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1-Benzyl-3-phenyl-1*H*-pyrazole-5-carboxylic acid

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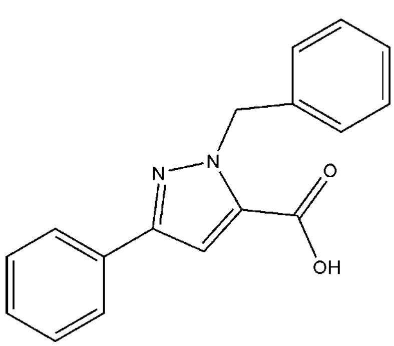
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.164; data-to-parameter ratio = 16.6.

In the title compound, $C_{17}H_{14}N_2O_2$, the pyrazole ring makes dihedral angles of 18.8 (1) and 81.1 (1)° with the phenyl and benzyl rings, respectively. In the crystal structure, carboxyl groups are connected by O—H···O hydrogen bonds, creating a centrosymmetric ring typical of organic carboxylic acids.

Related literature

For related literature, see: Jia *et al.* (2004); Cottineau *et al.* (2002); Finn *et al.* (2003); Wei *et al.* (2006); Ding *et al.* (2007).



Experimental

Crystal data

$C_{17}H_{14}N_2O_2$
M_r = 278.30
Monoclinic, $P2_1/n$
a = 13.1764 (5) Å
b = 5.3356 (2) Å
c = 20.6646 (7) Å
β = 106.132 (3)°
V = 1395.60 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.30 × 0.21 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.974, T_{max} = 0.985
8816 measured reflections
3175 independent reflections
1921 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.164
S = 0.90
3175 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1^{i}	0.82	1.85	2.662 (2)	173

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2120).

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supplementary materials

Acta Cryst. (2007). E**63**, o3473   [doi:10.1107/S1600536807033363]

1-Benzyl-3-phenyl-1*H*-pyrazole-5-carboxylic acid

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Comment

Pyrazole moiety plays an essential role in biologically active compounds. Many pyrazole derivatives are known to exhibit a wide range of biological properties such as anticoagulant (Jia *et al.*, 2004), antipyretic, antibacterial, hypoglycaemic, anti-hyperglycaemic, analgesic, anti-inflammatory, sedative-hypnotic (Cottineau *et al.*, 2002; Finn *et al.*, 2003), and antitumour (Wei *et al.*, 2006) activities. We report here the crystal structure of the title compound (I).

Experimental

A mixture of ethyl 1-benzyl-3-phenyl-1*H*-pyrazole-5-carboxylate (0.01 mol) and potassium hydroxide (0.02 mol) in ethanol (40 ml) was heated to reflux for 2 h (Ding *et al.*, 2007). The solvent was removed under reduced pressure and the residue was dissolved in water and acidified with hydrochloric acid (10%). The precipitate was filtered and dried to give a white solid (yield 80%). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a solution of the solid in acetone at room temperature for 6 d.

Refinement

All H atoms were placed at geometrically calculated positions and allowed to ride with C—H = 0.97 Å (for CH_2 groups), and O—H = 0.82 Å; their isotropic displacement parameters were set to 1.2 times (CH_2 groups) or 1.5 times (O—H groups) the equivalent displacement parameter of their parent atoms.

Figures

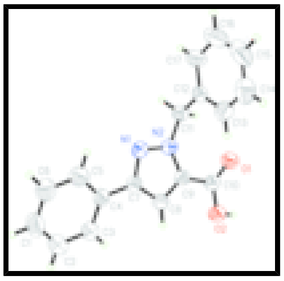

Fig. 1. The molecular strure of (I) showing displacement ellipsoids drawn at the 50% probability level.

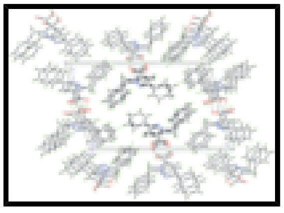

Fig. 2. Packing view of (I) along the *a* axis. Hydrogen bonds creating dimeric units are drawn as dashed lines. Hydrogen bonded rings are stacked perpendicular to the *c* axis forming hydrophilic channels.

