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N-Benzylcinnamamide

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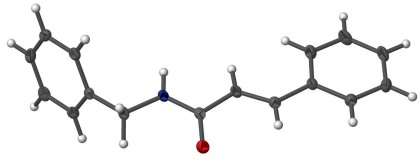
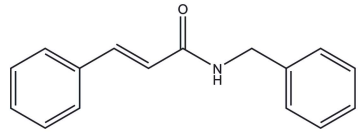
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{16}H_{15}NO$, there is a weak intramolecular C—H···O contact which leads to a planar acrylamide moiety. The phenyl ring forms an angle of 8.30 (2)° with the mean plane of the acrylamide moiety. The benzyl group is tilted against the cinnamamide unit, with the ring forming an angle of 77.11 (2)° with the cinnamamide unit mean plane. In the crystal, molecules are linked *via* N—H···O and C—H···O hydrogen bonds and C—H···π interactions, forming chains propagating along [001]. The chains are linked *via* further C—H···π interactions, forming layers parallel to the *ac* plane.

3D view



Chemical scheme



Structure description

The title compound, Fig. 1, has been shown to be a potential bombesin subtype 3 agonist (Kim *et al.* 2014), a matrix metalloproteinase inhibitor (Shi *et al.* 2013) and a 17β-hydroxysteroid dehydrogenase inhibitor (Kristan *et al.* 2006). Herein we report on the synthesis and crystal structure of the title compound. Other methods of synthesis of the title compound have been reported by Lagerlund *et al.* (2009).

In the title compound, Fig. 1, there is a weak intramolecular C3—H3···O1 contact (Fig. 1 and Table 1), which leads to a planar acrylamide structure (N1/O1/C1–C3). The phenyl ring (C4–C9) forms a dihedral angle of 8.30 (2)° with this acrylamide mean plane. The benzyl group is tilted against the cinnamamide mean plane, with the ring (C11–C16) forming a dihedral angle of 77.11 (3)° with the mean plane of the cinnamamide (N1/O1/C1–C9) moiety. The two phenyl rings are inclined to one another by 80.04 (2)°.

In the crystal, molecules are linked *via* N—H···O and C—H···O hydrogen bonds, forming chains along the *c*-axis direction (Fig. 2 and Table 1). Within the chains there are also C—H···π interactions present (Table 1 and Fig. 2). The (C4–C9) phenyl rings of two adjacent molecules form a dihedral angle of 57.38 (2)°, while the (C11–C16) benzyl rings

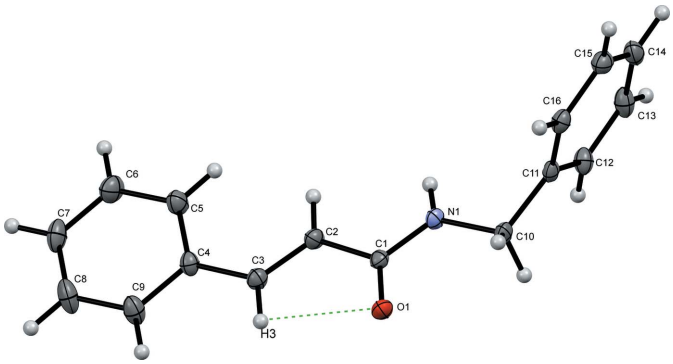


Figure 1
A view of the molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level. The intramolecular C—H···O contact is shown as a dashed line (see Table 1).

