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Crystal structure of 3-amino-2-propyl-quinazolin-4(3H)-one

Gamal A. El-Hiti,^{a*} Keith Smith,^b Amany S. Hegazy,^b
Saud A. Alanazi^a and Benson M. Kariuki^{b*}

^aCornea Research Chair, Department of Optometry, College of Applied Medical Sciences, King Saud University, PO Box 10219, Riyadh 11433, Saudi Arabia, and

^bSchool of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, Wales. *Correspondence e-mail: gelhiti@ksu.edu.sa, kariukib@cardiff.ac.uk

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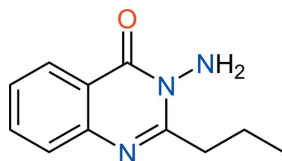
In the title molecule, C₁₁H₁₃N₃O, the propyl group is almost perpendicular to the quinazolin-4(3H)-one mean plane, making a dihedral angle of 88.98 (9)°. In the crystal, molecules related by an inversion centre are paired *via* π–π overlap, indicated by the short distances of 3.616 (5) and 3.619 (5) Å between the centroids of the aromatic rings of neighbouring molecules. Intermolecular N–H···N and N–H···O hydrogen bonds form R₆⁶(30) rings and C(5) chains, respectively, generating a three-dimensional network. Weak C–H···O interactions are also observed.

Keywords: crystal structure; quinazolin-4(3H)-one; hydrogen bonding; π–π overlap.

CCDC reference: 1411448

1. Related literature

For biological applications of related compounds, see: Sasmal *et al.* (2012); Rohini *et al.* (2010); Chandregowda *et al.* (2009); Gupta *et al.* (2008); Alagarsamy *et al.* (2007). For the synthesis of substituted quinazolin-4(3H)-ones, see: Ma *et al.* (2013); Adib *et al.* (2012); Xu *et al.* (2012); Kumar *et al.* (2011). For modification of the quinazolin-4(3H)-one ring system *via* lithiation, see: Smith *et al.* (2004, 1996, 1995). For the crystal structures for related compounds, see: El-Hiti *et al.* (2014); Yang *et al.* (2009); Coogan *et al.* (1999).



2. Experimental

2.1. Crystal data

C ₁₁ H ₁₃ N ₃ O	Z = 18
M _r = 203.24	Cu Kα radiation
Trigonal, R $\bar{3}$: H	μ = 0.67 mm ⁻¹
a = 24.1525 (5) Å	T = 296 K
c = 9.6500 (2) Å	0.34 × 0.25 × 0.19 mm
V = 4875.1 (2) Å ³	

2.2. Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector	3734 measured reflections
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)	2136 independent reflections
T _{min} = 0.975, T _{max} = 0.984	1913 reflections with I > 2σ(I)
	R _{int} = 0.013

2.3. Refinement

R[F ² > 2σ(F ²)] = 0.040	H atoms treated by a mixture of independent and constrained refinement
wR(F ²) = 0.120	Δρ _{max} = 0.17 e Å ⁻³
S = 1.06	Δρ _{min} = -0.15 e Å ⁻³
2136 reflections	
146 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

D–H···A	D–H	H···A	D···A	D–H···A
N3–H3A···N2 ⁱ	0.91 (2)	2.16 (2)	3.0677 (17)	176.1 (16)
N3–H3B···O1 ⁱⁱ	0.87 (2)	2.51 (2)	3.0599 (16)	122.0 (15)
C5–H5···O1 ⁱⁱⁱ	0.93	2.44	3.3163 (16)	157

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

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: CV5493).

