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2-Phenoxy-1,2,4-triazolo[1,5-*a*]quinazolin-5(4*H*)-one

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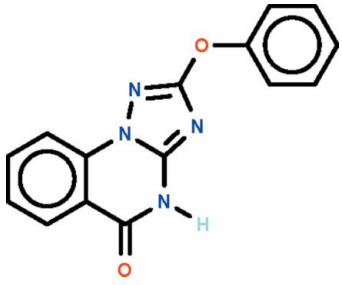
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.103; data-to-parameter ratio = 13.2.

The triazoloquinazole ring system in the title compound, $C_{15}H_{10}N_4O_2$ is approximately planar (r.m.s. deviation = 0.035 Å). The phenyl ring of the phenoxy substitutent is aligned at 59.3 (1)° with respect to this ring system. In the crystal, two molecules are linked about a center of inversion by a pair of N—H···O hydrogen bonds, generating a dimer.

Related literature

The synthesis was based on theat of a similar compound; see: Al-Salahi & Geffken (2011).



Experimental

Crystal data

$C_{15}H_{10}N_4O_2$ M_r = 278.27
Triclinic, $P\overline{1}$
a = 5.6985 (2) Å
b = 8.4328 (4) Å
c = 13.4322 (7) Å
α = 74.087 (4)°
β = 86.623 (4)°
γ = 89.284 (4)°
V = 619.66 (5) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 0.86 mm^{-1}
T = 294 K
0.30 × 0.30 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.783, T_{max} = 0.919
10219 measured reflections
2570 independent reflections
2408 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.103
S = 1.03
2570 reflections
194 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.88 (1)	1.90 (1)	2.775 (1)	174 (1)

Symmetry code: (i) $-x+2, -y+1, -z+1$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5917).

References

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Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2012). E**68**, o1808 [doi:10.1107/S1600536812021782]

2-Phenoxy-1,2,4-triazolo[1,5-*a*]quinazolin-5(4*H*)-one

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S1. Comment

The procedure for the synthesis of 2-(methylsulfanyl)-[1,2,4]triazolo[1,5-*a*]quinazolin-5-one uses dimethyl *N*-cyano-dithioimidocarbonate as one of the reactants (Al-Salahi & Geffken, 2011). The title phenoxy-substituted analog (Scheme I) is obtained with diphenyl *N*-cyanodithioimidocarbonate instead. The triazoloquinazole fused-ring system of $C_{15}H_{10}N_4O_2$ is planar. The phenyl ring of the phenoxy substitutent is aligned at 59.3 (1) ° with respect to this ring system. Two molecules are linked about a center of inversion by N–H···O hydrogen bonds to generate a dimer (Table 1).

S2. Experimental

Under ice-cold conditions, 2-hydrazinobenzoic acid (10 mmol, 1.52 g) was added to a solution of diphenyl *N*-cyano-dithioimidocarbonate (10 mmol, 2.38 g) in ethanol (20 ml). Triethylamine (30 mmol, 3.03 g) was added. The reaction mixture was stirred overnight at room temperature. Concentrated hydrochloric acid was added; the acidified mixture for heated for an hour. The mixture was poured into ice water; the solid that formed was collected and recrystallized from ethanol to give colorless crystals of 2-phenoxy-[1,2,4]triazolo[1,5-*a*]quinazolin-5-one. The procedure was based on that reported for 2-(methylsulfanyl)-[1,2,4]triazolo[1,5-*a*]quinazolin-5-one (Al-Salahi & Geffken, 2011).

S3. Refinement

All H-atom were located in a difference Fourier map. Carbon-bound H-atoms were placed in calculated positions [C–H 0.93 Å, U_{iso}(H) 1.2U_{eq}(C)] and were included in the refinement in the riding model approximation.

The amino H-atom was refined isotropically with a distance restraint of N–H 0.88±0.01 Å.

