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N-Phenyl-[1,1′-biphenyl]-2-carboxamide

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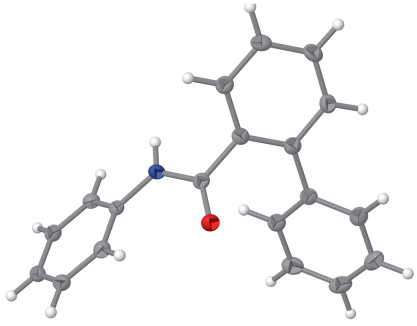
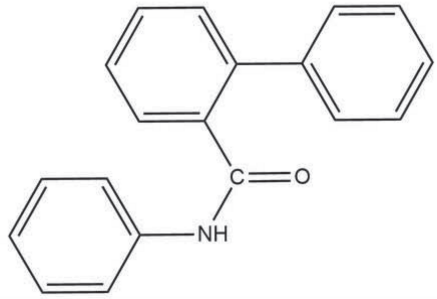
Structural data: full structural data are available from iucrdata.iucr.org

The title molecule, $C_{19}H_{15}NO$, contains a carboxamide fragment in which the amide N atom is bonded to a phenyl group, while the carbonyl C atom is attached to a biphenyl unit. In the crystal, molecules are linked by N—H···O hydrogen bonds, forming chains running parallel to the *a* axis. These chains are further connected by C—H···π interactions, resulting in a three-dimensional supramolecular network.

3D view



Chemical scheme



Structure description

Biphenyl derivatives represent an important class of aromatic compounds owing to their conformational flexibility and structural diversity (Jain *et al.*, 2017; Landeros-Rivera & Hernańdez-Trujillo, 2022). Functionalized biphenyl systems bearing carboxylic acid or amide groups have attracted considerable interest for their structural and coordination properties (Sienkiewicz-Gromiuk *et al.*, 2014; Wang *et al.*, 2004; Yu *et al.*, 2006), as well as for their biological relevance (Sharma *et al.*, 2010; van 't Hof *et al.*, 2004; Mukherjee *et al.*, 2016; Zhao *et al.*, 2017). The amide functional group is well known for its strong hydrogen-bonding ability and its role in directing supramolecular organization in the solid state. The combination of a biphenyl scaffold with an amide linkage provides a versatile structural platform capable of promoting intermolecular hydrogen bonding and π–π stacking interactions, which are key factors in supramolecular self-assembly processes (Gao *et al.*, 2022; Yao *et al.*, 2025). Recent crystallographic studies of substituted biphenyl derivatives further highlight the influence of these interactions on molecular conformation and crystal packing (Nodera *et al.*, 2025). In this context, we report herein the synthesis and crystal structure of the title comnpound, $C_{19}H_{15}NO$.

The title compound **1** crystallizes in the triclinic space group $P\overline{1}$ with one molecule in the asymmetric unit (Fig. 1). The molecular structure consists of a carboxamide fragment, C—N(H)—C(=O)—C, in which the amide N atom is bonded to a phenyl group and the

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

*Cg*1 is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.877 (16)	2.307 (16)	3.0790 (12)	146.9 (13)
C3—H3···O1	0.95	2.38	2.9035 (15)	114
C7—H7···O1^{i}	0.95	2.64	3.2433 (13)	122
C13—H13···*Cg*1^{ii}	0.95	2.78	3.5815 (13)	142
C24—H24···*Cg*1^{iii}	0.95	2.94	3.8444 (13)	160

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, -y+1, -z$; (iii) $-x+1, -y+1, -z+1$.

carbonyl C atom is bonded to a biphenyl unit. The C—N, N—C and C═O bond lengths are in agreement with those observed in related compounds (see below). The amide fragment C—N(H)—C(═O)—C is essentially planar, with the largest deviation from the mean plane being 0.0413 (5) Å for atom C2. The phenyl ring C2—C7 is twisted by 24.70 (4)° with respect to the amide mean plane, while the phenyl ring attached to the carbonyl group is inclined by 55.67 (4)°. The phenyl and biphenyl groups are in the *trans* position with respect to the C1—N1 bond. The dihedral angle between the biphenyl rings is 40.67 (6)°.