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supporting information

Acta Cryst. (2015). E71, o590–o591 [doi:10.1107/S2056989015013134]

Crystal structure of 3-amino-2-propylquinazolin-4(3H)-one

Gamal A. El-Hiti, Keith Smith, Amany S. Hegazy, Saud A. Alanazi and Benson M. Kariuki

S1. Introduction

Quinazolines have a range of biological activities such as anti-cancer (Chandregowda *et al.*, 2009), anti-bacterial (Rohini *et al.*, 2010), anti-inflammatory (Alagarsamy *et al.*, 2007), anti-obesity (Sasmal *et al.*, 2012) and anti-spasm (Gupta *et al.*, 2008). Synthesis of quinazolin-4(3H)-ones involves use of various synthetic procedures. Recent examples involve reactions of 2-aminobenzonitrile with carbon dioxide in water (Ma *et al.*, 2013), 2-bromobenzamides with formamide catalysed by CuI and 4-hydroxy-L-proline (Xu *et al.*, 2012) and isatoic anhydride, benzyl halides and primary amines under mild Kornblum conditions (Adib *et al.*, 2012). 2-Alkyl-3-aminoquinazolin-4(3H)-ones can be obtained from reactions of 2-alkyl-4H-3,1-benzoxazin-4-ones with hydrazine hydrate (Kumar *et al.*, 2011). Lithiation of 2-unsubstituted and 2-n-alkyl-3-acylaminoquinazolin-4(3H)-ones followed by reactions of the lithium reagents produced *in-situ* with electrophiles gave the corresponding substituted derivatives in high yields (Smith *et al.*, 2004, 1996, 1995). For the X-ray structures for related compounds, see: El-Hiti *et al.* (2014); Yang *et al.* (2009); Coogan *et al.* (1999).

S2. Experimental

S2.1. Synthesis and crystallization

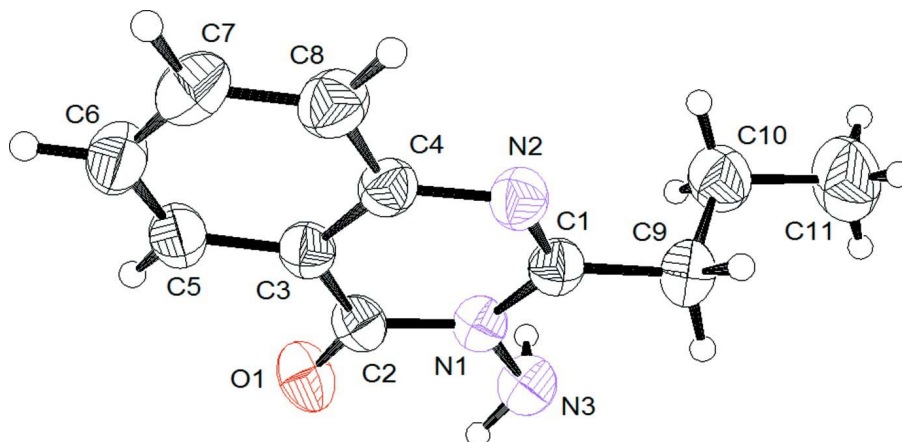
3-Amino-2-propylquinazolin-4(3H)-one was obtained in 82% yield by reaction of 2-propyl-4H-3,1-benzoxazin-4-one with excess hydrazine hydrate (three mole equivalents) in methanol under reflux conditions for 3 h (Kumar *et al.*, 2011). Crystallization from ethanol gave colourless crystals of the title compound. The NMR and mass spectral data for the title compound were identical with those reported (Kumar *et al.*, 2011).

S2.2. Refinement

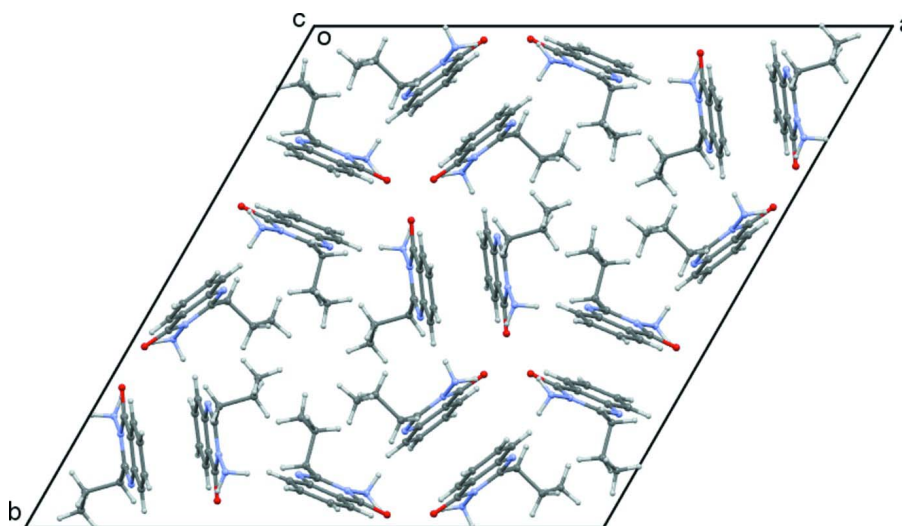
The amino hydrogen atoms were located in the difference Fourier map and refined freely. The rest of the H atoms were positioned geometrically and refined using a riding model with $U_{\text{iso}}(\text{H})$ constrained to be 1.2 times U_{eq} for the atom it is bonded to except for methyl groups where it was 1.5 times with free rotation about the C—C bond.