1-Benzyl-3-phenyl-1*H*-pyrazole-5-carboxylic acid

Crystal data

$C_{17}H_{14}N_2O_2$	F_{000} = 584
M_r = 278.30	D_x = 1.325 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 13.1764 (5) Å	Cell parameters from 2168 reflections
b = 5.3356 (2) Å	θ = 3.1–24.9º
c = 20.6646 (7) Å	μ = 0.09 mm^{-1}
β = 106.132 (3)º	T = 293 (2) K
V = 1395.60 (9) Å^3	Prism, colourless
Z = 4	0.30 × 0.21 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	3175 independent reflections
Radiation source: fine-focus sealed tube	1921 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 293(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (APEX2; Bruker, 2005)	$h = -17 \rightarrow 16$
T_{min} = 0.974, T_{max} = 0.985	$k = -6 \rightarrow 6$
8816 measured reflections	$l = -26 \rightarrow 24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.164	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.212P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.90	$(\Delta/\sigma)_{max}$ < 0.001
3175 reflections	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
191 parameters	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3797 (2)	−0.3005 (5)	0.34905 (13)	0.0702 (7)
H1	0.4076	−0.4120	0.3239	0.084*
C2	0.2974 (2)	−0.1482 (5)	0.31785 (12)	0.0722 (7)
H2	0.2690	−0.1573	0.2714	0.087*
C3	0.25613 (19)	0.0193 (4)	0.35477 (10)	0.0584 (6)
H3	0.2004	0.1230	0.3329	0.070*
C4	0.29696 (15)	0.0340 (4)	0.42403 (9)	0.0445 (5)
C5	0.37994 (17)	−0.1229 (4)	0.45512 (11)	0.0560 (6)
H5	0.4082	−0.1167	0.5016	0.067*
C6	0.42100 (19)	−0.2885 (5)	0.41757 (13)	0.0664 (6)
H6	0.4770	−0.3923	0.4389	0.080*
C7	0.25032 (14)	0.2085 (4)	0.46310 (9)	0.0411 (4)
C8	0.18501 (15)	0.4147 (4)	0.44101 (9)	0.0443 (5)
H8	0.1629	0.4779	0.3974	0.053*
C9	0.15998 (14)	0.5055 (4)	0.49666 (9)	0.0407 (4)
C10	0.09260 (14)	0.7196 (4)	0.50114 (9)	0.0419 (4)
C11	0.20965 (16)	0.3581 (4)	0.61995 (9)	0.0484 (5)
H11A	0.2045	0.1871	0.6347	0.058*
H11B	0.1475	0.4476	0.6237	0.058*
C12	0.30615 (15)	0.4784 (4)	0.66620 (9)	0.0440 (5)
C13	0.35187 (18)	0.6884 (4)	0.64740 (12)	0.0591 (6)
H13	0.3252	0.7545	0.6044	0.071*
C14	0.4374 (2)	0.8010 (5)	0.69235 (15)	0.0783 (8)
H14	0.4681	0.9425	0.6795	0.094*
C15	0.4771 (2)	0.7040 (6)	0.75619 (15)	0.0832 (9)
H15	0.5344	0.7804	0.7865	0.100*
C16	0.4325 (2)	0.4969 (6)	0.77479 (12)	0.0802 (8)
H16	0.4596	0.4313	0.8178	0.096*
C17	0.34734 (19)	0.3830 (5)	0.73023 (10)	0.0619 (6)
H17	0.3174	0.2409	0.7434	0.074*
N1	0.26556 (13)	0.1739 (3)	0.52914 (8)	0.0460 (4)
N2	0.21010 (12)	0.3551 (3)	0.54916 (7)	0.0435 (4)
O1	0.07681 (11)	0.7942 (3)	0.55347 (7)	0.0529 (4)
O2	0.04902 (11)	0.8197 (3)	0.44201 (6)	0.0549 (4)
H2A	0.0087	0.9321	0.4460	0.082*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0844 (17)	0.0574 (15)	0.0805 (17)	0.0054 (14)	0.0421 (15)	−0.0104 (13)
C2	0.0992 (19)	0.0666 (17)	0.0541 (14)	0.0088 (15)	0.0267 (13)	−0.0071 (12)
C3	0.0759 (14)	0.0518 (13)	0.0475 (12)	0.0096 (12)	0.0173 (11)	−0.0001 (10)
C4	0.0517 (11)	0.0373 (11)	0.0472 (11)	−0.0058 (9)	0.0178 (9)	−0.0008 (9)
C5	0.0554 (12)	0.0594 (14)	0.0533 (12)	0.0028 (11)	0.0153 (10)	0.0005 (10)
C6	0.0659 (14)	0.0633 (15)	0.0732 (16)	0.0148 (13)	0.0246 (12)	0.0009 (13)
C7	0.0462 (10)	0.0361 (10)	0.0402 (10)	−0.0043 (9)	0.0105 (8)	0.0014 (8)
C8	0.0501 (10)	0.0440 (11)	0.0376 (10)	−0.0045 (10)	0.0100 (8)	0.0013 (8)
C9	0.0418 (9)	0.0384 (10)	0.0408 (10)	−0.0021 (9)	0.0098 (8)	0.0023 (8)
C10	0.0389 (9)	0.0429 (11)	0.0427 (10)	−0.0034 (9)	0.0095 (8)	0.0027 (8)
C11	0.0578 (11)	0.0491 (12)	0.0408 (10)	0.0025 (10)	0.0181 (9)	0.0072 (9)
C12	0.0515 (11)	0.0426 (11)	0.0390 (10)	0.0077 (9)	0.0143 (8)	−0.0036 (8)
C13	0.0624 (13)	0.0492 (13)	0.0620 (14)	0.0024 (11)	0.0111 (11)	0.0015 (11)
C14	0.0727 (16)	0.0616 (16)	0.097 (2)	−0.0076 (14)	0.0183 (15)	−0.0156 (15)
C15	0.0659 (15)	0.095 (2)	0.0775 (19)	0.0039 (16)	0.0020 (14)	−0.0396 (17)
C16	0.0821 (18)	0.104 (2)	0.0454 (13)	0.0168 (18)	0.0029 (12)	−0.0116 (14)
C17	0.0740 (14)	0.0721 (16)	0.0393 (11)	0.0113 (13)	0.0153 (10)	0.0048 (11)
N1	0.0536 (9)	0.0406 (9)	0.0444 (9)	0.0036 (8)	0.0144 (7)	0.0027 (7)
N2	0.0502 (9)	0.0431 (9)	0.0380 (8)	0.0003 (8)	0.0136 (7)	0.0027 (7)
O1	0.0580 (8)	0.0570 (9)	0.0442 (8)	0.0094 (7)	0.0151 (7)	0.0011 (7)
O2	0.0626 (9)	0.0545 (9)	0.0446 (8)	0.0145 (7)	0.0098 (7)	0.0037 (6)

