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3-Phenyl-2-(1*H*-tetrazol-1-yl)propanoic acid monohydrate

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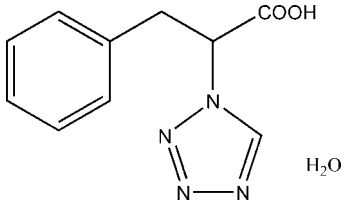
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.098; data-to-parameter ratio = 9.4.

In the title compound, $C_{10}H_{10}N_4O_2\cdot H_2O$, the dihedral angle between the tetrazole and benzene rings is 63.24 (11)°. The crystal structure is stabilized by intramolecular O—H···N and O—H···O hydrogen bonds.

Related literature

For background to the applications of tetrazole metal derivatives, see: Gaponik *et al.* (2006); Zhao *et al.* (2008); Xiao *et al.* (2009).



Experimental

Crystal data

$C_{10}H_{10}N_4O_2\cdot H_2O$
M_r = 236.24
Orthorhombic, $Pca2_1$
a = 24.001 (4) Å
b = 8.3769 (19) Å
c = 5.7455 (11) Å
V = 1155.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.40 × 0.25 × 0.10 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.972, T_{max} = 0.987
11450 measured reflections
1461 independent reflections
1237 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.098
S = 1.11
1461 reflections
155 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1W^{i}	0.82	1.74	2.552 (2)	174
O1W—H1B···N4^{ii}	0.92	1.98	2.903 (4)	177
O1W—H1A···N3^{iii}	0.89	2.12	3.003 (3)	171

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

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: RZ2488).

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supporting information

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3-Phenyl-2-(1*H*-tetrazol-1-yl)propanoic acid monohydrate

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S1. Comment

Recently tetrazoles have been area of interest of coordination chemistry because of various applications of their metal derivatives (Gaponik *et al.*, 2006; Zhao *et al.*, 2008). A great variety of tetrazoles, especially substituted ones, are investigated as ligands. Recently, we have reported a few tetrazole compounds (Xiao *et al.*, 2009). As an extension of our work on the structural characterization of tetrazole compounds, the 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 planes of the tetrazole and phenyl rings is 63.24 (0.11)°. The crystal structure (Fig. 2) is stabilized by intramolecular O—H···N and O—H···O hydrogen bonds (Table 1).

S2. Experimental

2-Amino-3-phenylpropanoic acid (1.65 g, 10 mmol) and triethoxymethane (2.96 g, 20 mmol) was added to a mixture of sodium azide (0.65 g, 10 mmol) in acetic acid. After 3 h at 80°C, the mixture was cooled to room temperature and poured into 50 ml HCl (30%) to afford a white precipitate of the title compound. Colourless crystals suitable for X-ray diffraction were obtained after 3 days by slow evaporation of an ethanol solution.

S3. Refinement

All H atoms were detected in a difference map, but were placed in calculated positions and refined using a riding motion approximation, with C—H = 0.93–0.97 Å, O—H = 0.82–0.92 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O). In the absence of significant anomalous dispersion effects, Friedel pairs were merged.