S3. Results and discussion

In the title compound (I) (Fig. 1), the propyl group is perpendicular to the quinazolin-4(3H)-one group with a dihedral angle of 88.98 (9)° between the least-squares planes of the two groups. In the crystal (Fig. 2), π – π overlap is observed for paired molecules with a centroid-centroid distance of *ca* 3.62 (1) Å between the benzene and pyrimidine rings of parallel 3-aminoquinazolin-4(3H)-one groups. N—H···N hydrogen bonds form $R_6^6(30)$ rings and N—H···O form C(5) chains to generate three dimensional packing. Weak C—H···O contacts (C(5)) are also observed.

**Figure 1**

View of (I) showing the atom labels and 50% probability displacement ellipsoids.

**Figure 2**

Crystal packing viewed along the *c* axis.

3-Amino-2-propylquinazolin-4(3H)-one

Crystal data

$C_{11}H_{13}N_3O$

$M_r = 203.24$

Trigonal, $R\bar{3}:H$

$a = 24.1525(5) \text{ \AA}$

$c = 9.6500(2) \text{ \AA}$

$V = 4875.1(2) \text{ \AA}^3$

$Z = 18$

$F(000) = 1944$

$D_x = 1.246 \text{ Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$

Cell parameters from 2040 reflections

$\theta = 5.0\text{--}74.1^\circ$

$\mu = 0.67 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Block, colourless

$0.34 \times 0.25 \times 0.19 \text{ mm}$

Data collection

Agilent SuperNova Dual Source
diffractometer with an Atlas detector

ω scans

Absorption correction: multi-scan
(*CrysAlis PRO*; Agilent, 2014)

$T_{\min} = 0.975$, $T_{\max} = 0.984$

3734 measured reflections

2136 independent reflections

1913 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.013$

$\theta_{\max} = 74.1^\circ$, $\theta_{\min} = 3.7^\circ$

$h = -21 \rightarrow 30$

$k = -26 \rightarrow 18$

$l = -11 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.120$

$S = 1.06$

2136 reflections

146 parameters

0 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 1.4157P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.17 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.15 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXL2013* (Sheldrick,
2015), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00114 (10)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.23343 (6)	0.11120 (6)	0.00970 (12)	0.0453 (3)
C2	0.28221 (6)	0.06090 (5)	0.14259 (13)	0.0457 (3)
C3	0.27352 (5)	0.09197 (5)	0.26270 (12)	0.0440 (3)
C4	0.24674 (6)	0.13113 (6)	0.24439 (12)	0.0450 (3)
C5	0.29168 (6)	0.08293 (7)	0.39466 (14)	0.0535 (3)
H5	0.3089	0.0563	0.4064	0.064*
C6	0.28403 (7)	0.11345 (8)	0.50654 (14)	0.0618 (4)
H6	0.2958	0.1074	0.5946	0.074*
C7	0.25865 (8)	0.15367 (8)	0.48822 (14)	0.0630 (4)
H7	0.2544	0.1749	0.5643	0.076*
C8	0.23997 (7)	0.16241 (7)	0.36013 (14)	0.0567 (3)
H8	0.2228	0.1891	0.3498	0.068*
C9	0.20961 (7)	0.11882 (6)	-0.12831 (14)	0.0546 (3)
H9A	0.2357	0.1157	-0.2009	0.066*
H9B	0.2141	0.1610	-0.1337	0.066*
C10	0.13977 (8)	0.06846 (8)	-0.15299 (18)	0.0697 (4)
H10A	0.1359	0.0265	-0.1554	0.084*
H10B	0.1141	0.0691	-0.0763	0.084*
C11	0.11417 (10)	0.07946 (12)	-0.2869 (2)	0.0996 (7)
H11A	0.1222	0.1226	-0.2894	0.149*
H11B	0.0690	0.0503	-0.2924	0.149*

