Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Benzamido-1-benzoyl-1*H*-pyrrol-2(5*H*)-one

Marta Kasunič,* Bojan Verček, Irena Mušič and Amalija Golobič

Faculty of Chemistry and Chemical Technology, University of Ljubljana, Aškerčeva 5, 1000 Ljubljana, Slovenia
Correspondence e-mail: marta.kasunic@fkkt.uni-lj.si

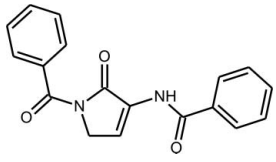
Received 18 February 2010; accepted 19 February 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.132; data-to-parameter ratio = 17.5.

In the title compound, $C_{18}H_{14}N_2O_3$, one of the phenyl rings is almost coplanar with the pyrrole ring [dihedral angle = 2.56 (14)°], whereas the other one is tilted by 63.01 (6)° with respect to the pyrrole ring. Since the NH group is shielded from possible acceptors, this group is not involved in hydrogen bonding.

Related literature

For the synthesis of 1,5-dihydro-2*H*-pyrrol-2-ones, see: Gao *et al.* (1997); Alizadeh *et al.* (2006); Nedolya *et al.* (2002); Mušič *et al.* (1998).



Experimental

Crystal data

$C_{18}H_{14}N_2O_3$
M_r = 306.31
Monoclinic, $P2_1/c$
a = 20.966 (2) Å
b = 5.8891 (7) Å
c = 12.329 (1) Å
β = 95.908 (8)°
V = 1514.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.58 × 0.36 × 0.09 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
13450 measured reflections
3648 independent reflections
2119 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
3 standard reflections every 333.3 min
intensity decay: 1.1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.132
S = 1.00
3648 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: the *XRAY76* System (Stewart *et al.*, 1976); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Ministry of Higher Education, Science and Technology of the Republic of Slovenia (grants P1–0175 and MR-29397).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5197).

References

Alizadeh, A., Movahedi, F., Masrouri, H. & Zhu, L. G. (2006). *Synthesis*, pp. 3431–3436.
Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Gao, Y., Shirai, M. & Sato, F. (1997). *Tetrahedron Lett.* **38**, 6849–6852.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Mušič, I., Golobič, A. & Verček, B. (1998). *Heterocycles*, **48**, 353–358.
Nedolya, N. A., Brandsma, L. & Tolmachev, S. V. (2002). *Russ. J. Org. Chem.* **38**, 948–949.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stewart, R. F., Machin, P. A., Dickinson, C. W., Ammon, H. L., Heck, H. & Flack, H. (1976). *The XRAY76 System*. Technical Report TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland, USA.

supporting information

Acta Cryst. (2010). E**66**, o687 [doi:10.1107/S1600536810006483]

3-Benzamido-1-benzoyl-1*H*-pyrrol-2(5*H*)-one

Marta Kasunič, Bojan Verček, Irena Mušič and Amalija Golobič

S1. Comment

1,5-dihydro-2H-pyrrol-2-ones comprise a family of lactams which are found as substructures in several natural products with promising pharmalogical properties. Several reports on synthesis of substituted 1,5-dihydro-2H-pyrrol-2-ones exist and these compounds can be prepared *via* different synthetic pathways (e.g. Gao *et al.*, 1997; Alizadeh *et al.*, 2006; Nedolya *et al.*, 2002), Mušič *et al.* (1998). The asymmetry unit of the title compound with atom labelling scheme can be seen in Fig. 1.

S2. Experimental

The title compound was prepared according to the procedure by Mušič *et al.* (1998). The crystals, suitable for X-ray structure analysis, were obtained by slow crystallization from the mixture of acetonitrile and hexane at room temperature.

S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms [C—H = 0.97 for methylene and 0.93 Å for aromatic hydrogens, respectively, N—H = 0.86 Å and U_{iso}(H) = 1.2 times U_{eq}(C, N)].

