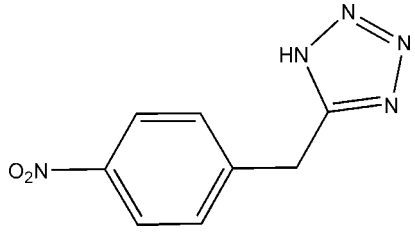
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.058; wR factor = 0.128; data-to-parameter ratio = 15.1.

In the title compound, $C_8H_7N_5O_2$, the dihedral angle between the benzene and tetrazole rings is 63.13 (8)°. The crystal structure exhibits intermolecular N—H···N hydrogen bonds which lead to the formation of one-dimensional chains along the [010] direction.

Related literature

For the applications of tetrazoles, see: Demko & Sharpless (2001). For our previous work on this class of compounds, see: Zhao *et al.* (2008).



Experimental

Crystal data

$C_8H_7N_5O_2$
M_r = 205.19
Monoclinic, $P2_1/c$
a = 6.3393 (10) Å
b = 4.9381 (6) Å
c = 28.801 (4) Å
β = 101.905 (14)°
V = 882.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 K
0.50 × 0.42 × 0.28 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.982, T_{max} = 0.990
8583 measured reflections
2088 independent reflections
1823 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.128
S = 1.20
2088 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N4^{i}	0.87	1.94	2.803 (2)	176

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL/PC*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2321).

References

Demko, Z. P. & Sharpless, K. B. (2001). *Org. Lett.* **3**, 4091–4094.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhao, H., Qu, Z. R., Ye, H. Y. & Xiong, R. G. (2008). *Chem. Soc. Rev.* **37**, 84–100.

supporting information

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5-(4-Nitrobenzyl)-1*H*-1,2,3,4-tetrazole

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S1. Comment

Tetrazole ligands have found a wide range of application in medicine chemistry, coordination chemistry and material chemistry (Demko & Sharpless, 2001). As part of an ongoing program in our laboratory to explore the structural characterization of the tetrazole-related compounds (Zhao *et al.*, 2008), the crystal structure of the title compound is reported here.

In the molecule of the title compound (Fig. 1) bond lengths and angles have normal values. The dihedral angle between the benzene ring and tetrazole ring is 63.13 (8)°. The crystal structure exhibits intermolecular N—H···N hydrogen bonds which lead to the formation of one dimensional chains along the [010] direction. (Fig. 2; Table 1).

S2. Experimental

A mixture of 2-(4-nitrophenyl)acetonitrile (20 mmol), NaN_3 (22 mmol) and NH_4Cl (22 mmol) in DMF (15 ml) was heated at 120°C for 20 h then cooled and the solvent removed under vacuum. The residue was poured into water (20 ml) to give the crude title compound. Colourless prismatic crystals suitable for X-ray analysis were obtained by slow evaporation of a 95% ethanol/water solution.

S3. Refinement

All H atoms were detected in a difference map, but were placed in calculated positions and refined using a riding motion approxmation, with C—H = 0.93–0.97 Å, with U_{iso}(H) = 1.2U_{eq}(C); N—H = 0.87 Å, with U_{iso}(H) = 1.5U_{eq}(N).