H11C	0.1351	0.0724	-0.3639	0.149*
N1	0.25905 (5)	0.07168 (5)	0.01918 (10)	0.0447 (3)
N2	0.22710 (5)	0.14035 (5)	0.11608 (11)	0.0486 (3)
N3	0.26483 (7)	0.04247 (6)	-0.10370 (12)	0.0550 (3)
O1	0.30729 (5)	0.02780 (5)	0.14300 (11)	0.0625 (3)
H3A	0.2287 (9)	0.0033 (10)	-0.1045 (18)	0.069 (5)*
H3B	0.2972 (10)	0.0370 (9)	-0.087 (2)	0.069 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0447 (6)	0.0405 (6)	0.0464 (6)	0.0179 (5)	-0.0012 (5)	0.0016 (4)
C2	0.0425 (6)	0.0391 (5)	0.0518 (7)	0.0177 (5)	-0.0073 (5)	-0.0046 (5)
C3	0.0400 (6)	0.0401 (6)	0.0462 (6)	0.0158 (5)	-0.0028 (4)	-0.0002 (4)
C4	0.0441 (6)	0.0438 (6)	0.0439 (6)	0.0196 (5)	0.0021 (4)	0.0025 (4)
C5	0.0514 (7)	0.0554 (7)	0.0518 (7)	0.0253 (6)	-0.0067 (5)	0.0018 (5)
C6	0.0650 (8)	0.0724 (9)	0.0432 (7)	0.0307 (7)	-0.0043 (6)	0.0016 (6)
C7	0.0736 (9)	0.0695 (9)	0.0450 (7)	0.0350 (7)	0.0067 (6)	-0.0039 (6)
C8	0.0653 (8)	0.0603 (8)	0.0504 (7)	0.0358 (7)	0.0057 (6)	-0.0003 (6)
C9	0.0631 (8)	0.0512 (7)	0.0486 (7)	0.0279 (6)	-0.0060 (5)	0.0022 (5)
C10	0.0616 (9)	0.0732 (10)	0.0692 (9)	0.0300 (8)	-0.0086 (7)	0.0004 (7)
C11	0.0780 (12)	0.1036 (15)	0.0986 (15)	0.0315 (11)	-0.0333 (11)	0.0058 (12)
N1	0.0467 (5)	0.0401 (5)	0.0434 (5)	0.0189 (4)	-0.0036 (4)	-0.0052 (4)
N2	0.0546 (6)	0.0488 (6)	0.0462 (6)	0.0287 (5)	0.0001 (4)	0.0023 (4)
N3	0.0630 (7)	0.0499 (6)	0.0494 (6)	0.0263 (6)	-0.0042 (5)	-0.0120 (4)
O1	0.0729 (6)	0.0611 (6)	0.0683 (6)	0.0446 (5)	-0.0198 (5)	-0.0166 (4)

Geometric parameters (Å, °)

C1—N2	1.2963 (16)	C7—H7	0.9300
C1—N1	1.3760 (16)	C8—H8	0.9300
C1—C9	1.4981 (17)	C9—C10	1.526 (2)
C2—O1	1.2209 (15)	C9—H9A	0.9700
C2—N1	1.3945 (16)	C9—H9B	0.9700
C2—C3	1.4520 (17)	C10—C11	1.512 (2)
C3—C4	1.3984 (18)	C10—H10A	0.9700
C3—C5	1.3991 (18)	C10—H10B	0.9700
C4—N2	1.3832 (16)	C11—H11A	0.9600
C4—C8	1.4032 (18)	C11—H11B	0.9600
C5—C6	1.371 (2)	C11—H11C	0.9600
C5—H5	0.9300	N1—N3	1.4219 (14)
C6—C7	1.395 (2)	N3—H3A	0.91 (2)
C6—H6	0.9300	N3—H3B	0.87 (2)
C7—C8	1.368 (2)		
N2—C1—N1	122.69 (11)	C1—C9—H9A	109.1
N2—C1—C9	118.73 (11)	C10—C9—H9A	109.1
N1—C1—C9	118.53 (11)	C1—C9—H9B	109.1

