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N-(Pyrazin-2-yl)adamantane-1-carboxamide

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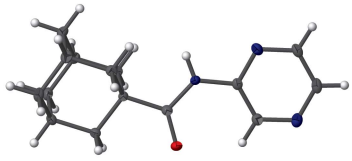
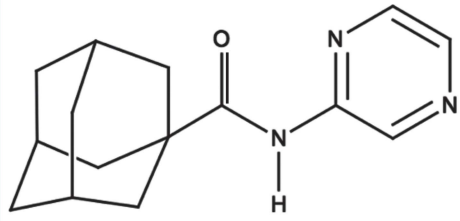
Molecules of the title compound, $C_{15}H_{19}N_3O$, are composed of an adamantine unit and a pyrazine ring connected to each other through an amide bond. The H—N—C═O moiety is close to planar [C—N—C—O and C—N—C—C torsion angles of 4.7 (2) and −173.8 (1)°, respectively]. The N3—C5 bond has partial double-bond character [1.370 (1) Å]. The geometries of the pyrazine ring and the adamantane substituent are normal and in good agreement with closely related structures. In the crystal, molecules are connected by N—H···O hydrogen bonds, forming zigzag chains in the [001] direction and are arranged in a herringbone fashion.

3D view



Chemical scheme



Structure description

Adamantane compounds have garnered considerable interest from the pharmacological community owning to their antiviral activity (*e.g.* Shchelkanov *et al.*, 2014). In the molecular structure presented herein, the adamantane component and its meaningful steric hindrance represents a geometric restriction for N—H···O═C hydrogen-bond formation. These interactions are the most interesting hydrogen bonding in biochemistry, as they stabilize the secondary structure of peptides (Pauling *et al.*, 1951). From the structural chemistry point of view, the strength and geometry of the interaction can be easily modified by use of bulky substituents (like adamantane) of the carboxyamide unit (Ośmiałowski *et al.*, 2010, 2013).

In the asymmetric unit of the title compound (Fig. 1), there is one independent molecule. The molecule is composed of an adamantane unit and a pyrazine ring connected to each other through the amide bond. The H—N—C═O bond is close to planar, with C1—N3—C5—O1 and C1—N3—C5—C6 torsion angles of 4.7 (2) and −173.8 (1)°, respectively. The N3—C5 [1.370 (1) Å] bond has partial double-bond character and pyramidalization of N3 is not observed. The geometries of the pyrazine ring and the adamantane

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1^{i}	0.86	2.22	3.0732 (13)	174
C3—H3···N1^{ii}	0.93	2.64	3.5179 (16)	157
C4—H4···O1	0.93	2.27	2.8612 (14)	121

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

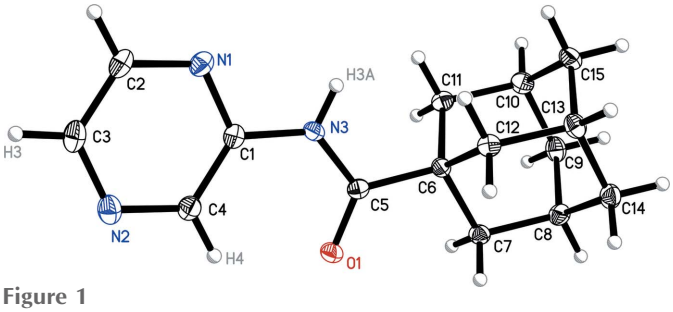


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

substituent are typical and the C—C and C—N bond lengths are normal and in good agreement with the average literature values (Allen, 2002) and with those of closely related structures (*e.g.* Cati & Stoeckli-Evans, 2014; Wang & Stoeckli-Evans, 2016; SiMa, 2009; Zheng & Wang, 2009). In the crystal, molecules of the title compound form zigzag chains in the [001] direction through an N3—H3A···O1^{i} hydrogen bond [symmetry code: (i) $x, -y, z-\frac{1}{2}$] (Table 1). Chains are linked to each other by C3—H3···N1^{ii} interactions [symmetry code: (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$], arranging the molecules in a herringbone packing arrangement (Fig. 2).