Geometric parameters (Å, °)

C1—C2	1.365 (3)	C10—O2	1.311 (2)
C1—C6	1.370 (3)	C11—N2	1.465 (2)
C1—H1	0.9300	C11—C12	1.506 (3)
C2—C3	1.381 (3)	C11—H11A	0.9700
C2—H2	0.9300	C11—H11B	0.9700
C3—C4	1.384 (3)	C12—C13	1.378 (3)
C3—H3	0.9300	C12—C17	1.380 (3)
C4—C5	1.385 (3)	C13—C14	1.383 (3)
C4—C7	1.474 (3)	C13—H13	0.9300
C5—C6	1.381 (3)	C14—C15	1.378 (4)
C5—H5	0.9300	C14—H14	0.9300
C6—H6	0.9300	C15—C16	1.356 (4)
C7—N1	1.336 (2)	C15—H15	0.9300
C7—C8	1.393 (3)	C16—C17	1.379 (3)
C8—C9	1.370 (2)	C16—H16	0.9300
C8—H8	0.9300	C17—H17	0.9300
C9—N2	1.363 (2)	N1—N2	1.345 (2)
C9—C10	1.465 (3)	O2—H2A	0.8200
C10—O1	1.223 (2)		
C2—C1—C6	119.7 (2)	N2—C11—C12	113.68 (15)