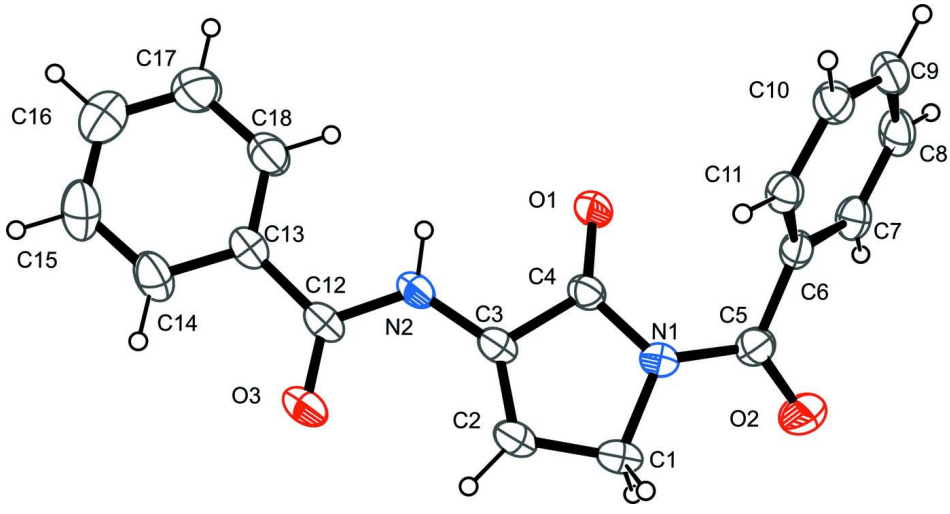


Figure 1

The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are drawn as small spheres of arbitrary radii.

3-Benzamido-1-benzoyl-1*H*-pyrrol-2(5*H*)-one

Crystal data

$C_{18}H_{14}N_2O_3$
$M_r = 306.31$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 20.966$ (2) Å
$b = 5.8891$ (7) Å
$c = 12.329$ (1) Å
$\beta = 95.908$ (8)°
$V = 1514.2$ (3) Å^3
$Z = 4$
$F(000) = 640$
$D_x = 1.344$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 75 reflections
$\theta = 8.0$–$15.3°$
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Plate, pale yellow
0.58 × 0.36 × 0.09 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans [width (0.85 + 0.3tanθ)]
13450 measured reflections
3648 independent reflections
2119 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.0°$
$h = -27 \rightarrow 27$
$k = -7 \rightarrow 7$
$l = -16 \rightarrow 14$
3 standard reflections every 333.3 min
intensity decay: 1.1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.132$
$S = 1.00$
3648 reflections
209 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
$w = 1/[\sigma^2(F_o^2) + (0.0676P)^2 + 0.1617P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELX97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.029 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.80491 (6)	0.1771 (2)	0.90089 (10)	0.0492 (3)
N2	0.69375 (7)	0.6347 (2)	0.88815 (11)	0.0554 (4)
H2	0.6985	0.6820	0.8235	0.066*

O1	0.77372 (6)	0.4192 (2)	0.75402 (9)	0.0632 (4)
O2	0.85617 (8)	−0.1579 (2)	0.90309 (12)	0.0846 (5)
O3	0.64221 (7)	0.6962 (3)	1.03607 (10)	0.0784 (4)
C1	0.78338 (8)	0.1439 (3)	1.00943 (12)	0.0534 (4)
H1A	0.8190	0.1548	1.0660	0.064*
H1B	0.7627	−0.0024	1.0147	0.064*
C2	0.73736 (8)	0.3319 (3)	1.01751 (13)	0.0550 (4)
H2A	0.7162	0.3627	1.0785	0.066*
C3	0.73060 (7)	0.4501 (3)	0.92579 (12)	0.0483 (4)
C4	0.77164 (7)	0.3562 (3)	0.84693 (12)	0.0472 (4)
C5	0.84667 (8)	0.0250 (3)	0.85911 (13)	0.0534 (4)
C6	0.88045 (7)	0.0966 (3)	0.76467 (12)	0.0453 (4)
C7	0.88460 (8)	−0.0552 (3)	0.67966 (14)	0.0549 (4)
H7	0.8640	−0.1950	0.6800	0.066*
C8	0.91946 (9)	0.0018 (3)	0.59465 (14)	0.0634 (5)
H8	0.9210	−0.0975	0.5363	0.076*
C9	0.95206 (9)	0.2049 (3)	0.59581 (15)	0.0619 (5)
H9	0.9763	0.2408	0.5391	0.074*
C10	0.94882 (8)	0.3549 (3)	0.68073 (14)	0.0555 (4)
H10	0.9712	0.4913	0.6817	0.067*
C11	0.91240 (7)	0.3029 (3)	0.76453 (12)	0.0487 (4)
H11	0.9093	0.4061	0.8208	0.058*
C12	0.65088 (8)	0.7482 (3)	0.94360 (13)	0.0528 (4)
C13	0.61696 (8)	0.9416 (3)	0.88463 (13)	0.0512 (4)
C14	0.57527 (10)	1.0680 (4)	0.93989 (16)	0.0712 (6)
H14	0.5678	1.0268	1.0103	0.085*
C15	0.54448 (12)	1.2550 (4)	0.8915 (2)	0.0884 (7)
H15	0.5166	1.3397	0.9294	0.106*
C16	0.55488 (11)	1.3153 (4)	0.7884 (2)	0.0860 (7)
H16	0.5347	1.4425	0.7561	0.103*
C17	0.59485 (12)	1.1893 (5)	0.7325 (2)	0.0956 (8)
H17	0.6015	1.2299	0.6616	0.115*
C18	0.62549 (10)	1.0025 (4)	0.77981 (16)	0.0770 (6)
H18	0.6523	0.9165	0.7403	0.092*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0550 (8)	0.0540 (8)	0.0394 (7)	0.0026 (7)	0.0086 (6)	0.0046 (6)
N2	0.0570 (8)	0.0713 (10)	0.0406 (7)	0.0103 (7)	0.0184 (6)	0.0029 (7)
O1	0.0735 (8)	0.0808 (9)	0.0375 (6)	0.0250 (7)	0.0167 (5)	0.0084 (6)
O2	0.1141 (12)	0.0581 (8)	0.0851 (10)	0.0181 (8)	0.0264 (9)	0.0236 (7)
O3	0.0878 (10)	0.1034 (11)	0.0492 (7)	0.0198 (8)	0.0315 (7)	0.0071 (7)
C1	0.0575 (10)	0.0645 (11)	0.0387 (8)	−0.0111 (8)	0.0071 (7)	0.0064 (8)
C2	0.0519 (9)	0.0741 (11)	0.0409 (8)	−0.0055 (9)	0.0139 (7)	0.0004 (8)
C3	0.0457 (8)	0.0620 (11)	0.0385 (8)	−0.0033 (8)	0.0105 (6)	−0.0017 (7)
C4	0.0489 (9)	0.0573 (10)	0.0361 (8)	0.0018 (8)	0.0075 (6)	−0.0009 (7)
C5	0.0589 (10)	0.0492 (10)	0.0515 (9)	0.0025 (8)	0.0031 (8)	0.0027 (8)