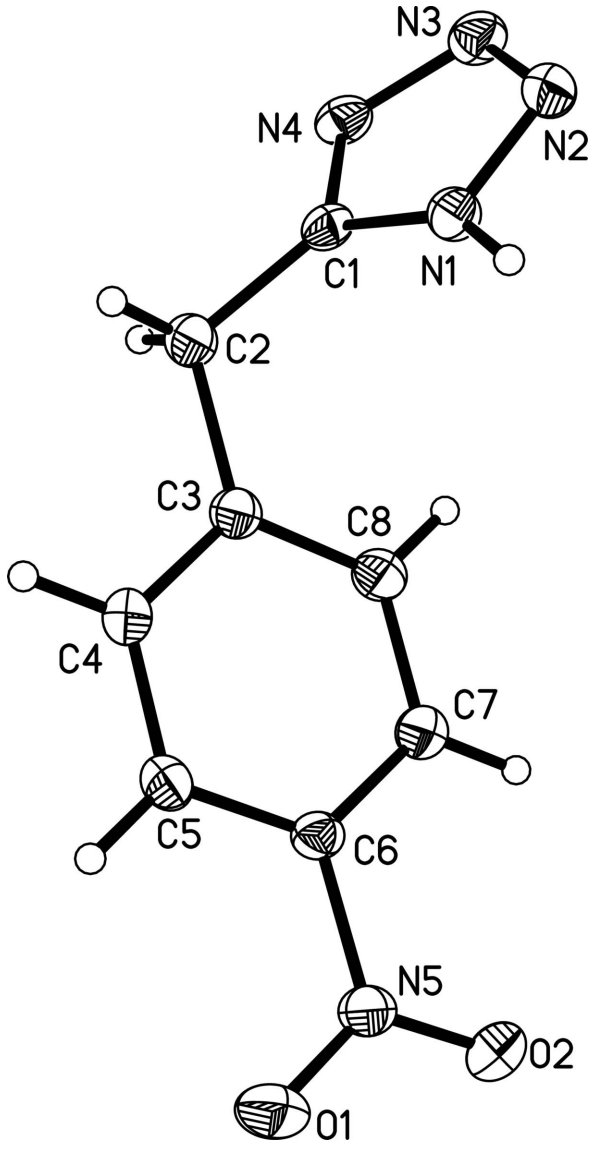

Figure 1

The molecular structure of the title compound, showing the atomic numbering scheme. The displacement ellipsoids are drawn at the 30% probability level.

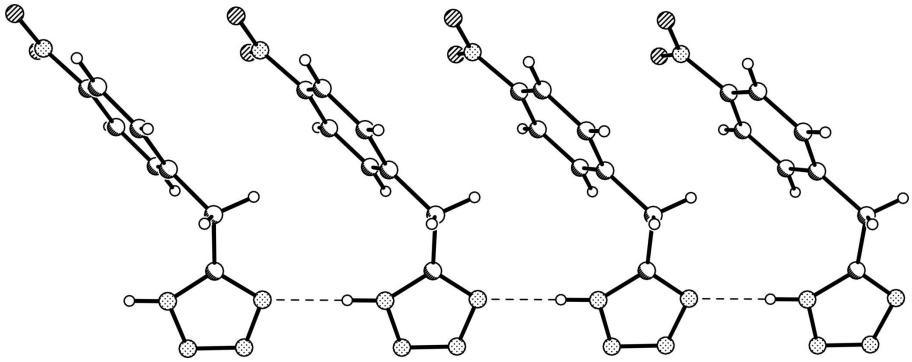

Figure 2

Diagram of the molecules linked into one-dimensional chain by a simple N—H···N interaction.