Synthesis and crystallization

N-(Pyrazin-2-yl)adamantane-1-carboxamide was obtained by reaction of aminopyrazine with 1-adamantanecarbonyl chloride (equimolar amounts added dropwise) in dichloromethane as a solvent containing triethylamine (1.2 molar equivalent). The reaction was performed at room temperature for 24 h. The solvent was then removed under reduced pressure and the residual was treated with saturated Na_2CO_3 solution. The water layer was extracted with chloroform and the organic phase was evaporated to dryness. The residual solid was recrystallized from ethanol solution.

Refinement

All H atoms were found in a difference map but set to idealized positions and treated as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^3 H atoms, and N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N). Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{19}N_3O$
M_r	257.34
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	100
a, *b*, *c* (Å)	27.3649 (9), 9.4960 (3), 10.0932 (3)
β (°)	97.371 (3)
V (Å^3)	2601.11 (14)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.35 × 0.20 × 0.15
Data collection	
Diffractometer	Oxford Diffraction Xcalibur
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7922, 2288, 1872
R_{int}	0.017
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.082, 1.06
No. of reflections	2288
No. of parameters	172
H-atom treatment	H-atom parameters not refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.20

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), and *XP* in *SHELXTL* (Sheldrick, 2008).

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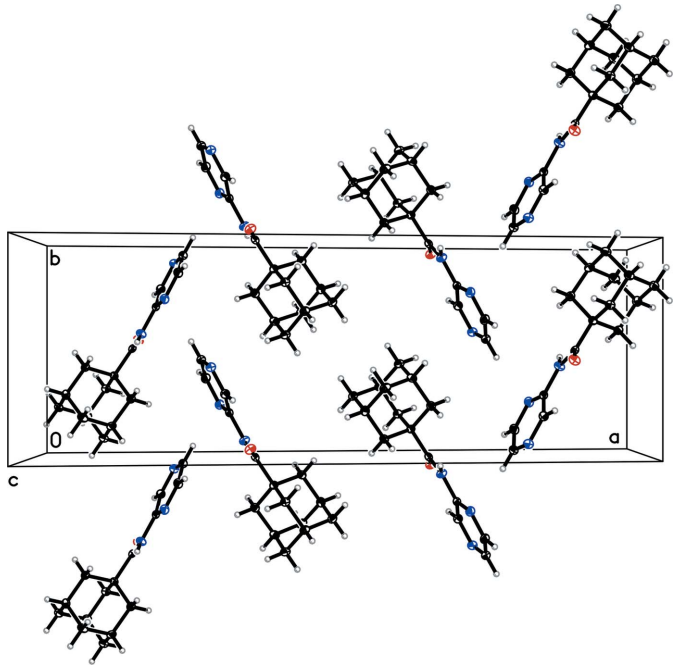

Figure 2
The crystal packing of the title compound, viewed along the *c* axis.

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full crystallographic data

IUCrData (2016). **1**, x161258 [doi:10.1107/S241431461601258X]