C6	0.0466 (8)	0.0432 (8)	0.0457 (8)	0.0093 (7)	0.0027 (6)	−0.0018 (7)
C7	0.0574 (10)	0.0444 (9)	0.0625 (11)	0.0076 (8)	0.0048 (8)	−0.0092 (8)
C8	0.0682 (12)	0.0659 (12)	0.0566 (11)	0.0189 (10)	0.0093 (9)	−0.0179 (9)
C9	0.0539 (10)	0.0758 (13)	0.0584 (11)	0.0125 (9)	0.0168 (8)	0.0003 (9)
C10	0.0486 (9)	0.0561 (10)	0.0624 (10)	−0.0002 (8)	0.0089 (8)	0.0008 (8)
C11	0.0514 (9)	0.0466 (9)	0.0475 (9)	0.0047 (7)	0.0026 (7)	−0.0060 (7)
C12	0.0484 (9)	0.0688 (11)	0.0432 (9)	−0.0040 (8)	0.0152 (7)	−0.0079 (8)
C13	0.0446 (8)	0.0621 (10)	0.0479 (9)	−0.0041 (8)	0.0098 (7)	−0.0112 (8)
C14	0.0744 (13)	0.0822 (14)	0.0590 (11)	0.0110 (11)	0.0160 (9)	−0.0205 (10)
C15	0.0897 (17)	0.0788 (15)	0.0968 (17)	0.0231 (13)	0.0096 (13)	−0.0297 (13)
C16	0.0808 (16)	0.0710 (14)	0.1039 (19)	0.0063 (12)	−0.0011 (13)	0.0066 (13)
C17	0.0862 (16)	0.116 (2)	0.0873 (16)	0.0289 (15)	0.0238 (13)	0.0341 (15)
C18	0.0704 (12)	0.1031 (16)	0.0608 (11)	0.0271 (12)	0.0233 (10)	0.0130 (11)

Geometric parameters (Å, º)

N1—C5	1.388 (2)	C8—C9	1.377 (3)
N1—C4	1.395 (2)	C8—H8	0.9300
N1—C1	1.4687 (19)	C9—C10	1.377 (2)
N2—C12	1.360 (2)	C9—H9	0.9300
N2—C3	1.385 (2)	C10—C11	1.381 (2)
N2—H2	0.8600	C10—H10	0.9300
O1—C4	1.2091 (18)	C11—H11	0.9300
O2—C5	1.213 (2)	C12—C13	1.492 (2)
O3—C12	1.2121 (19)	C13—C18	1.370 (2)
C1—C2	1.479 (3)	C13—C14	1.380 (2)
C1—H1A	0.9700	C14—C15	1.381 (3)
C1—H1B	0.9700	C14—H14	0.9300
C2—C3	1.323 (2)	C15—C16	1.358 (3)
C2—H2A	0.9300	C15—H15	0.9300
C3—C4	1.471 (2)	C16—C17	1.359 (3)
C5—C6	1.485 (2)	C16—H16	0.9300
C6—C11	1.387 (2)	C17—C18	1.373 (3)
C6—C7	1.387 (2)	C17—H17	0.9300
C7—C8	1.379 (2)	C18—H18	0.9300
C7—H7	0.9300		
C5—N1—C4	127.91 (13)	C7—C8—H8	119.8
C5—N1—C1	121.13 (13)	C8—C9—C10	120.13 (17)
C4—N1—C1	110.46 (13)	C8—C9—H9	119.9
C12—N2—C3	126.31 (14)	C10—C9—H9	119.9
C12—N2—H2	116.8	C9—C10—C11	120.07 (17)
C3—N2—H2	116.8	C9—C10—H10	120.0
N1—C1—C2	103.04 (13)	C11—C10—H10	120.0
N1—C1—H1A	111.2	C10—C11—C6	119.96 (15)
C2—C1—H1A	111.2	C10—C11—H11	120.0
N1—C1—H1B	111.2	C6—C11—H11	120.0
C2—C1—H1B	111.2	O3—C12—N2	121.29 (17)