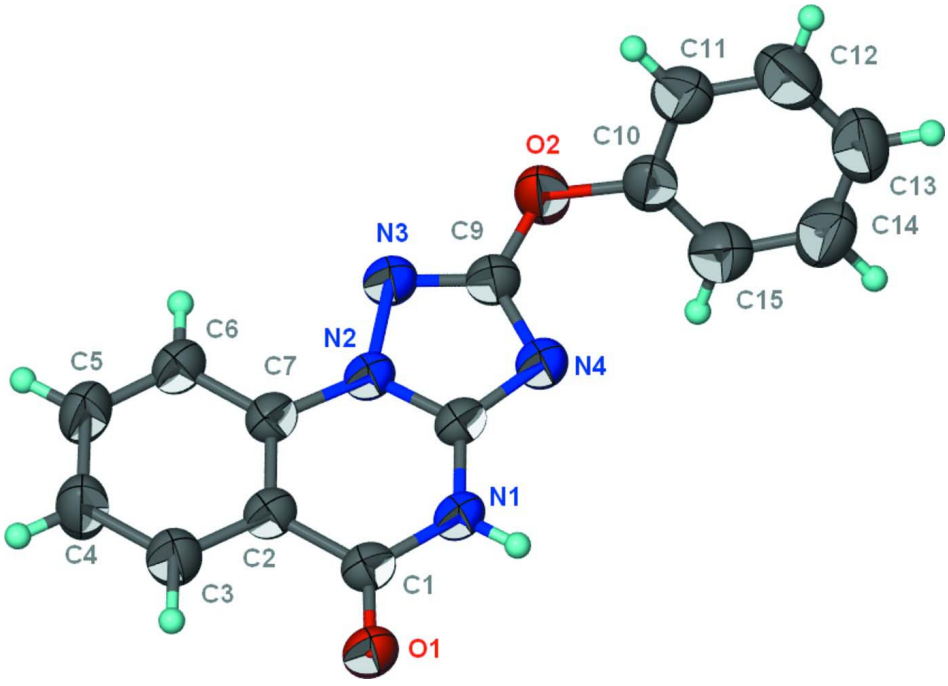

Figure 1

Anitropic displacement ellipsoid plot (Barbour, 2001) of $C_{15}H_{10}N_4O_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Phenoxy-1,2,4-triazolo[1,5-*a*]quinazolin-5(4*H*)-one