N-(Pyrazin-2-yl)adamantane-1-carboxamide

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Crystal data

$C_{15}H_{19}N_3O$
M_r = 257.34
Monoclinic, $C2/c$
a = 27.3649 (9) Å
b = 9.4960 (3) Å
c = 10.0932 (3) Å
β = 97.371 (3)°
V = 2601.11 (14) Å^3
Z = 8
$F(000)$ = 1104
D_x = 1.314 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7922 reflections
θ = 3.0–25.2°
μ = 0.09 mm^{-1}
T = 100 K
Irregular, colourless
0.35 × 0.20 × 0.15 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.07 pixels mm^{-1}
ω scan
7922 measured reflections
2288 independent reflections
1872 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.0°, θ_{min} = 3.0°
h = −32→32
k = −11→11
l = −7→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.082
S = 1.06
2288 reflections
172 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 not refined
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.2928P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 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. 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.35335 (3)	0.04607 (8)	0.64164 (8)	0.0171 (2)
N1	0.29623 (4)	0.23922 (11)	0.28328 (9)	0.0166 (2)
N2	0.28733 (4)	0.41834 (11)	0.49820 (10)	0.0192 (3)
N3	0.33971 (4)	0.07518 (10)	0.41681 (9)	0.0148 (2)
H3A	0.3433	0.0354	0.3421	0.018*
C1	0.31491 (4)	0.20496 (12)	0.40801 (11)	0.0134 (3)
C2	0.27321 (4)	0.36365 (13)	0.26772 (12)	0.0183 (3)
H2	0.2599	0.3915	0.1823	0.022*
C3	0.26850 (4)	0.45175 (13)	0.37355 (12)	0.0189 (3)
H3	0.2518	0.5366	0.3579	0.023*
C4	0.31065 (4)	0.29484 (12)	0.51542 (12)	0.0162 (3)
H4	0.3243	0.2681	0.6008	0.019*
C5	0.35891 (4)	0.00418 (12)	0.52975 (11)	0.0127 (3)
C6	0.38861 (4)	−0.12766 (12)	0.50667 (11)	0.0125 (3)
C7	0.40850 (4)	−0.19418 (12)	0.64151 (11)	0.0144 (3)
H7A	0.4286	−0.1261	0.6955	0.017*
H7B	0.3812	−0.2204	0.6889	0.017*
C8	0.43941 (4)	−0.32477 (12)	0.62024 (12)	0.0159 (3)
H8	0.4516	−0.3661	0.7071	0.019*
C9	0.40736 (5)	−0.43301 (13)	0.53643 (12)	0.0185 (3)
H9A	0.4266	−0.5166	0.5237	0.022*
H9B	0.3798	−0.4603	0.5824	0.022*
C10	0.38834 (4)	−0.36779 (13)	0.40072 (12)	0.0172 (3)
H10	0.3682	−0.4370	0.3463	0.021*
C11	0.35678 (4)	−0.23827 (12)	0.42266 (11)	0.0151 (3)
H11A	0.3293	−0.2659	0.4687	0.018*
H11B	0.3437	−0.1980	0.3371	0.018*
C12	0.43293 (4)	−0.08611 (12)	0.43399 (12)	0.0142 (3)
H12A	0.4211	−0.0445	0.3480	0.017*
H12B	0.4530	−0.0167	0.4865	0.017*
C13	0.46409 (4)	−0.21676 (13)	0.41374 (12)	0.0167 (3)
H13	0.4921	−0.1897	0.3676	0.020*
C14	0.48310 (4)	−0.28214 (13)	0.54869 (12)	0.0173 (3)
H14A	0.5035	−0.2147	0.6027	0.021*
H14B	0.5030	−0.3642	0.5356	0.021*
C15	0.43197 (4)	−0.32405 (13)	0.32845 (12)	0.0186 (3)
H15A	0.4199	−0.2827	0.2426	0.022*
H15B	0.4515	−0.4063	0.3129	0.022*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0218 (5)	0.0182 (5)	0.0112 (4)	0.0040 (4)	0.0026 (3)	−0.0009 (3)
N1	0.0157 (5)	0.0181 (6)	0.0158 (5)	0.0006 (4)	0.0013 (4)	0.0036 (4)
N2	0.0182 (6)	0.0149 (6)	0.0245 (6)	0.0007 (4)	0.0031 (5)	−0.0003 (4)

