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2-Phenyl-2H-1,2,3-triazole-4-carboxylic acid

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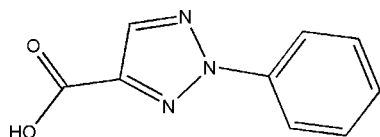
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.043; wR factor = 0.110; data-to-parameter ratio = 13.1.

In the title compound, $\text{C}_9\text{H}_7\text{N}_3\text{O}_2$, the dihedral angle between the triazole and phenyl ring planes is $4.72(6)^\circ$. In the crystal structure, classical inversion dimers arise from $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds between carboxylic acid groups.

Related literature

For related literature, see: Himanshu *et al.* (2002); Olesen *et al.* (2003); Tian *et al.* (2005). For the synthesis, see: Riebsomer & Sumrell (1948).



Experimental

Crystal data

$\text{C}_9\text{H}_7\text{N}_3\text{O}_2$
 $M_r = 189.18$
 Monoclinic, $P2_1/c$
 $a = 10.3239(16)$ Å
 $b = 5.2878(8)$ Å
 $c = 16.762(3)$ Å
 $\beta = 102.059(3)^\circ$

$V = 894.9(3)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 295(2)$ K
 $0.24 \times 0.14 \times 0.12$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\min} = 0.976$, $T_{\max} = 0.985$

4595 measured reflections
 1662 independent reflections
 1285 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.110$
 $S = 1.04$
 1662 reflections

127 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.13$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O2}-\text{H2}\cdots\text{O1}^i$	0.82	1.81	2.6295 (17)	176

Symmetry code: (i) $-x, -y - 1, -z + 2$.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2597).

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supplementary materials

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2-Phenyl-2H-1,2,3-triazole-4-carboxylic acid

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Comment

2-Substituted 1,2,3-triazole-4-carboxylic acids and their derivatives have received much attention due to their biological activities (Olesen *et al.*, 2003; Tian *et al.*, 2005). We report herein the crystal structure of the title compound, (I), (Fig. 1).

The bond lengths and angles for (I) are within normal ranges (Himanshu, *et al.*, 2002). The carboxyl group is inclined at an angle of 6.72 (11)° with respect to the attached triazole ring, and the dihedral angle between the triazole and phenyl planes is 4.72 (6)°. The classical hydrogen-bonded carboxylic acid dimers [O...O = 2.6295 (17) Å], characterized by an $R^2_2(8)$ pattern, predominantly stabilize the supramolecular assembly (Table 1).

Experimental

The title compound was prepared from phenyl-D-glucosazone according to the reported method (Riebsomer & Sumrell, 1948). Colourless prisms of (I) were obtained by slow evaporation of a 95% ethanol/water solution at room temperature.

Refinement

H atoms were placed at calculated positions (C—H = 0.93 Å, O—H = 0.82 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{O})$.

Figures

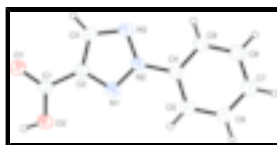


Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level for the non-hydrogen atoms.

2-Phenyl-2H-1,2,3-triazole-4-carboxylic acid

Crystal data

$\text{C}_9\text{H}_7\text{N}_3\text{O}_2$

$M_r = 189.18$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.3239$ (16) Å

$b = 5.2878$ (8) Å

$F_{000} = 392$

$D_x = 1.404$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 582 reflections

$\theta = 2.5$ – 22.5°

$\mu = 0.10$ mm⁻¹

supplementary materials

$c = 16.762$ (3) Å
 $\beta = 102.059$ (3)°
 $V = 894.9$ (3) Å³
 $Z = 4$

$T = 295$ (2) K
Prism, colourless
 $0.24 \times 0.14 \times 0.12$ mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
 $T = 295$ (2) K
 φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\min} = 0.976$, $T_{\max} = 0.985$
4595 measured reflections

1662 independent reflections
1285 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\text{max}} = 25.5^\circ$
 $\theta_{\text{min}} = 2.0^\circ$
 $h = -12 \rightarrow 12$
 $k = -6 \rightarrow 6$
 $l = -20 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.110$
 $S = 1.04$
1662 reflections
127 parameters
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
 $w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 0.1068P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.15199 (11)	-0.3925 (2)	1.02747 (7)	0.0582 (4)