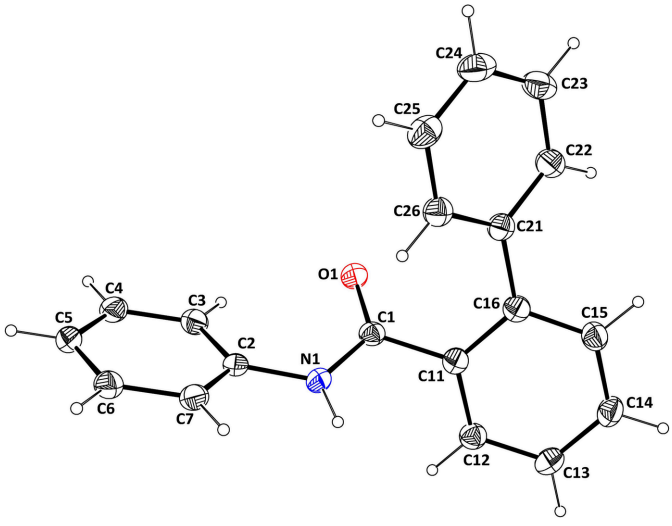


Figure 1
Molecular structure of the title compound with the labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

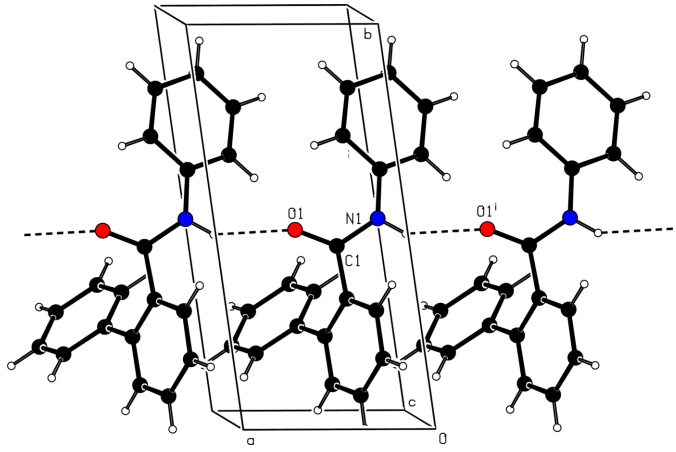


Figure 2
Partial packing view showing the formation of N—H···O hydrogen-bonded chains running parallel to the *a* axis. Symmetry code as in Table 1.

In the crystal, molecules are linked by N1—H1···O1 hydrogen bonds, generating chains running parallel to the *a* axis (Table 1, Fig. 2). A weak C7—H7···O1 contact also contributes to the crystal packing. In addition, weak C—H···π interactions (Table 1) involving atoms C13 and C24 and the centroid of the C2—C7 phenyl ring further consolidate the packing. These interactions connect the N—H···O hydrogen-bonded chains into a three-dimensional supramolecular network.

A search of the Cambridge Structural Database (CSD, version 5.36; Groom *et al.*, 2016), based on the Ph—NH—C(═O)—C(*R*) fragment, revealed ten related structures containing a phenyl group attached to the amide N atom and different substituents attached to the carbonyl C atom. A comparison of selected bond lengths and angles is given in Table 2.

Synthesis and crystallization

2-Biphenylcarboxylic acid (1.63 g, 10 mmol) was dissolved in toluene (50 ml) and treated dropwise with thionyl chloride $SOCl_2$ (1.67 ml, 15 mmol) under stirring at 323–333 K. The reaction mixture was maintained at this temperature to allow

Table 2
Comparison of selected distances and angles (Å, °) in related compounds having a similar C(Ph)—NH—C(O)—C(*R*) fragment.