N3	0.0198 (5)	0.0142 (5)	0.0104 (5)	0.0040 (4)	0.0018 (4)	−0.0011 (4)
C1	0.0113 (6)	0.0131 (6)	0.0161 (6)	−0.0008 (5)	0.0025 (5)	0.0019 (5)
C2	0.0158 (6)	0.0186 (7)	0.0200 (7)	0.0018 (5)	0.0000 (5)	0.0063 (5)
C3	0.0149 (6)	0.0142 (6)	0.0273 (7)	0.0009 (5)	0.0019 (5)	0.0035 (5)
C4	0.0158 (6)	0.0155 (6)	0.0170 (6)	0.0002 (5)	0.0008 (5)	0.0008 (5)
C5	0.0118 (6)	0.0132 (6)	0.0131 (6)	−0.0026 (5)	0.0009 (5)	−0.0001 (5)
C6	0.0135 (6)	0.0123 (6)	0.0118 (6)	0.0012 (5)	0.0021 (5)	0.0000 (5)
C7	0.0170 (6)	0.0139 (6)	0.0122 (6)	0.0006 (5)	0.0018 (5)	0.0004 (5)
C8	0.0182 (6)	0.0145 (7)	0.0146 (6)	0.0022 (5)	0.0003 (5)	0.0024 (5)
C9	0.0193 (6)	0.0127 (6)	0.0238 (7)	0.0021 (5)	0.0042 (5)	0.0001 (5)
C10	0.0185 (7)	0.0131 (7)	0.0193 (6)	−0.0021 (5)	0.0002 (5)	−0.0040 (5)
C11	0.0153 (6)	0.0152 (6)	0.0144 (6)	−0.0013 (5)	0.0007 (5)	0.0003 (5)
C12	0.0152 (6)	0.0136 (6)	0.0140 (6)	−0.0013 (5)	0.0024 (5)	0.0013 (5)
C13	0.0149 (6)	0.0183 (7)	0.0177 (6)	0.0002 (5)	0.0058 (5)	−0.0005 (5)
C14	0.0160 (6)	0.0146 (6)	0.0211 (6)	0.0022 (5)	0.0012 (5)	−0.0020 (5)
C15	0.0227 (7)	0.0169 (6)	0.0164 (6)	0.0041 (5)	0.0031 (5)	−0.0038 (5)

Geometric parameters (Å, º)

O1—C5	1.2252 (14)	C8—C9	1.5332 (16)
N1—C1	1.3368 (14)	C8—H8	0.9800
N1—C2	1.3387 (16)	C9—C10	1.5322 (16)
N2—C3	1.3353 (16)	C9—H9A	0.9700
N2—C4	1.3358 (15)	C9—H9B	0.9700
N3—C5	1.3698 (14)	C10—C15	1.5340 (17)
N3—C1	1.4042 (15)	C10—C11	1.5351 (17)
N3—H3A	0.8600	C10—H10	0.9800
C1—C4	1.3963 (16)	C11—H11A	0.9700
C2—C3	1.3758 (18)	C11—H11B	0.9700
C2—H2	0.9300	C12—C13	1.5339 (16)
C3—H3	0.9300	C12—H12A	0.9700
C4—H4	0.9300	C12—H12B	0.9700
C5—C6	1.5267 (16)	C13—C14	1.5263 (16)
C6—C7	1.5354 (15)	C13—C15	1.5354 (16)
C6—C11	1.5464 (16)	C13—H13	0.9800
C6—C12	1.5468 (16)	C14—H14A	0.9700
C7—C8	1.5316 (16)	C14—H14B	0.9700
C7—H7A	0.9700	C15—H15A	0.9700
C7—H7B	0.9700	C15—H15B	0.9700
C8—C14	1.5286 (17)		
C1—N1—C2	116.27 (10)	C8—C9—H9A	109.9
C3—N2—C4	116.83 (11)	C10—C9—H9B	109.9
C5—N3—C1	127.97 (10)	C8—C9—H9B	109.9
C5—N3—H3A	116.0	H9A—C9—H9B	108.3
C1—N3—H3A	116.0	C9—C10—C15	109.80 (9)
N1—C1—C4	121.50 (11)	C9—C10—C11	109.13 (10)
N1—C1—N3	113.36 (10)	C15—C10—C11	109.76 (10)