C2—C1—H1	120.2	N2—C11—H11A	108.8
C6—C1—H1	120.2	C12—C11—H11A	108.8
C1—C2—C3	120.5 (2)	N2—C11—H11B	108.8
C1—C2—H2	119.8	C12—C11—H11B	108.8
C3—C2—H2	119.8	H11A—C11—H11B	107.7
C2—C3—C4	120.5 (2)	C13—C12—C17	118.9 (2)
C2—C3—H3	119.7	C13—C12—C11	121.73 (18)
C4—C3—H3	119.7	C17—C12—C11	119.29 (19)
C3—C4—C5	118.38 (19)	C12—C13—C14	120.2 (2)
C3—C4—C7	120.05 (18)	C12—C13—H13	119.9
C5—C4—C7	121.55 (18)	C14—C13—H13	119.9
C6—C5—C4	120.5 (2)	C15—C14—C13	120.1 (3)
C6—C5—H5	119.7	C15—C14—H14	119.9
C4—C5—H5	119.7	C13—C14—H14	119.9
C1—C6—C5	120.4 (2)	C16—C15—C14	119.9 (3)
C1—C6—H6	119.8	C16—C15—H15	120.1
C5—C6—H6	119.8	C14—C15—H15	120.1
N1—C7—C8	110.35 (16)	C15—C16—C17	120.4 (3)
N1—C7—C4	120.34 (17)	C15—C16—H16	119.8
C8—C7—C4	129.27 (17)	C17—C16—H16	119.8
C9—C8—C7	105.97 (16)	C16—C17—C12	120.5 (2)
C9—C8—H8	127.0	C16—C17—H17	119.7
C7—C8—H8	127.0	C12—C17—H17	119.7
N2—C9—C8	106.46 (16)	C7—N1—N2	105.94 (15)
N2—C9—C10	125.21 (16)	N1—N2—C9	111.28 (14)
C8—C9—C10	128.33 (17)	N1—N2—C11	117.94 (15)
O1—C10—O2	123.60 (18)	C9—N2—C11	130.75 (16)
O1—C10—C9	124.37 (17)	C10—O2—H2A	109.5
O2—C10—C9	112.02 (16)		

C6—C1—C2—C3	0.5 (4)	N2—C11—C12—C13	38.8 (3)
C1—C2—C3—C4	−0.5 (4)	N2—C11—C12—C17	−144.13 (18)
C2—C3—C4—C5	0.0 (3)	C17—C12—C13—C14	−0.2 (3)
C2—C3—C4—C7	−178.3 (2)	C11—C12—C13—C14	176.9 (2)
C3—C4—C5—C6	0.4 (3)	C12—C13—C14—C15	−0.1 (4)
C7—C4—C5—C6	178.70 (19)	C13—C14—C15—C16	0.3 (4)
C2—C1—C6—C5	−0.1 (4)	C14—C15—C16—C17	−0.2 (4)
C4—C5—C6—C1	−0.4 (4)	C15—C16—C17—C12	−0.2 (4)
C3—C4—C7—N1	159.65 (19)	C13—C12—C17—C16	0.4 (3)
C5—C4—C7—N1	−18.6 (3)	C11—C12—C17—C16	−176.8 (2)
C3—C4—C7—C8	−17.8 (3)	C8—C7—N1—N2	0.4 (2)
C5—C4—C7—C8	163.97 (19)	C4—C7—N1—N2	−177.49 (16)
N1—C7—C8—C9	−0.4 (2)	C7—N1—N2—C9	−0.3 (2)
C4—C7—C8—C9	177.26 (18)	C7—N1—N2—C11	178.09 (16)
C7—C8—C9—N2	0.2 (2)	C8—C9—N2—N1	0.0 (2)
C7—C8—C9—C10	−179.40 (17)	C10—C9—N2—N1	179.64 (16)
N2—C9—C10—O1	3.0 (3)	C8—C9—N2—C11	−178.03 (18)
C8—C9—C10—O1	−177.48 (19)	C10—C9—N2—C11	1.6 (3)
N2—C9—C10—O2	−175.67 (17)	C12—C11—N2—N1	81.3 (2)
C8—C9—C10—O2	3.9 (3)	C12—C11—N2—C9	−100.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1^{i}	0.82	1.85	2.662 (2)	173