5-(4-Nitrobenzyl)-1*H*-1,2,3,4-tetrazole

Crystal data

$C_8H_7N_5O_2$
$M_r = 205.19$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.3393\ (10)$ Å
$b = 4.9381\ (6)$ Å
$c = 28.801\ (4)$ Å
$\beta = 101.905\ (14)°$
$V = 882.2\ (2)$ Å^3
$Z = 4$
$F(000) = 424$
$D_x = 1.545$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2188 reflections
$\theta = 3.2–27.5°$
$\mu = 0.12$ mm^{-1}
$T = 295$ K
Prism, pale yellow
0.50 × 0.42 × 0.28 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.982$, $T_{max} = 0.990$
8583 measured reflections
2088 independent reflections
1823 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.9°$
$h = -8\rightarrow8$
$k = -6\rightarrow6$
$l = -37\rightarrow37$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.128$
$S = 1.20$
2088 reflections
138 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 0.5689P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.037 (6)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.6521 (3)	−0.0440 (4)	0.23878 (6)	0.0537 (5)
O2	0.3476 (3)	0.0031 (4)	0.18977 (6)	0.0538 (5)
N1	0.7922 (3)	0.6457 (3)	0.02183 (6)	0.0340 (4)
H1	0.7833	0.4706	0.0214	0.051*
N2	0.7245 (3)	0.7302 (4)	−0.02353 (6)	0.0402 (4)
N3	0.7205 (3)	0.9910 (4)	−0.02326 (6)	0.0413 (5)
N4	0.7847 (3)	1.0783 (3)	0.02209 (6)	0.0358 (4)
N5	0.5369 (3)	0.0619 (4)	0.20421 (6)	0.0367 (4)
C1	0.8285 (3)	0.8620 (4)	0.04930 (7)	0.0297 (4)
C2	0.9119 (4)	0.8641 (4)	0.10150 (7)	0.0399 (5)
H2A	0.8881	1.0425	0.1135	0.048*
H2B	1.0664	0.8337	0.1076	0.048*
C3	0.8111 (3)	0.6555 (4)	0.12886 (7)	0.0327 (4)
C4	0.9324 (3)	0.5398 (4)	0.16973 (7)	0.0369 (5)
H4	1.0754	0.5918	0.1802	0.044*
C5	0.8439 (3)	0.3485 (4)	0.19519 (7)	0.0371 (5)
H5	0.9255	0.2715	0.2225	0.044*
C6	0.6314 (3)	0.2747 (4)	0.17898 (7)	0.0316 (4)
C7	0.5058 (3)	0.3865 (5)	0.13898 (7)	0.0382 (5)
H7	0.3629	0.3337	0.1288	0.046*
C8	0.5962 (3)	0.5790 (4)	0.11420 (7)	0.0386 (5)
H8	0.5124	0.6585	0.0874	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0614 (10)	0.0516 (10)	0.0475 (9)	−0.0025 (8)	0.0098 (8)	0.0188 (8)
O2	0.0503 (9)	0.0592 (11)	0.0516 (9)	−0.0227 (8)	0.0099 (8)	0.0033 (8)
N1	0.0432 (9)	0.0243 (8)	0.0348 (9)	−0.0038 (7)	0.0085 (7)	−0.0009 (7)
N2	0.0465 (10)	0.0401 (10)	0.0332 (9)	−0.0083 (8)	0.0064 (7)	0.0007 (8)
N3	0.0388 (9)	0.0413 (10)	0.0421 (10)	−0.0031 (8)	0.0041 (8)	0.0134 (8)
N4	0.0354 (9)	0.0301 (9)	0.0430 (9)	−0.0003 (7)	0.0104 (7)	0.0087 (7)
N5	0.0476 (10)	0.0317 (9)	0.0326 (9)	−0.0050 (8)	0.0127 (7)	−0.0009 (7)
C1	0.0318 (9)	0.0234 (9)	0.0352 (10)	−0.0035 (7)	0.0102 (7)	0.0009 (7)
C2	0.0530 (12)	0.0330 (11)	0.0332 (10)	−0.0122 (9)	0.0074 (9)	−0.0023 (9)
C3	0.0406 (10)	0.0278 (10)	0.0301 (9)	−0.0033 (8)	0.0083 (8)	−0.0022 (8)

C4	0.0354 (10)	0.0395 (11)	0.0336 (10)	−0.0073 (9)	0.0021 (8)	−0.0012 (9)
C5	0.0408 (11)	0.0385 (11)	0.0290 (9)	−0.0031 (9)	0.0006 (8)	0.0024 (8)
C6	0.0400 (10)	0.0268 (9)	0.0292 (9)	−0.0033 (8)	0.0102 (8)	−0.0006 (7)
C7	0.0333 (10)	0.0439 (12)	0.0365 (10)	−0.0045 (9)	0.0048 (8)	0.0031 (9)
C8	0.0389 (10)	0.0395 (12)	0.0350 (10)	−0.0010 (9)	0.0018 (8)	0.0090 (9)