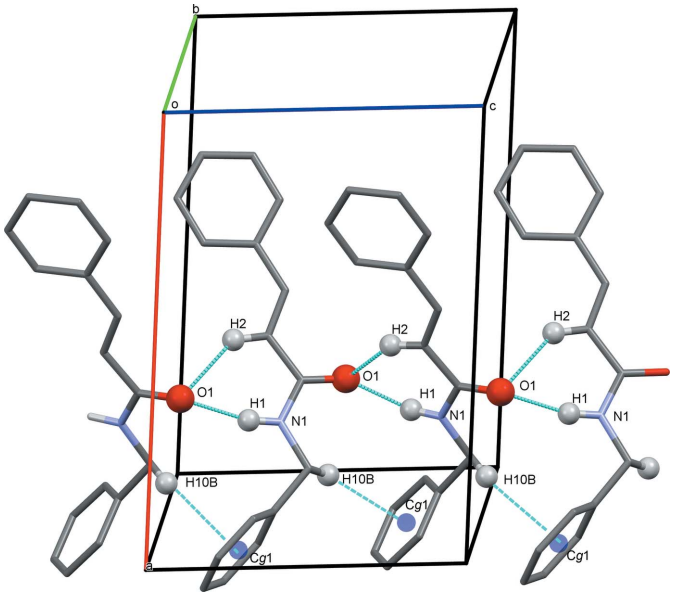


Figure 2
A partial view of the formation of the molecular chains propagating along the *c*-axis direction, formed by intermolecular N—H···O and C—H···O hydrogen bonds and C—H···π interactions (dashed lines; see Table 1). H atoms not involved in these interactions have been omitted for clarity.

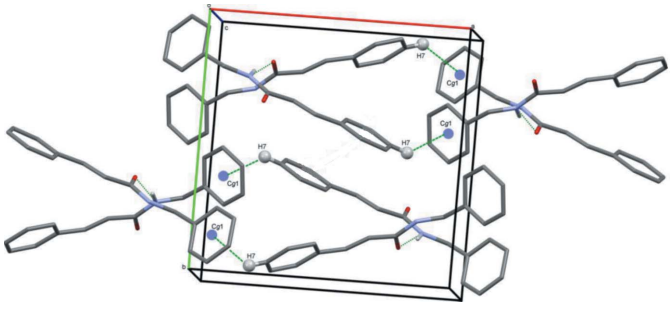


Figure 3
A partial view along the *c* axis of the crystal packing of the title compound, showing the chains linked *via* C—H···π interactions along the *a*-axis direction (intermolecular contacts are shown as dashed lines; see Table 1). H atoms not involved in these interactions have been omitted for clarity.

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

*Cg*1 is the centroid of the benzyl ring C11–C16.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1	0.95	2.52	2.8559 (11)	101
N1—H1···O1^{i}	0.889 (14)	2.009 (14)	2.880 (1)	166.3 (13)
C2—H2···O1^{i}	0.95	2.45	3.2126 (11)	138
C10—H10*B*···*Cg*1^{ii}	0.99	2.81	3.7058 (10)	151
C7—H7···*Cg*1^{iii}	0.95	2.88	3.6303 (12)	137

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $x-1, -y+\frac{3}{2}, z-\frac{1}{2}$.

are inclined to one another by 34.00 (2)°. The chains are linked *via* further C—H···π interactions, forming layers parallel to the *ac* plane (Table 1 and Fig. 3).

Synthesis and crystallization

The title compound was synthesized using a modified Appel reaction: To triphenylphosphine (PPh_3, 980 mg, 3.74 mmol) in dry CH_2Cl_2 (12 ml) was added bromotrichloromethane ($BrCCl_3$, 750 mg, 3.78 mmol), and the subsequent solution was stirred at room temperature for 35 min. Then, cinnamic acid (500 mg, 3.38 mmol) was added, and the mixture was heated at reflux for 45 min. Thereafter, benzylamine (720 mg, 6.73 mmol) was added dropwise *via* a syringe. The mixture was stirred at reflux for 14 h. Thereafter, the cooled mixture was subjected directly to column chromatographic separation to

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{15}NO$
M_r	237.29
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, *b*, *c* (Å)	12.4817 (6), 12.3107 (6), 8.5737 (4)
β (°)	94.276 (1)
V (Å^3)	1313.75 (11)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.3 × 0.1 × 0.1
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.705, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19856, 3249, 3010
R_{int}	0.018
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.038, 0.098, 1.04
No. of reflections	3249
No. of parameters	167
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.18

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2013* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

give the title compound as colourless needles [yield 655 mg, 82%; m.p. 386–387 K (382–383 K reported by Saito *et al.* (2008)]. Crystals used for the X-ray analysis were grown from a solution in ether/hexane/CH_2Cl_2.