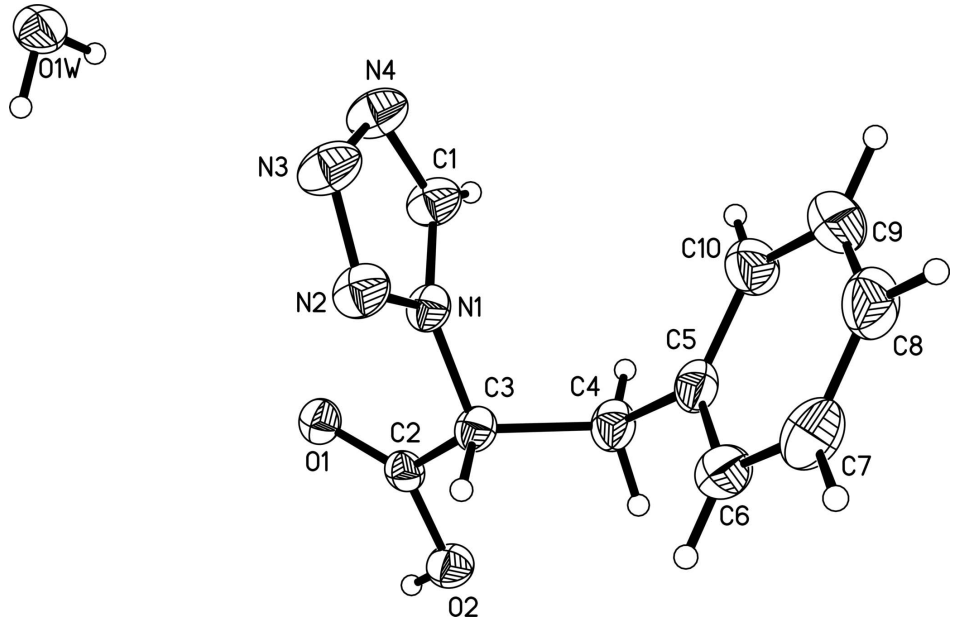

Figure 1

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

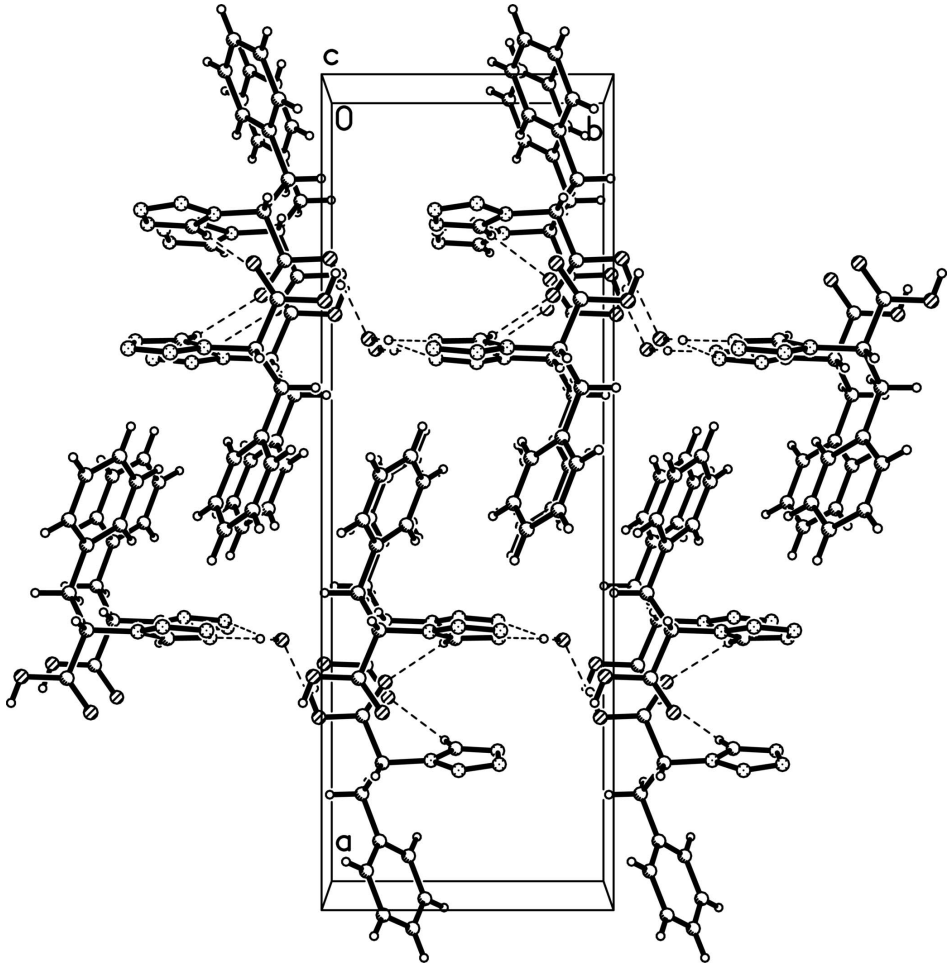

Figure 2

Packing diagram of the title compound, showing the structure down the *c* axis. Intermolecular hydrogen bonds are shown as dashed lines.

3-Phenyl-2-(1*H*-tetrazol-1-yl)propanoic acid monohydrate

Crystal data

$C_{10}H_{10}N_4O_2·H_2O$
M_r = 236.24
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
a = 24.001 (4) Å
b = 8.3769 (19) Å
c = 5.7455 (11) Å
V = 1155.1 (4) Å^3
Z = 4
$F(000)$ = 496
D_x = 1.358 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2576 reflections
θ = 2.4–27.5°
μ = 0.10 mm^{-1}
T = 293 K
Prism, colourless
0.40 × 0.25 × 0.10 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)

T_{min} = 0.972, T_{max} = 0.987
11450 measured reflections
1461 independent reflections
1237 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