Compound	N—C(O)	N—C(Ph)	C═O	C(O)—C(*R*)	C—N—C	N—C—C
1	1.3626 (14)	1.4198 (14)	1.2283 (13)	1.5001 (15)	126.70 (9)	114.07 (9)
CIBPIM	1.332	1.400	1.234	1.508	127.1	114.0
CIBPIM01	1.340	1.421	1.232	1.505	128.2	114.9
LASHEU	1.335	1.431	1.236	1.495	122.1	118.5
MANDIP	1.354	1.409	1.232	1.487	128.4	115.0
MANDIP01	1.350	1.416	1.237	1.497	127.3	115.3
MANDIP02	1.352	1.410	1.233	1.500	127.8	114.3
MANDIP03	1.353	1.412	1.233	1.499	127.9	114.1
NUKVOH	1.355	1.420	1.226	1.595	125.4	115.8
YEGJID	1.353	1.424	1.225	1.493	124.8	115.4
YEGJID01	1.352	1.418	1.237	1.492	126.3	114.5

References: CIBPIM: Smith *et al.* (1983); CIBPIM01: Bocelli *et al.* (1989); LASHEU: Panini *et al.* (2012); MANDIP: Goswami *et al.* (2005); MANDIP01: Fellowes (2020); MANDIP02: Romito & Bonifazi (2023); MANDIP03: Clarke *et al.* (2024); NUKVOH: McKay *et al.* (2020); YEGJID: Azumaya *et al.* (1994); YEGJID01: Gowda *et al.* (2008).

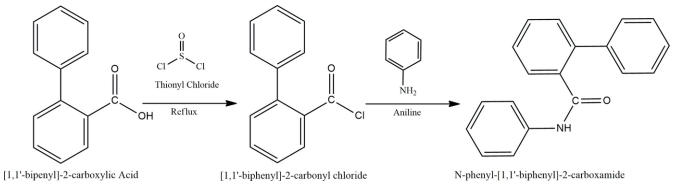


Figure 3
Synthesis of *N*-phenyl-[1,1′-biphenyl]-2-carboxamide.

formation of the corresponding acyl chloride. Aniline (1.03 g, 10 mmol) was then added dropwise, and the mixture was heated under reflux for 3 h. After completion of the reaction, the solvent was removed under reduced pressure. The crude solid was purified by recrystallization from ethanol solution to afford the title amide as a white solid (yield = 80%). Crystals suitable for single-crystal X-ray diffraction were obtained by slow evaporation of a solution of the compound in ethanol at room temperature. The reaction scheme is shown in Fig. 3.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{15}NO$
M_r	273.32
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	5.2935 (1), 12.0493 (2), 12.3713 (3)
α, β, γ (°)	65.411 (2), 80.417 (2), 80.644 (1)
V (Å^3)	703.67 (3)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.62
Crystal size (mm)	0.18 × 0.06 × 0.04
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.84, 1.0
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20896, 2252, 2084
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.581
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.031, 0.081, 1.05
No. of reflections	2252
No. of parameters	194
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.11, −0.20

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEPIII* (Burnett & Johnson, 1996); *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2020).