Geometric parameters (Å, º)

O1—N5	1.224 (2)	C2—H2B	0.9700
O2—N5	1.221 (2)	C3—C4	1.389 (3)
N1—C1	1.321 (2)	C3—C8	1.392 (3)
N1—N2	1.354 (2)	C4—C5	1.384 (3)
N1—H1	0.8666	C4—H4	0.9300
N2—N3	1.288 (3)	C5—C6	1.381 (3)
N3—N4	1.356 (3)	C5—H5	0.9300
N4—C1	1.320 (2)	C6—C7	1.374 (3)
N5—C6	1.473 (2)	C7—C8	1.382 (3)
C1—C2	1.487 (3)	C7—H7	0.9300
C2—C3	1.516 (3)	C8—H8	0.9300
C2—H2A	0.9700		

C1—N1—N2	108.07 (16)	C4—C3—C8	118.78 (18)
C1—N1—H1	145.0	C4—C3—C2	120.03 (18)
N2—N1—H1	106.6	C8—C3—C2	121.18 (18)
N3—N2—N1	107.76 (17)	C5—C4—C3	121.02 (18)
N2—N3—N4	108.73 (16)	C5—C4—H4	119.5
C1—N4—N3	107.42 (16)	C3—C4—H4	119.5
O2—N5—O1	123.73 (18)	C6—C5—C4	118.38 (18)
O2—N5—C6	118.18 (17)	C6—C5—H5	120.8
O1—N5—C6	118.08 (17)	C4—C5—H5	120.8
N4—C1—N1	108.02 (17)	C7—C6—C5	122.25 (18)
N4—C1—C2	125.59 (18)	C7—C6—N5	118.43 (17)
N1—C1—C2	126.35 (17)	C5—C6—N5	119.28 (17)
C1—C2—C3	114.87 (16)	C6—C7—C8	118.63 (19)
C1—C2—H2A	108.6	C6—C7—H7	120.7
C3—C2—H2A	108.5	C8—C7—H7	120.7
C1—C2—H2B	108.6	C7—C8—C3	120.92 (18)
C3—C2—H2B	108.6	C7—C8—H8	119.5
H2A—C2—H2B	107.5	C3—C8—H8	119.5

C1—N1—N2—N3	0.1 (2)	C3—C4—C5—C6	0.0 (3)
N1—N2—N3—N4	−0.2 (2)	C4—C5—C6—C7	−0.7 (3)
N2—N3—N4—C1	0.2 (2)	C4—C5—C6—N5	177.08 (18)
N3—N4—C1—N1	−0.2 (2)	O2—N5—C6—C7	−3.4 (3)
N3—N4—C1—C2	177.72 (18)	O1—N5—C6—C7	177.28 (19)
N2—N1—C1—N4	0.1 (2)	O2—N5—C6—C5	178.74 (19)
N2—N1—C1—C2	−177.80 (18)	O1—N5—C6—C5	−0.5 (3)
N4—C1—C2—C3	138.7 (2)	C5—C6—C7—C8	0.1 (3)

N1—C1—C2—C3	−43.8 (3)	N5—C6—C7—C8	−177.64 (19)
C1—C2—C3—C4	147.51 (19)	C6—C7—C8—C3	1.1 (3)
C1—C2—C3—C8	−33.4 (3)	C4—C3—C8—C7	−1.7 (3)
C8—C3—C4—C5	1.1 (3)	C2—C3—C8—C7	179.3 (2)
C2—C3—C4—C5	−179.8 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N4^{i}	0.87	1.94	2.803 (2)	176

Symmetry code: (i) *x*, *y*−1, *z*.