Spectroscopic data: IR ν_{max} (KBr/cm^{-1}) 3280 (*bs*, NH), 3080, 2921, 1654, 1614, 1541, 1450, 1348, 1230, 1213, 979, 751, 696; δ_H (400 MHz, $CDCl_3$) 4.56 (2*H*, *d*, ^3J = 5.6 Hz), 6.06 (1*H*, *bs*, NH), 6.42 (1*H*, *d*, ^3J = 16.0 Hz), 7.25–7.30 (3*H*, *m*), 7.47–7.48 (2*H*, *m*), 7.66 (1*H*, *d*, ^3J = 16.0 Hz); δ_H (100.5 MHz, $CDCl_3$) 43.8 (−), 120.4 (CH), 127.6 (CH), 127.8 (2 C, CH), 127.9 (2 C, CH), 128.7 (2 C, CH), 128.8 (2 C, CH), 129.7 (CH), 134.7 (C_{quat}), 138.1 (C_{quat}), 141.4 (CH), 165.8 (C_{quat}, CO); MS (FAB, 3-nitrobenzyl alcohol) 238 (MH^+).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2016). **1**, x160647 [doi:10.1107/S2414314616006477]

N-Benzylcinnamamide

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N-Benzyl-3-phenylprop-2-enamide

Crystal data

$C_{16}H_{15}NO$
M_r = 237.29
Monoclinic, $P2_1/c$
a = 12.4817 (6) Å
b = 12.3107 (6) Å
c = 8.5737 (4) Å
β = 94.276 (1)°
V = 1313.75 (11) Å^3
Z = 4
$F(000)$ = 504
D_x = 1.200 Mg m^{-3}
Melting point: 386 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9967 reflections
θ = 2.3–28.8°
μ = 0.08 mm^{-1}
T = 100 K
Needle, colourless
0.3 × 0.1 × 0.1 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.705, T_{max} = 0.746
19856 measured reflections
3249 independent reflections
3010 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 28.9°, θ_{min} = 1.6°
h = −16→16
k = −16→16
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.098
S = 1.04
3249 reflections
167 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 0.5467P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.75871 (7)	0.79875 (7)	0.39369 (10)	0.01464 (18)
C10	0.93424 (7)	0.71049 (8)	0.43422 (10)	0.01744 (19)
C11	1.01755 (7)	0.66577 (7)	0.33259 (10)	0.01582 (18)
C12	1.01050 (7)	0.55828 (8)	0.28088 (12)	0.0199 (2)
C13	1.08325 (8)	0.51807 (8)	0.18015 (12)	0.0237 (2)
C14	1.16460 (8)	0.58402 (9)	0.13148 (11)	0.0231 (2)
C15	1.17303 (8)	0.69091 (9)	0.18333 (11)	0.0216 (2)
C16	1.09960 (7)	0.73147 (8)	0.28338 (11)	0.01817 (19)
C2	0.66405 (7)	0.81776 (8)	0.28144 (10)	0.01739 (19)
C3	0.57548 (7)	0.86518 (8)	0.32619 (11)	0.01755 (19)
C4	0.47794 (7)	0.89036 (8)	0.22575 (11)	0.01776 (19)
C5	0.46773 (8)	0.86615 (9)	0.06536 (12)	0.0228 (2)
C6	0.37579 (8)	0.89571 (10)	−0.02580 (13)	0.0269 (2)
C7	0.29287 (8)	0.95052 (9)	0.04032 (14)	0.0271 (2)
C8	0.30175 (8)	0.97456 (9)	0.19887 (15)	0.0291 (2)
C9	0.39331 (8)	0.94385 (9)	0.29075 (13)	0.0246 (2)
H1	0.8262 (11)	0.7126 (11)	0.2406 (17)	0.027 (3)*
H10A	0.9172	0.6556	0.5130	0.021*
H10B	0.9628	0.7759	0.4902	0.021*
H12	0.9557	0.5123	0.3148	0.024*
H13	1.0773	0.4451	0.1444	0.028*
H14	1.2144	0.5562	0.0630	0.028*
H15	1.2287	0.7362	0.1506	0.026*
H16	1.1055	0.8046	0.3184	0.022*
H2	0.6668	0.7957	0.1756	0.021*
H3	0.5753	0.8846	0.4334	0.021*
H5	0.5241	0.8293	0.0189	0.027*
H6	0.3694	0.8784	−0.1341	0.032*
H7	0.2305	0.9714	−0.0228	0.033*
H8	0.2454	1.0120	0.2446	0.035*
H9	0.3983	0.9595	0.3995	0.030*
N1	0.83680 (6)	0.73863 (7)	0.33718 (9)	0.01585 (17)
O1	0.76568 (5)	0.83631 (6)	0.52847 (7)	0.01820 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0185 (3)	0.0229 (3)	0.0130 (3)	0.0016 (3)	−0.0005 (2)	−0.0003 (2)
N1	0.0136 (4)	0.0202 (4)	0.0132 (3)	0.0014 (3)	−0.0027 (3)	−0.0016 (3)
C1	0.0137 (4)	0.0159 (4)	0.0143 (4)	−0.0010 (3)	0.0002 (3)	0.0029 (3)
C2	0.0148 (4)	0.0234 (5)	0.0136 (4)	0.0005 (3)	−0.0016 (3)	−0.0006 (3)
C3	0.0168 (4)	0.0197 (4)	0.0158 (4)	0.0008 (3)	−0.0012 (3)	−0.0017 (3)
C4	0.0141 (4)	0.0179 (4)	0.0208 (4)	0.0008 (3)	−0.0017 (3)	−0.0017 (3)
C5	0.0167 (4)	0.0302 (5)	0.0211 (5)	0.0029 (4)	−0.0011 (3)	−0.0026 (4)
C6	0.0208 (5)	0.0359 (6)	0.0231 (5)	−0.0010 (4)	−0.0055 (4)	0.0009 (4)