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full crystallographic data

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Crystal data

$C_{19}H_{15}NO$
M_r = 273.32
Triclinic, $P\overline{1}$
a = 5.2935 (1) Å
b = 12.0493 (2) Å
c = 12.3713 (3) Å
α = 65.411 (2)°
β = 80.417 (2)°
γ = 80.644 (1)°
V = 703.67 (3) Å^3
Z = 2
$F(000)$ = 288
D_x = 1.290 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 15231 reflections
θ = 4.0–63.5°
μ = 0.62 mm^{-1}
T = 100 K
Needle, colorless
0.18 × 0.06 × 0.04 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.84, T_{max} = 1.0
20896 measured reflections
2252 independent reflections
2084 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 63.7°, θ_{min} = 4.0°
h = −6→6
k = −13→13
l = −14→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.081
S = 1.05
2252 reflections
194 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.1624P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-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. Hydrogen atoms bonded to carbon atoms were placed at geometrically idealized positions and refined using a riding model, with Uiso(H) = 1.2Ueq(C). The amide H atom was located in a difference-Fourier map and freely refined.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.56138 (14)	0.48552 (7)	0.15047 (7)	0.0233 (2)
N1	0.12096 (18)	0.51216 (8)	0.16680 (8)	0.0204 (2)
H1	−0.016 (3)	0.4735 (12)	0.1824 (11)	0.026 (3)*
C1	0.3539 (2)	0.44452 (10)	0.16721 (9)	0.0191 (3)
C2	0.0753 (2)	0.63423 (10)	0.15990 (10)	0.0198 (3)
C3	0.2518 (2)	0.72007 (10)	0.10018 (10)	0.0227 (3)
H3	0.411682	0.698081	0.062454	0.027*
C4	0.1921 (2)	0.83811 (10)	0.09629 (11)	0.0246 (3)
H4	0.312790	0.896678	0.055944	0.029*
C5	−0.0406 (2)	0.87187 (10)	0.15028 (10)	0.0243 (3)
H5	−0.079582	0.952895	0.147088	0.029*
C6	−0.2159 (2)	0.78608 (10)	0.20900 (10)	0.0239 (3)
H6	−0.376344	0.808549	0.245972	0.029*
C7	−0.1588 (2)	0.66771 (10)	0.21413 (10)	0.0220 (3)
H7	−0.279691	0.609315	0.254787	0.026*
C11	0.33708 (19)	0.31320 (10)	0.19073 (10)	0.0194 (3)
C12	0.2034 (2)	0.28790 (10)	0.11718 (10)	0.0222 (3)
H12	0.112167	0.353274	0.058094	0.027*
C13	0.2018 (2)	0.16830 (10)	0.12918 (11)	0.0246 (3)
H13	0.112241	0.151757	0.077916	0.029*
C14	0.3319 (2)	0.07337 (10)	0.21654 (11)	0.0253 (3)
H14	0.333382	−0.008692	0.224702	0.030*
C15	0.4600 (2)	0.09738 (10)	0.29225 (11)	0.0239 (3)
H15	0.545952	0.030985	0.352639	0.029*
C16	0.4657 (2)	0.21702 (10)	0.28175 (10)	0.0204 (3)
C21	0.5881 (2)	0.23759 (10)	0.37111 (10)	0.0210 (3)
C22	0.8175 (2)	0.16885 (10)	0.41265 (10)	0.0251 (3)
H22	0.901319	0.111695	0.380268	0.030*
C23	0.9242 (2)	0.18298 (11)	0.50042 (11)	0.0303 (3)
H23	1.079857	0.135190	0.527985	0.036*
C24	0.8061 (2)	0.26608 (12)	0.54823 (11)	0.0327 (3)
H24	0.880431	0.276035	0.608025	0.039*
C25	0.5781 (2)	0.33477 (11)	0.50809 (11)	0.0296 (3)
H25	0.495631	0.391962	0.540670	0.035*
C26	0.4698 (2)	0.32056 (10)	0.42091 (10)	0.0239 (3)
H26	0.312917	0.367838	0.394535	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0196 (4)	0.0220 (4)	0.0287 (5)	−0.0038 (3)	−0.0038 (3)	−0.0094 (3)
N1	0.0181 (5)	0.0181 (5)	0.0260 (5)	−0.0042 (4)	−0.0032 (4)	−0.0088 (4)
C1	0.0205 (6)	0.0205 (5)	0.0167 (6)	−0.0028 (4)	−0.0033 (4)	−0.0071 (4)
C2	0.0219 (6)	0.0187 (5)	0.0207 (6)	−0.0005 (4)	−0.0086 (4)	−0.0081 (5)
C3	0.0204 (6)	0.0222 (6)	0.0248 (6)	−0.0020 (4)	−0.0048 (5)	−0.0079 (5)
C4	0.0259 (6)	0.0203 (6)	0.0268 (6)	−0.0056 (5)	−0.0081 (5)	−0.0056 (5)
C5	0.0290 (6)	0.0194 (6)	0.0273 (6)	0.0005 (5)	−0.0114 (5)	−0.0101 (5)
C6	0.0232 (6)	0.0256 (6)	0.0257 (6)	0.0007 (5)	−0.0059 (5)	−0.0129 (5)
C7	0.0215 (6)	0.0228 (6)	0.0231 (6)	−0.0041 (4)	−0.0045 (5)	−0.0091 (5)
C11	0.0170 (5)	0.0205 (6)	0.0208 (6)	−0.0030 (4)	0.0011 (4)	−0.0090 (5)
C12	0.0222 (6)	0.0228 (6)	0.0212 (6)	−0.0032 (4)	−0.0028 (5)	−0.0081 (5)
C13	0.0264 (6)	0.0266 (6)	0.0258 (6)	−0.0062 (5)	−0.0023 (5)	−0.0143 (5)
C14	0.0266 (6)	0.0207 (6)	0.0314 (7)	−0.0029 (5)	−0.0010 (5)	−0.0139 (5)
C15	0.0217 (6)	0.0205 (6)	0.0278 (6)	0.0001 (4)	−0.0034 (5)	−0.0086 (5)
C16	0.0160 (5)	0.0224 (6)	0.0228 (6)	−0.0023 (4)	0.0006 (4)	−0.0099 (5)
C21	0.0206 (5)	0.0202 (5)	0.0201 (6)	−0.0059 (4)	−0.0010 (4)	−0.0052 (4)
C22	0.0214 (6)	0.0245 (6)	0.0255 (6)	−0.0051 (5)	−0.0026 (5)	−0.0053 (5)
C23	0.0250 (6)	0.0325 (7)	0.0271 (7)	−0.0087 (5)	−0.0077 (5)	−0.0020 (5)
C24	0.0379 (7)	0.0376 (7)	0.0235 (7)	−0.0158 (6)	−0.0076 (5)	−0.0072 (6)
C25	0.0377 (7)	0.0301 (6)	0.0229 (6)	−0.0112 (5)	−0.0011 (5)	−0.0107 (5)
C26	0.0242 (6)	0.0239 (6)	0.0228 (6)	−0.0048 (5)	−0.0019 (5)	−0.0078 (5)