H1A—C1—H1B	109.1	O3—C12—C13	122.77 (15)
C3—C2—C1	110.47 (14)	N2—C12—C13	115.92 (14)
C3—C2—H2A	124.8	C18—C13—C14	118.38 (18)
C1—C2—H2A	124.8	C18—C13—C12	123.87 (16)
C2—C3—N2	134.92 (15)	C14—C13—C12	117.74 (16)
C2—C3—C4	110.40 (15)	C15—C14—C13	120.6 (2)
N2—C3—C4	114.67 (13)	C15—C14—H14	119.7
O1—C4—N1	128.21 (15)	C13—C14—H14	119.7
O1—C4—C3	126.27 (15)	C16—C15—C14	120.0 (2)
N1—C4—C3	105.48 (13)	C16—C15—H15	120.0
O2—C5—N1	119.19 (16)	C14—C15—H15	120.0
O2—C5—C6	122.21 (16)	C15—C16—C17	119.9 (2)
N1—C5—C6	118.54 (14)	C15—C16—H16	120.0
C11—C6—C7	119.70 (15)	C17—C16—H16	120.0
C11—C6—C5	121.26 (14)	C16—C17—C18	120.5 (2)
C7—C6—C5	118.79 (15)	C16—C17—H17	119.7
C8—C7—C6	119.78 (17)	C18—C17—H17	119.7
C8—C7—H7	120.1	C13—C18—C17	120.6 (2)
C6—C7—H7	120.1	C13—C18—H18	119.7
C9—C8—C7	120.31 (16)	C17—C18—H18	119.7
C9—C8—H8	119.8		

C5—N1—C1—C2	−176.46 (15)	C11—C6—C7—C8	−1.2 (2)
C4—N1—C1—C2	−3.92 (17)	C5—C6—C7—C8	−175.60 (15)
N1—C1—C2—C3	2.68 (19)	C6—C7—C8—C9	2.4 (3)
C1—C2—C3—N2	178.14 (18)	C7—C8—C9—C10	−1.5 (3)
C1—C2—C3—C4	−0.6 (2)	C8—C9—C10—C11	−0.6 (3)
C12—N2—C3—C2	−0.5 (3)	C9—C10—C11—C6	1.8 (2)
C12—N2—C3—C4	178.20 (15)	C7—C6—C11—C10	−0.9 (2)
C5—N1—C4—O1	−2.2 (3)	C5—C6—C11—C10	173.38 (15)
C1—N1—C4—O1	−174.11 (17)	C3—N2—C12—O3	1.6 (3)
C5—N1—C4—C3	175.56 (15)	C3—N2—C12—C13	−179.80 (15)
C1—N1—C4—C3	3.67 (17)	O3—C12—C13—C18	−179.38 (19)
C2—C3—C4—O1	175.90 (17)	N2—C12—C13—C18	2.0 (3)
N2—C3—C4—O1	−3.1 (3)	O3—C12—C13—C14	1.6 (3)
C2—C3—C4—N1	−1.93 (19)	N2—C12—C13—C14	−177.04 (16)
N2—C3—C4—N1	179.08 (13)	C18—C13—C14—C15	−1.9 (3)
C4—N1—C5—O2	−157.39 (17)	C12—C13—C14—C15	177.23 (18)
C1—N1—C5—O2	13.7 (2)	C13—C14—C15—C16	0.4 (3)
C4—N1—C5—C6	25.3 (2)	C14—C15—C16—C17	1.0 (4)
C1—N1—C5—C6	−163.60 (14)	C15—C16—C17—C18	−0.7 (4)
O2—C5—C6—C11	−127.91 (19)	C14—C13—C18—C17	2.1 (3)
N1—C5—C6—C11	49.3 (2)	C12—C13—C18—C17	−176.9 (2)
O2—C5—C6—C7	46.4 (2)	C16—C17—C18—C13	−0.9 (4)
N1—C5—C6—C7	−136.36 (16)		