O2	-0.00876 (11)	-0.2424 (3)	0.92851 (8)	0.0645 (4)
H2	-0.0504	-0.3605	0.9425	0.097*
N1	0.16466 (12)	0.1176 (3)	0.89183 (8)	0.0484 (4)
N2	0.27159 (12)	0.2601 (3)	0.89746 (8)	0.0473 (4)
N3	0.37074 (14)	0.2079 (3)	0.96051 (9)	0.0600 (4)
C1	0.10945 (15)	-0.2398 (3)	0.97275 (10)	0.0458 (4)
C2	0.19676 (15)	-0.0394 (3)	0.95531 (10)	0.0465 (4)
C3	0.32355 (17)	0.0180 (4)	0.99697 (12)	0.0590 (5)
H3	0.3687	-0.0645	1.0435	0.071*
C4	0.28259 (16)	0.4517 (3)	0.83914 (10)	0.0476 (4)
C5	0.18146 (18)	0.4835 (4)	0.77184 (11)	0.0624 (5)
H5	0.1064	0.3818	0.7641	0.075*
C6	0.1937 (2)	0.6685 (5)	0.71632 (12)	0.0737 (6)
H6	0.1262	0.6923	0.6707	0.088*
C7	0.3044 (2)	0.8186 (4)	0.72739 (12)	0.0691 (6)
H7	0.3118	0.9430	0.6894	0.083*
C8	0.40415 (19)	0.7846 (4)	0.79474 (12)	0.0642 (5)
H8	0.4792	0.8862	0.8021	0.077*
C9	0.39421 (16)	0.6013 (4)	0.85153 (11)	0.0556 (5)
H9	0.4616	0.5791	0.8974	0.067*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0524 (7)	0.0605 (8)	0.0577 (8)	-0.0031 (6)	0.0021 (6)	0.0080 (7)
O2	0.0465 (7)	0.0701 (10)	0.0718 (9)	-0.0097 (6)	0.0007 (6)	0.0139 (7)
N1	0.0399 (7)	0.0538 (9)	0.0511 (9)	-0.0042 (7)	0.0082 (6)	-0.0020 (7)
N2	0.0388 (7)	0.0517 (9)	0.0500 (8)	-0.0035 (6)	0.0062 (6)	-0.0020 (7)
N3	0.0431 (8)	0.0686 (11)	0.0621 (10)	-0.0061 (8)	-0.0028 (7)	0.0079 (8)
C1	0.0409 (9)	0.0513 (11)	0.0446 (9)	0.0018 (8)	0.0078 (7)	-0.0032 (8)
C2	0.0405 (9)	0.0506 (11)	0.0483 (9)	0.0020 (8)	0.0088 (7)	-0.0030 (8)
C3	0.0481 (10)	0.0658 (13)	0.0586 (11)	-0.0025 (9)	0.0010 (8)	0.0100 (10)
C4	0.0464 (9)	0.0495 (11)	0.0481 (9)	-0.0027 (8)	0.0125 (7)	-0.0047 (8)
C5	0.0547 (10)	0.0712 (14)	0.0574 (11)	-0.0120 (10)	0.0029 (9)	0.0051 (10)
C6	0.0723 (13)	0.0844 (17)	0.0585 (12)	-0.0112 (12)	0.0000 (10)	0.0109 (11)
C7	0.0805 (14)	0.0661 (14)	0.0612 (12)	-0.0103 (11)	0.0157 (10)	0.0084 (10)
C8	0.0627 (11)	0.0621 (13)	0.0693 (13)	-0.0147 (10)	0.0172 (10)	-0.0036 (10)
C9	0.0500 (10)	0.0593 (12)	0.0566 (11)	-0.0082 (9)	0.0089 (8)	-0.0051 (9)

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

O1—C1	1.2320 (19)	C4—C9	1.377 (2)
O2—C1	1.2889 (18)	C4—C5	1.378 (2)
O2—H2	0.8200	C5—C6	1.374 (3)
N1—N2	1.3235 (18)	C5—H5	0.9300
N1—C2	1.336 (2)	C6—C7	1.372 (3)
N2—N3	1.3376 (18)	C6—H6	0.9300
N2—C4	1.428 (2)	C7—C8	1.372 (3)
N3—C3	1.320 (2)	C7—H7	0.9300

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C1—C2	1.460 (2)	C8—C9	1.377 (3)
C2—C3	1.383 (2)	C8—H8	0.9300
C3—H3	0.9300	C9—H9	0.9300
C1—O2—H2	109.5	C5—C4—N2	119.47 (15)
N2—N1—C2	103.47 (12)	C6—C5—C4	118.69 (18)
N1—N2—N3	115.33 (14)	C6—C5—H5	120.7
N1—N2—C4	122.63 (13)	C4—C5—H5	120.7
N3—N2—C4	122.02 (13)	C7—C6—C5	120.82 (19)
C3—N3—N2	103.15 (14)	C7—C6—H6	119.6
O1—C1—O2	124.68 (16)	C5—C6—H6	119.6
O1—C1—C2	119.06 (15)	C8—C7—C6	119.75 (19)
O2—C1—C2	116.26 (15)	C8—C7—H7	120.1
N1—C2—C3	108.47 (15)	C6—C7—H7	120.1
N1—C2—C1	123.37 (14)	C7—C8—C9	120.66 (18)
C3—C2—C1	128.12 (16)	C7—C8—H8	119.7
N3—C3—C2	109.58 (16)	C9—C8—H8	119.7
N3—C3—H3	125.2	C8—C9—C4	118.74 (17)
C2—C3—H3	125.2	C8—C9—H9	120.6
C9—C4—C5	121.34 (17)	C4—C9—H9	120.6
C9—C4—N2	119.19 (15)		
C2—N1—N2—N3	-0.43 (19)	N1—N2—C4—C9	176.55 (15)
C2—N1—N2—C4	177.77 (14)	N3—N2—C4—C9	-5.4 (2)
N1—N2—N3—C3	0.4 (2)	N1—N2—C4—C5	-3.3 (2)
C4—N2—N3—C3	-177.78 (16)	N3—N2—C4—C5	174.78 (16)
N2—N1—C2—C3	0.24 (18)	C9—C4—C5—C6	0.2 (3)
N2—N1—C2—C1	-177.93 (15)	N2—C4—C5—C6	-179.94 (18)
O1—C1—C2—N1	172.56 (15)	C4—C5—C6—C7	0.1 (3)
O2—C1—C2—N1	-7.5 (2)	C5—C6—C7—C8	-0.2 (3)
O1—C1—C2—C3	-5.2 (3)	C6—C7—C8—C9	-0.1 (3)
O2—C1—C2—C3	174.74 (17)	C7—C8—C9—C4	0.4 (3)
N2—N3—C3—C2	-0.3 (2)	C5—C4—C9—C8	-0.5 (3)
N1—C2—C3—N3	0.0 (2)	N2—C4—C9—C8	179.67 (16)
C1—C2—C3—N3	178.07 (17)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O2-H2\cdots O1^i$	0.82	1.81	2.6295 (17)	176

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

Fig. 1