Geometric parameters (Å, º)

O1—C1	1.2283 (13)	C12—C13	1.3872 (16)
N1—C1	1.3626 (14)	C13—C14	1.3833 (17)
N1—C2	1.4198 (14)	C14—C15	1.3864 (16)
C1—C11	1.5001 (15)	C15—C16	1.3975 (15)
C2—C7	1.3905 (16)	C16—C21	1.4906 (16)
C2—C3	1.3920 (16)	C21—C22	1.3969 (15)
C3—C4	1.3882 (16)	C21—C26	1.3970 (16)
C4—C5	1.3851 (17)	C22—C23	1.3844 (17)
C5—C6	1.3857 (16)	C23—C24	1.3820 (19)
C6—C7	1.3859 (15)	C24—C25	1.3862 (18)
C11—C12	1.3919 (16)	C25—C26	1.3828 (17)
C11—C16	1.4098 (16)		
C1—N1—C2	126.70 (9)	C13—C12—C11	120.74 (10)
O1—C1—N1	123.91 (10)	C14—C13—C12	119.33 (11)
O1—C1—C11	122.02 (9)	C13—C14—C15	120.33 (10)
N1—C1—C11	114.07 (9)	C14—C15—C16	121.51 (10)
C7—C2—C3	119.80 (10)	C15—C16—C11	117.62 (10)
C7—C2—N1	117.46 (10)	C15—C16—C21	119.56 (10)
C3—C2—N1	122.73 (10)	C11—C16—C21	122.66 (10)
C4—C3—C2	119.36 (10)	C22—C21—C26	118.06 (10)

C5—C4—C3	121.06 (10)	C22—C21—C16	120.66 (10)
C4—C5—C6	119.23 (10)	C26—C21—C16	121.17 (10)
C5—C6—C7	120.42 (11)	C23—C22—C21	120.80 (11)
C6—C7—C2	120.13 (10)	C24—C23—C22	120.51 (11)
C12—C11—C16	120.43 (10)	C23—C24—C25	119.35 (11)
C12—C11—C1	118.88 (9)	C26—C25—C24	120.40 (12)
C16—C11—C1	120.61 (10)	C25—C26—C21	120.88 (11)

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1	0.95	2.38	2.9035 (15)	114
C7—H7···O1^{i}	0.95	2.64	3.2433 (13)	122
N1—H1···O1^{i}	0.877 (16)	2.307 (16)	3.0790 (12)	146.9 (13)
C13—H13···*Cg*1^{ii}	0.95	2.78	3.5815 (13)	142
C24—H24···*Cg*1^{iii}	0.95	2.94	3.8444 (13)	160

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, -y+1, -z$; (iii) $-x+1, -y+1, -z+1$.