O1—C2—N1	120.11 (11)	C10—C9—H9B	109.1
O1—C2—C3	125.67 (12)	H9A—C9—H9B	107.9
N1—C2—C3	114.21 (10)	C11—C10—C9	112.30 (15)
C4—C3—C5	120.51 (12)	C11—C10—H10A	109.1
C4—C3—C2	118.94 (11)	C9—C10—H10A	109.1
C5—C3—C2	120.55 (11)	C11—C10—H10B	109.1
N2—C4—C3	122.27 (11)	C9—C10—H10B	109.1
N2—C4—C8	118.95 (12)	H10A—C10—H10B	107.9
C3—C4—C8	118.78 (12)	C10—C11—H11A	109.5
C6—C5—C3	119.73 (13)	C10—C11—H11B	109.5
C6—C5—H5	120.1	H11A—C11—H11B	109.5
C3—C5—H5	120.1	C10—C11—H11C	109.5
C5—C6—C7	119.93 (13)	H11A—C11—H11C	109.5
C5—C6—H6	120.0	H11B—C11—H11C	109.5
C7—C6—H6	120.0	C1—N1—C2	123.22 (10)
C8—C7—C6	121.04 (13)	C1—N1—N3	118.60 (10)
C8—C7—H7	119.5	C2—N1—N3	118.13 (10)
C6—C7—H7	119.5	C1—N2—C4	118.58 (11)
C7—C8—C4	119.99 (13)	N1—N3—H3A	104.0 (11)
C7—C8—H8	120.0	N1—N3—H3B	103.8 (13)
C4—C8—H8	120.0	H3A—N3—H3B	108.1 (17)
C1—C9—C10	112.34 (12)		
O1—C2—C3—C4	176.78 (12)	N2—C1—C9—C10	-89.31 (15)
N1—C2—C3—C4	-3.10 (16)	N1—C1—C9—C10	88.39 (15)
O1—C2—C3—C5	-3.2 (2)	C1—C9—C10—C11	175.23 (16)
N1—C2—C3—C5	176.95 (11)	N2—C1—N1—C2	-1.99 (18)
C5—C3—C4—N2	-178.79 (11)	C9—C1—N1—C2	-179.59 (11)
C2—C3—C4—N2	1.26 (17)	N2—C1—N1—N3	-179.17 (11)
C5—C3—C4—C8	1.61 (18)	C9—C1—N1—N3	3.23 (16)
C2—C3—C4—C8	-178.34 (11)	O1—C2—N1—C1	-176.35 (11)
C4—C3—C5—C6	-0.98 (19)	C3—C2—N1—C1	3.54 (16)
C2—C3—C5—C6	178.97 (12)	O1—C2—N1—N3	0.84 (17)
C3—C5—C6—C7	-0.4 (2)	C3—C2—N1—N3	-179.27 (10)
C5—C6—C7—C8	1.2 (2)	N1—C1—N2—C4	-0.22 (18)
C6—C7—C8—C4	-0.6 (2)	C9—C1—N2—C4	177.38 (11)
N2—C4—C8—C7	179.55 (13)	C3—C4—N2—C1	0.51 (18)
C3—C4—C8—C7	-0.8 (2)	C8—C4—N2—C1	-179.89 (12)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H3A...N2 ⁱ	0.91 (2)	2.16 (2)	3.0677 (17)	176.1 (16)
N3—H3B...O1 ⁱⁱ	0.87 (2)	2.51 (2)	3.0599 (16)	122.0 (15)
C5—H5...O1 ⁱⁱⁱ	0.93	2.44	3.3163 (16)	157

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