C4—C1—N3	125.11 (11)	C9—C10—H10	109.4
N1—C2—C3	122.36 (11)	C15—C10—H10	109.4
N1—C2—H2	118.8	C11—C10—H10	109.4
C3—C2—H2	118.8	C10—C11—C6	109.61 (9)
N2—C3—C2	121.59 (12)	C10—C11—H11A	109.7
N2—C3—H3	119.2	C6—C11—H11A	109.7
C2—C3—H3	119.2	C10—C11—H11B	109.7
N2—C4—C1	121.45 (11)	C6—C11—H11B	109.7
N2—C4—H4	119.3	H11A—C11—H11B	108.2
C1—C4—H4	119.3	C13—C12—C6	109.87 (9)
O1—C5—N3	121.84 (11)	C13—C12—H12A	109.7
O1—C5—C6	122.58 (10)	C6—C12—H12A	109.7
N3—C5—C6	115.57 (10)	C13—C12—H12B	109.7
C5—C6—C7	109.71 (9)	C6—C12—H12B	109.7
C5—C6—C11	111.55 (9)	H12A—C12—H12B	108.2
C7—C6—C11	108.50 (9)	C14—C13—C12	109.99 (10)
C5—C6—C12	109.16 (9)	C14—C13—C15	109.60 (10)
C7—C6—C12	108.36 (9)	C12—C13—C15	108.87 (9)
C11—C6—C12	109.50 (9)	C14—C13—H13	109.5
C8—C7—C6	110.38 (10)	C12—C13—H13	109.5
C8—C7—H7A	109.6	C15—C13—H13	109.5
C6—C7—H7A	109.6	C13—C14—C8	109.36 (9)
C8—C7—H7B	109.6	C13—C14—H14A	109.8
C6—C7—H7B	109.6	C8—C14—H14A	109.8
H7A—C7—H7B	108.1	C13—C14—H14B	109.8
C14—C8—C7	109.35 (10)	C8—C14—H14B	109.8
C14—C8—C9	110.09 (10)	H14A—C14—H14B	108.3
C7—C8—C9	109.46 (10)	C10—C15—C13	109.73 (9)
C14—C8—H8	109.3	C10—C15—H15A	109.7
C7—C8—H8	109.3	C13—C15—H15A	109.7
C9—C8—H8	109.3	C10—C15—H15B	109.7
C10—C9—C8	109.08 (10)	C13—C15—H15B	109.7
C10—C9—H9A	109.9	H15A—C15—H15B	108.2

C2—N1—C1—C4	−0.24 (16)	C14—C8—C9—C10	−59.90 (12)
C2—N1—C1—N3	−178.33 (10)	C7—C8—C9—C10	60.32 (12)
C5—N3—C1—N1	−173.52 (10)	C8—C9—C10—C15	59.24 (13)
C5—N3—C1—C4	8.47 (19)	C8—C9—C10—C11	−61.11 (12)
C1—N1—C2—C3	−0.46 (17)	C9—C10—C11—C6	61.22 (12)
C4—N2—C3—C2	−0.49 (17)	C15—C10—C11—C6	−59.15 (12)
N1—C2—C3—N2	0.86 (19)	C5—C6—C11—C10	179.30 (9)
C3—N2—C4—C1	−0.20 (17)	C7—C6—C11—C10	−59.73 (12)
N1—C1—C4—N2	0.59 (18)	C12—C6—C11—C10	58.36 (12)
N3—C1—C4—N2	178.45 (11)	C5—C6—C12—C13	178.29 (9)
C1—N3—C5—O1	4.70 (18)	C7—C6—C12—C13	58.86 (12)
C1—N3—C5—C6	−173.80 (10)	C11—C6—C12—C13	−59.32 (12)
O1—C5—C6—C7	0.46 (15)	C6—C12—C13—C14	−59.77 (12)
N3—C5—C6—C7	178.96 (9)	C6—C12—C13—C15	60.33 (12)

O1—C5—C6—C11	120.72 (12)	C12—C13—C14—C8	59.94 (12)
N3—C5—C6—C11	−60.79 (13)	C15—C13—C14—C8	−59.71 (12)
O1—C5—C6—C12	−118.14 (12)	C7—C8—C14—C13	−59.99 (12)
N3—C5—C6—C12	60.36 (12)	C9—C8—C14—C13	60.31 (12)
C5—C6—C7—C8	−178.69 (9)	C9—C10—C15—C13	−59.34 (13)
C11—C6—C7—C8	59.21 (12)	C11—C10—C15—C13	60.63 (12)
C12—C6—C7—C8	−59.60 (12)	C14—C13—C15—C10	59.45 (12)
C6—C7—C8—C14	60.67 (12)	C12—C13—C15—C10	−60.89 (12)
C6—C7—C8—C9	−60.01 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1^{i}	0.86	2.22	3.0732 (13)	174
C3—H3···N1^{ii}	0.93	2.64	3.5179 (16)	157
C4—H4···O1	0.93	2.27	2.8612 (14)	121

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