C7	0.0172 (5)	0.0255 (5)	0.0370 (6)	0.0014 (4)	−0.0090 (4)	0.0026 (4)
C8	0.0177 (5)	0.0262 (5)	0.0426 (6)	0.0072 (4)	−0.0036 (4)	−0.0093 (5)
C9	0.0192 (5)	0.0266 (5)	0.0275 (5)	0.0045 (4)	−0.0024 (4)	−0.0095 (4)
C10	0.0155 (4)	0.0218 (4)	0.0144 (4)	0.0040 (3)	−0.0031 (3)	0.0004 (3)
C11	0.0143 (4)	0.0179 (4)	0.0145 (4)	0.0035 (3)	−0.0042 (3)	0.0004 (3)
C12	0.0151 (4)	0.0181 (4)	0.0258 (5)	0.0000 (3)	−0.0037 (3)	−0.0006 (4)
C13	0.0212 (5)	0.0201 (5)	0.0286 (5)	0.0053 (4)	−0.0052 (4)	−0.0067 (4)
C14	0.0186 (4)	0.0306 (5)	0.0200 (4)	0.0082 (4)	−0.0004 (3)	−0.0025 (4)
C15	0.0176 (4)	0.0269 (5)	0.0200 (4)	0.0004 (4)	−0.0006 (3)	0.0044 (4)
C16	0.0186 (4)	0.0174 (4)	0.0177 (4)	0.0006 (3)	−0.0037 (3)	0.0008 (3)

Geometric parameters (Å, º)