Crystal data

$C_{15}H_{10}N_4O_2$
$M_r = 278.27$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.6985$ (2) Å
$b = 8.4328$ (4) Å
$c = 13.4322$ (7) Å
$\alpha = 74.087$ (4)°
$\beta = 86.623$ (4)°
$\gamma = 89.284$ (4)°
$V = 619.66$ (5) Å^3
$Z = 2$
$F(000) = 288$
$D_x = 1.491$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 6342 reflections
$\theta = 5.5$–$76.8°$
$\mu = 0.86$ mm^{-1}
$T = 294$ K
Prism, colorless
0.30 × 0.30 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min} = 0.783$, $T_{max} = 0.919$
10219 measured reflections
2570 independent reflections
2408 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 77.0°$, $\theta_{min} = 5.5°$
$h = -7 \rightarrow 7$
$k = -10 \rightarrow 10$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.103$
$S = 1.03$
2570 reflections
194 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.101P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.99321 (13)	0.65595 (10)	0.38673 (6)	0.0434 (2)
O2	0.05541 (15)	0.63656 (11)	0.73718 (7)	0.0575 (3)
N1	0.72791 (14)	0.61117 (11)	0.52356 (7)	0.0368 (2)
H1	0.815 (2)	0.5287 (14)	0.5565 (10)	0.052 (4)*
N2	0.39197 (14)	0.77669 (10)	0.51740 (7)	0.0357 (2)
N3	0.19077 (15)	0.78851 (11)	0.57764 (7)	0.0407 (2)
N4	0.42432 (15)	0.57551 (11)	0.66105 (7)	0.0392 (2)
C1	0.80686 (17)	0.69434 (12)	0.42497 (8)	0.0357 (2)
C2	0.65586 (18)	0.82833 (13)	0.36907 (8)	0.0371 (2)
C3	0.7175 (2)	0.91440 (15)	0.26696 (9)	0.0478 (3)
H3A	0.8541	0.8874	0.2340	0.057*
C4	0.5757 (2)	1.03986 (17)	0.21472 (10)	0.0559 (3)
H4	0.6164	1.0970	0.1463	0.067*
C5	0.3716 (2)	1.08128 (15)	0.26419 (10)	0.0509 (3)
H5	0.2790	1.1674	0.2285	0.061*
C6	0.30459 (19)	0.99747 (14)	0.36443 (9)	0.0423 (3)
H6	0.1673	1.0250	0.3967	0.051*
C7	0.44778 (18)	0.86996 (13)	0.41660 (8)	0.0354 (2)
C8	0.52273 (17)	0.64985 (12)	0.56919 (8)	0.0342 (2)
C9	0.22415 (18)	0.66579 (14)	0.66014 (8)	0.0400 (2)
C10	0.0660 (2)	0.49527 (15)	0.82080 (9)	0.0453 (3)
C11	−0.1218 (2)	0.38863 (17)	0.83833 (10)	0.0524 (3)
H11	−0.2437	0.4075	0.7934	0.063*
C12	−0.1261 (3)	0.25285 (19)	0.92387 (11)	0.0621 (4)
H12	−0.2514	0.1790	0.9366	0.075*
C13	0.0546 (3)	0.22606 (19)	0.99069 (11)	0.0664 (4)
H13	0.0512	0.1346	1.0482	0.080*
C14	0.2391 (3)	0.3353 (2)	0.97164 (11)	0.0663 (4)
H14	0.3603	0.3175	1.0169	0.080*
C15	0.2473 (2)	0.47089 (19)	0.88648 (11)	0.0567 (3)
H15	0.3729	0.5445	0.8736	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0337 (4)	0.0480 (4)	0.0435 (4)	0.0121 (3)	0.0022 (3)	−0.0057 (3)
O2	0.0464 (5)	0.0600 (5)	0.0506 (5)	0.0199 (4)	0.0148 (4)	0.0065 (4)
N1	0.0287 (4)	0.0391 (5)	0.0391 (5)	0.0091 (3)	−0.0027 (3)	−0.0053 (4)
N2	0.0288 (4)	0.0379 (5)	0.0377 (5)	0.0075 (3)	−0.0014 (3)	−0.0064 (4)
N3	0.0319 (4)	0.0454 (5)	0.0410 (5)	0.0097 (4)	0.0023 (4)	−0.0066 (4)
N4	0.0330 (4)	0.0414 (5)	0.0391 (5)	0.0073 (3)	0.0000 (4)	−0.0048 (4)
C1	0.0299 (5)	0.0376 (5)	0.0387 (5)	0.0045 (4)	−0.0023 (4)	−0.0091 (4)
C2	0.0323 (5)	0.0376 (5)	0.0395 (5)	0.0055 (4)	−0.0028 (4)	−0.0076 (4)
C3	0.0434 (6)	0.0502 (6)	0.0433 (6)	0.0114 (5)	0.0036 (5)	−0.0038 (5)
C4	0.0558 (7)	0.0581 (7)	0.0420 (6)	0.0153 (6)	0.0037 (5)	0.0044 (5)
C5	0.0482 (7)	0.0486 (6)	0.0481 (7)	0.0159 (5)	−0.0059 (5)	0.0000 (5)
C6	0.0356 (5)	0.0414 (6)	0.0461 (6)	0.0098 (4)	−0.0036 (4)	−0.0058 (5)
C7	0.0313 (5)	0.0357 (5)	0.0379 (5)	0.0035 (4)	−0.0036 (4)	−0.0077 (4)
C8	0.0280 (5)	0.0360 (5)	0.0377 (5)	0.0052 (4)	−0.0042 (4)	−0.0085 (4)
C9	0.0322 (5)	0.0442 (6)	0.0401 (5)	0.0066 (4)	0.0025 (4)	−0.0069 (4)
C10	0.0416 (6)	0.0515 (6)	0.0373 (6)	0.0114 (5)	0.0062 (4)	−0.0053 (5)
C11	0.0428 (6)	0.0679 (8)	0.0431 (6)	0.0044 (5)	0.0020 (5)	−0.0104 (6)
C12	0.0593 (8)	0.0625 (8)	0.0578 (8)	−0.0047 (6)	0.0123 (6)	−0.0082 (6)
C13	0.0724 (9)	0.0666 (9)	0.0466 (7)	0.0142 (7)	0.0078 (6)	0.0043 (6)
C14	0.0580 (8)	0.0876 (11)	0.0464 (7)	0.0160 (7)	−0.0100 (6)	−0.0061 (7)
C15	0.0468 (7)	0.0675 (8)	0.0525 (7)	0.0017 (6)	−0.0024 (5)	−0.0112 (6)

Geometric parameters (Å, º)

O1—C1	1.2307 (12)	C4—C5	1.3938 (17)
O2—C9	1.3435 (13)	C4—H4	0.9300
O2—C10	1.3990 (14)	C5—C6	1.3721 (17)
N1—C8	1.3656 (13)	C5—H5	0.9300
N1—C1	1.3699 (13)	C6—C7	1.3947 (14)
N1—H1	0.878 (9)	C6—H6	0.9300
N2—C8	1.3477 (12)	C10—C15	1.3753 (18)
N2—N3	1.3824 (12)	C10—C11	1.3738 (18)
N2—C7	1.3874 (14)	C11—C12	1.3813 (19)
N3—C9	1.3139 (14)	C11—H11	0.9300
N4—C8	1.3164 (14)	C12—C13	1.382 (2)
N4—C9	1.3622 (13)	C12—H12	0.9300
C1—C2	1.4722 (14)	C13—C14	1.372 (2)
C2—C3	1.3910 (16)	C13—H13	0.9300
C2—C7	1.4000 (14)	C14—C15	1.377 (2)
C3—C4	1.3794 (17)	C14—H14	0.9300
C3—H3A	0.9300	C15—H15	0.9300
C9—O2—C10	119.95 (9)	N2—C7—C6	122.26 (10)
C8—N1—C1	122.69 (8)	N2—C7—C2	116.34 (9)
C8—N1—H1	120.6 (9)	C6—C7—C2	121.40 (10)