θ_{max} = 27.5°, θ_{min} = 2.4°
h = −30→31
k = −10→10
l = −7→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.098
S = 1.11
1461 reflections
155 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
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.0812P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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}
C1	0.17744 (13)	0.5430 (3)	0.8029 (6)	0.0523 (7)
H1	0.1849	0.5834	0.6553	0.063*
C2	0.22253 (10)	0.8730 (3)	0.9938 (5)	0.0370 (5)
C3	0.16456 (9)	0.8029 (3)	1.0194 (5)	0.0385 (6)
H3	0.1523	0.8234	1.1793	0.046*
C4	0.12188 (11)	0.8794 (3)	0.8571 (6)	0.0494 (7)
H4A	0.1215	0.9937	0.8834	0.059*
H4B	0.1332	0.8612	0.6972	0.059*
C5	0.06378 (11)	0.8150 (3)	0.8910 (5)	0.0466 (6)
C6	0.03288 (12)	0.8572 (4)	1.0852 (6)	0.0605 (8)
H6	0.0480	0.9258	1.1957	0.073*
C7	−0.02045 (13)	0.7972 (4)	1.1151 (7)	0.0738 (11)
H7	−0.0410	0.8264	1.2455	0.089*
C8	−0.04305 (13)	0.6958 (4)	0.9550 (8)	0.0714 (10)
H8	−0.0787	0.6551	0.9767	0.086*
C9	−0.01295 (13)	0.6545 (4)	0.7634 (8)	0.0728 (10)
H9	−0.0282	0.5858	0.6535	0.087*
C10	0.03997 (12)	0.7138 (4)	0.7312 (6)	0.0617 (8)
H10	0.0600	0.6850	0.5991	0.074*
N1	0.16699 (8)	0.6303 (2)	0.9891 (4)	0.0398 (5)

N2	0.15902 (10)	0.5316 (3)	1.1690 (5)	0.0540 (7)
N3	0.16442 (12)	0.3885 (3)	1.0871 (5)	0.0611 (7)
N4	0.17577 (12)	0.3922 (3)	0.8561 (5)	0.0594 (7)
O1	0.26404 (6)	0.79317 (19)	0.9755 (4)	0.0431 (4)
O2	0.22055 (7)	1.02860 (19)	0.9997 (5)	0.0489 (4)
H2	0.2522	1.0647	0.9909	0.073*
O1W	0.31635 (8)	0.1603 (2)	0.9820 (4)	0.0574 (5)
H1A	0.3191	0.2341	0.8710	0.086*
H1B	0.3195	0.2313	1.1033	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0678 (18)	0.0421 (16)	0.0470 (17)	0.0014 (14)	0.0082 (15)	0.0055 (13)
C2	0.0443 (12)	0.0387 (12)	0.0281 (11)	−0.0003 (9)	−0.0035 (12)	0.0023 (13)
C3	0.0404 (12)	0.0343 (11)	0.0408 (15)	0.0011 (9)	0.0001 (11)	0.0066 (11)
C4	0.0468 (14)	0.0435 (14)	0.0579 (17)	0.0004 (11)	−0.0052 (13)	0.0097 (14)
C5	0.0420 (14)	0.0426 (14)	0.0553 (16)	0.0051 (11)	−0.0044 (13)	0.0077 (13)
C6	0.0555 (18)	0.0553 (17)	0.071 (2)	0.0057 (14)	0.0008 (17)	−0.0098 (16)
C7	0.058 (2)	0.081 (2)	0.082 (3)	0.0169 (17)	0.0193 (19)	−0.001 (2)
C8	0.0429 (15)	0.074 (2)	0.098 (3)	−0.0014 (14)	0.000 (2)	0.004 (2)
C9	0.055 (2)	0.078 (2)	0.086 (3)	−0.0076 (16)	−0.012 (2)	−0.012 (2)
C10	0.0507 (17)	0.072 (2)	0.0621 (19)	0.0008 (15)	−0.0013 (16)	−0.0097 (17)
N1	0.0407 (10)	0.0357 (10)	0.0429 (11)	−0.0008 (8)	0.0012 (11)	0.0081 (11)
N2	0.0709 (17)	0.0437 (14)	0.0473 (13)	0.0007 (12)	0.0061 (13)	0.0108 (12)
N3	0.0820 (18)	0.0393 (14)	0.0619 (16)	0.0022 (12)	0.0129 (15)	0.0076 (13)
N4	0.0760 (17)	0.0398 (14)	0.0624 (17)	0.0014 (12)	0.0127 (14)	0.0033 (13)
O1	0.0433 (10)	0.0469 (9)	0.0391 (9)	0.0032 (7)	0.0022 (9)	0.0037 (9)
O2	0.0489 (9)	0.0371 (9)	0.0607 (11)	−0.0051 (7)	−0.0016 (12)	−0.0002 (11)
O1W	0.0674 (12)	0.0484 (10)	0.0564 (11)	−0.0175 (8)	−0.0066 (13)	0.0071 (12)