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

Fig. 1

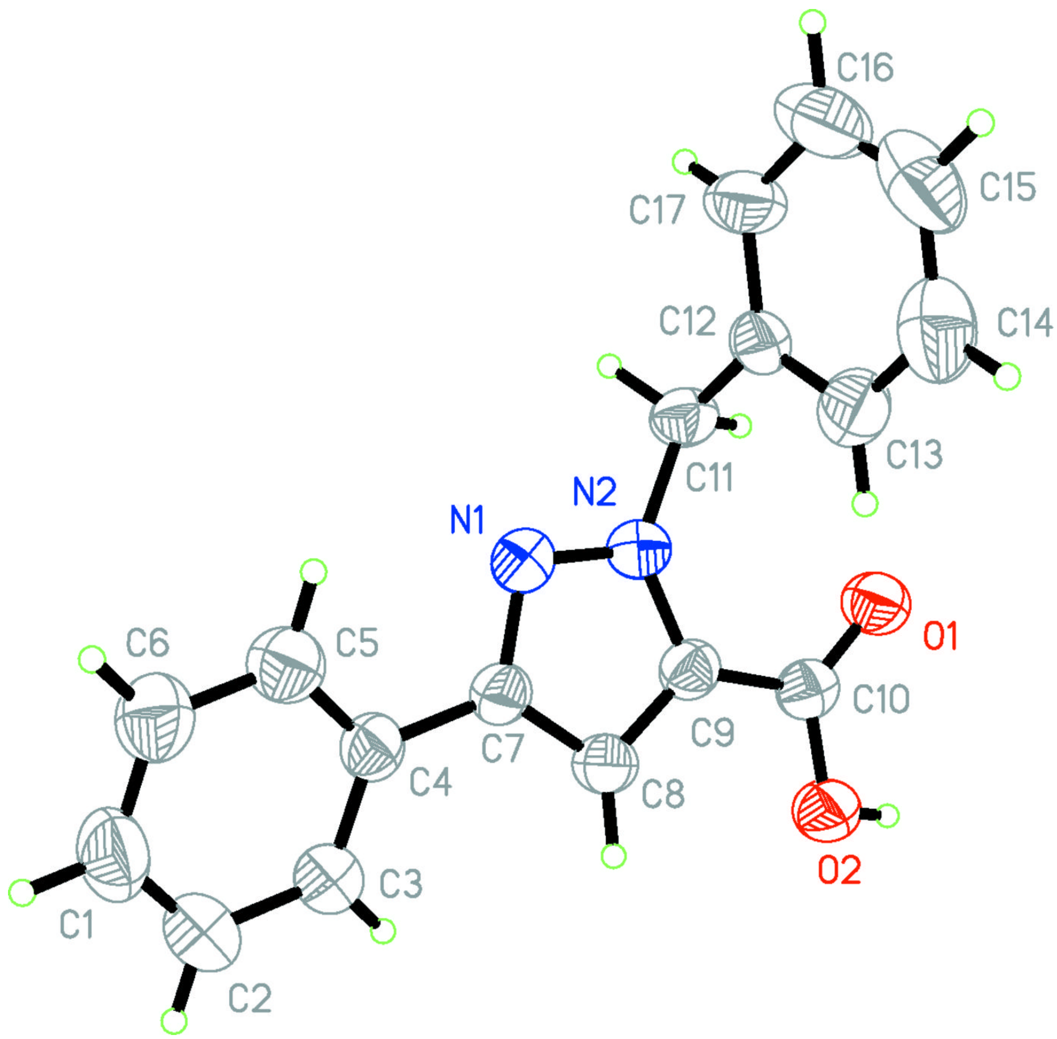
C16
C15
C17
C12
C14
C11
C13
N2
N1
O1
C6
C5
C10
C9
C7
C4
C8
O2
C3
C1
C2

Fig. 2