C1—N1—H1	116.7 (9)	N4—C8—N2	111.92 (9)
C8—N2—N3	109.16 (8)	N4—C8—N1	128.29 (9)
C8—N2—C7	123.88 (9)	N2—C8—N1	119.77 (9)
N3—N2—C7	126.79 (8)	N3—C9—O2	117.36 (9)
C9—N3—N2	100.32 (8)	N3—C9—N4	118.04 (9)
C8—N4—C9	100.54 (8)	O2—C9—N4	124.59 (10)
O1—C1—N1	120.70 (9)	C15—C10—C11	121.75 (12)
O1—C1—C2	123.08 (10)	C15—C10—O2	121.40 (12)
N1—C1—C2	116.22 (9)	C11—C10—O2	116.68 (11)
C3—C2—C7	118.94 (10)	C10—C11—C12	118.73 (12)
C3—C2—C1	120.02 (10)	C10—C11—H11	120.6
C7—C2—C1	121.04 (10)	C12—C11—H11	120.6
C4—C3—C2	119.93 (11)	C11—C12—C13	120.38 (14)
C4—C3—H3A	120.0	C11—C12—H12	119.8
C2—C3—H3A	120.0	C13—C12—H12	119.8
C3—C4—C5	120.17 (12)	C14—C13—C12	119.61 (13)
C3—C4—H4	119.9	C14—C13—H13	120.2
C5—C4—H4	119.9	C12—C13—H13	120.2
C6—C5—C4	121.30 (11)	C13—C14—C15	120.89 (13)
C6—C5—H5	119.4	C13—C14—H14	119.6
C4—C5—H5	119.4	C15—C14—H14	119.6
C5—C6—C7	118.26 (11)	C10—C15—C14	118.62 (13)
C5—C6—H6	120.9	C10—C15—H15	120.7
C7—C6—H6	120.9	C14—C15—H15	120.7

C8—N2—N3—C9	0.14 (11)	C9—N4—C8—N1	−177.91 (10)
C7—N2—N3—C9	175.59 (10)	N3—N2—C8—N4	−0.50 (12)
C8—N1—C1—O1	179.78 (9)	C7—N2—C8—N4	−176.12 (9)
C8—N1—C1—C2	−0.77 (15)	N3—N2—C8—N1	178.16 (8)
O1—C1—C2—C3	2.27 (17)	C7—N2—C8—N1	2.54 (16)
N1—C1—C2—C3	−177.17 (10)	C1—N1—C8—N4	177.01 (10)
O1—C1—C2—C7	−178.59 (10)	C1—N1—C8—N2	−1.40 (15)
N1—C1—C2—C7	1.98 (15)	N2—N3—C9—O2	−178.60 (10)
C7—C2—C3—C4	0.81 (19)	N2—N3—C9—N4	0.27 (13)
C1—C2—C3—C4	179.98 (12)	C10—O2—C9—N3	171.70 (11)
C2—C3—C4—C5	0.4 (2)	C10—O2—C9—N4	−7.09 (18)
C3—C4—C5—C6	−1.2 (2)	C8—N4—C9—N3	−0.55 (13)
C4—C5—C6—C7	0.7 (2)	C8—N4—C9—O2	178.22 (11)
C8—N2—C7—C6	178.15 (10)	C9—O2—C10—C15	63.17 (17)
N3—N2—C7—C6	3.32 (17)	C9—O2—C10—C11	−121.42 (12)
C8—N2—C7—C2	−1.29 (15)	C15—C10—C11—C12	−0.6 (2)
N3—N2—C7—C2	−176.12 (9)	O2—C10—C11—C12	−175.96 (11)
C5—C6—C7—N2	−178.86 (10)	C10—C11—C12—C13	0.5 (2)
C5—C6—C7—C2	0.55 (17)	C11—C12—C13—C14	0.0 (2)
C3—C2—C7—N2	178.15 (9)	C12—C13—C14—C15	−0.3 (2)
C1—C2—C7—N2	−1.00 (15)	C11—C10—C15—C14	0.2 (2)
C3—C2—C7—C6	−1.29 (17)	O2—C10—C15—C14	175.40 (12)
C1—C2—C7—C6	179.55 (10)	C13—C14—C15—C10	0.2 (2)

C9—N4—C8—N2	0.60 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88 (1)	1.90 (1)	2.775 (1)	174 (1)

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.