Geometric parameters (Å, º)

C1—N4	1.301 (4)	C6—H6	0.9300
C1—N1	1.320 (4)	C7—C8	1.365 (5)
C1—H1	0.9300	C7—H7	0.9300
C2—O1	1.205 (3)	C8—C9	1.362 (6)
C2—O2	1.305 (3)	C8—H8	0.9300
C2—C3	1.517 (3)	C9—C10	1.376 (4)
C3—N1	1.457 (3)	C9—H9	0.9300
C3—C4	1.526 (4)	C10—H10	0.9300
C3—H3	0.9800	N1—N2	1.337 (3)
C4—C5	1.508 (4)	N2—N3	1.294 (4)
C4—H4A	0.9700	N3—N4	1.355 (4)
C4—H4B	0.9700	O2—H2	0.8200
C5—C10	1.374 (4)	O1W—H1A	0.8904
C5—C6	1.385 (4)	O1W—H1B	0.9193
C6—C7	1.385 (4)		

N4—C1—N1	110.0 (3)	C5—C6—H6	119.9
N4—C1—H1	125.0	C7—C6—H6	119.9
N1—C1—H1	125.0	C8—C7—C6	120.6 (3)
O1—C2—O2	126.0 (2)	C8—C7—H7	119.7
O1—C2—C3	123.48 (19)	C6—C7—H7	119.7
O2—C2—C3	110.55 (18)	C9—C8—C7	119.5 (3)
N1—C3—C2	109.64 (18)	C9—C8—H8	120.3
N1—C3—C4	111.7 (2)	C7—C8—H8	120.3
C2—C3—C4	113.2 (2)	C8—C9—C10	120.4 (3)
N1—C3—H3	107.3	C8—C9—H9	119.8
C2—C3—H3	107.3	C10—C9—H9	119.8
C4—C3—H3	107.3	C5—C10—C9	121.1 (3)
C5—C4—C3	113.1 (2)	C5—C10—H10	119.4
C5—C4—H4A	109.0	C9—C10—H10	119.4
C3—C4—H4A	109.0	C1—N1—N2	108.12 (19)
C5—C4—H4B	109.0	C1—N1—C3	130.9 (2)
C3—C4—H4B	109.0	N2—N1—C3	121.0 (2)
H4A—C4—H4B	107.8	N3—N2—N1	106.1 (2)
C10—C5—C6	118.2 (3)	N2—N3—N4	110.8 (3)
C10—C5—C4	121.2 (3)	C1—N4—N3	105.0 (3)
C6—C5—C4	120.5 (3)	C2—O2—H2	109.5
C5—C6—C7	120.1 (3)	H1A—O1W—H1B	95.0

O1—C2—C3—N1	−7.0 (4)	C4—C5—C10—C9	179.6 (3)
O2—C2—C3—N1	174.4 (2)	C8—C9—C10—C5	0.3 (5)
O1—C2—C3—C4	−132.5 (3)	N4—C1—N1—N2	0.8 (3)
O2—C2—C3—C4	48.9 (3)	N4—C1—N1—C3	179.4 (2)
N1—C3—C4—C5	58.4 (3)	C2—C3—N1—C1	−68.8 (3)
C2—C3—C4—C5	−177.2 (2)	C4—C3—N1—C1	57.5 (3)
C3—C4—C5—C10	−106.6 (3)	C2—C3—N1—N2	109.7 (3)
C3—C4—C5—C6	73.5 (3)	C4—C3—N1—N2	−124.0 (3)
C10—C5—C6—C7	0.3 (5)	C1—N1—N2—N3	−0.4 (3)
C4—C5—C6—C7	−179.9 (3)	C3—N1—N2—N3	−179.2 (2)
C5—C6—C7—C8	0.3 (5)	N1—N2—N3—N4	0.0 (3)
C6—C7—C8—C9	−0.6 (6)	N1—C1—N4—N3	−0.8 (4)
C7—C8—C9—C10	0.3 (6)	N2—N3—N4—C1	0.5 (4)
C6—C5—C10—C9	−0.6 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1*W*^{i}	0.82	1.74	2.552 (2)	174
O1*W*—H1*B*···N4^{ii}	0.92	1.98	2.903 (4)	177
O1*W*—H1*A*···N3^{iii}	0.89	2.12	3.003 (3)	171

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