C1—C2	1.4857 (12)	C3—H3	0.9500
C10—H10A	0.9900	C3—C4	1.4709 (12)
C10—H10B	0.9900	C4—C5	1.4036 (13)
C10—C11	1.5096 (12)	C4—C9	1.3956 (13)
C11—C12	1.3963 (13)	C5—H5	0.9500
C11—C16	1.3948 (13)	C5—C6	1.3879 (14)
C12—H12	0.9500	C6—H6	0.9500
C12—C13	1.3901 (14)	C6—C7	1.3911 (15)
C13—H13	0.9500	C7—H7	0.9500
C13—C14	1.3884 (15)	C7—C8	1.3876 (17)
C14—H14	0.9500	C8—H8	0.9500
C14—C15	1.3904 (15)	C8—C9	1.3912 (14)
C15—H15	0.9500	C9—H9	0.9500
C15—C16	1.3937 (14)	N1—H1	0.889 (14)
C16—H16	0.9500	N1—C1	1.3427 (12)
C2—H2	0.9500	N1—C10	1.4631 (11)
C2—C3	1.3317 (13)	O1—C1	1.2417 (11)
C1—N1—H1	118.3 (9)	C4—C9—H9	119.5
C1—N1—C10	121.36 (8)	C8—C9—C4	121.09 (10)
C10—N1—H1	120.3 (9)	C8—C9—H9	119.5
O1—C1—N1	122.59 (8)	N1—C10—H10A	109.7
O1—C1—C2	122.78 (8)	N1—C10—H10B	109.7
N1—C1—C2	114.63 (8)	N1—C10—C11	109.71 (7)
C1—C2—H2	119.3	H10A—C10—H10B	108.2
C3—C2—C1	121.30 (8)	C11—C10—H10A	109.7
C3—C2—H2	119.3	C11—C10—H10B	109.7
C2—C3—H3	116.8	C12—C11—C10	119.94 (8)
C2—C3—C4	126.33 (9)	C16—C11—C10	121.07 (8)
C4—C3—H3	116.8	C16—C11—C12	118.94 (9)
C5—C4—C3	122.66 (8)	C11—C12—H12	119.8
C9—C4—C3	118.93 (8)	C13—C12—C11	120.41 (9)
C9—C4—C5	118.38 (9)	C13—C12—H12	119.8
C4—C5—H5	119.8	C12—C13—H13	119.8
C6—C5—C4	120.46 (9)	C14—C13—C12	120.31 (9)

C6—C5—H5	119.8	C14—C13—H13	119.8
C5—C6—H6	119.8	C13—C14—H14	120.1
C5—C6—C7	120.45 (10)	C13—C14—C15	119.80 (9)
C7—C6—H6	119.8	C15—C14—H14	120.1
C6—C7—H7	120.2	C14—C15—H15	120.1
C8—C7—C6	119.68 (9)	C14—C15—C16	119.89 (9)
C8—C7—H7	120.2	C16—C15—H15	120.1
C7—C8—H8	120.0	C11—C16—H16	119.7
C7—C8—C9	119.93 (10)	C15—C16—C11	120.65 (9)
C9—C8—H8	120.0	C15—C16—H16	119.7
C1—C2—C3—C4	178.62 (9)	C2—C3—C4—C5	−0.12 (16)
C1—N1—C10—C11	−167.08 (8)	C3—C4—C9—C8	176.57 (10)
C10—C11—C16—C15	−176.84 (8)	C3—C4—C5—C6	−177.25 (10)
C10—C11—C12—C13	176.38 (8)	C4—C5—C6—C7	0.51 (17)
C10—N1—C1—C2	−178.57 (8)	C5—C6—C7—C8	−0.77 (17)
C10—N1—C1—O1	2.12 (14)	C5—C4—C9—C8	−1.25 (16)
C11—C12—C13—C14	0.85 (15)	C6—C7—C8—C9	0.01 (17)
C12—C13—C14—C15	−0.25 (15)	C7—C8—C9—C4	1.01 (17)
C12—C11—C16—C15	0.45 (13)	C9—C4—C5—C6	0.49 (16)
C13—C14—C15—C16	−0.23 (14)	N1—C10—C11—C16	98.18 (10)
C14—C15—C16—C11	0.13 (14)	N1—C10—C11—C12	−79.08 (10)
C16—C11—C12—C13	−0.94 (13)	N1—C1—C2—C3	172.24 (9)
C2—C3—C4—C9	−177.84 (10)	O1—C1—C2—C3	−8.45 (15)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the benzyl ring C11–C16.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1	0.95	2.52	2.8559 (11)	101
N1—H1···O1^{i}	0.889 (14)	2.009 (14)	2.880 (1)	166.3 (13)
C2—H2···O1^{i}	0.95	2.45	3.2126 (11)	138
C10—H10*B*···*Cg*1^{ii}	0.99	2.81	3.7058 (10)	151
C7—H7···*Cg*1^{iii}	0.95	2.88	3.6303 (12)	137

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) *x*, −*y*+3/2, *z*+1/2; (iii) *x*−1, −*y*+3/2, *z*−1/2.