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2-Phenyl-7-(4-pyridylmethylamino)-1,2,4-triazolo[1,5-*a*][1,3,5]triazin-5(4*H*)-one[1]

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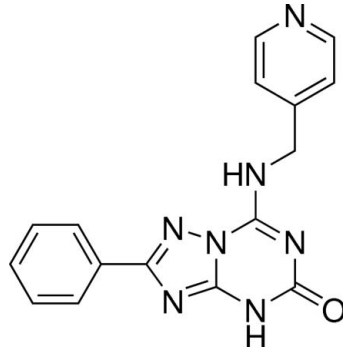
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.007 Å; R factor = 0.067; wR factor = 0.145; data-to-parameter ratio = 8.1.

In the title compound, $C_{16}H_{13}N_7O$, the 1,2,4-triazolo[1,5-*a*]-[1,3,5]triazine heterocyclic system is essentially planar (r.m.s. deviation = 0.0375 Å). The attached benzene ring lies almost in the mean plane of 1,2,4-triazolo[1,5-*a*][1,3,5]triazine [dihedral angle = 1.36 (23)°], while the pyridine ring is turned out of this plane by the aminomethyl bridge [dihedral angle = 69.22 (9)°]. The amino group H atom is involved in intramolecular hydrogen bonding with a triazole N atom. In the crystal, molecules are connected *via* C(=O)NH···N hydrogen bonds into $C(11)$ chains parallel to [100]. The amino group H atom acts as a hydrogen-bond donor, forming an NH···O=C hydrogen bond with the carbonyl O atom, which links the molecules into $C(6)$ chains running along [011] and [01$\bar{1}$].

Related literature

For review on the synthesis and biological activity of 1,2,4-triazolo[1,5-*a*][1,3,5]triazines, see: Dolzhenko *et al.* (2006). For our work on the synthesis, crystal structure studies and biological activity of 1,2,4-triazolo[1,5-*a*][1,3,5]triazine, see: Dolzhenko *et al.* (2007*a*,*b*, 2008). For graph-set analysis of hydrogen bonding, see: Bernstein *et al.* (1995). For a related structure, see: Dolzhenko *et al.* (2011).



Experimental

Crystal data

$C_{16}H_{13}N_7O$
M_r = 319.33
Orthorhombic, $Pna2_1$
a = 22.142 (8) Å
b = 11.016 (4) Å
c = 5.992 (2) Å
V = 1461.5 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 K
0.58 × 0.36 × 0.04 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.945, T_{max} = 0.996
9607 measured reflections
1830 independent reflections
1530 reflections with $I > 2\sigma(I)$
R_{int} = 0.088

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.145
S = 1.19
1830 reflections
225 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5*N*···N7^{i}	0.90 (4)	1.89 (4)	2.782 (5)	173 (4)
N6—H6*N*···O1^{ii}	0.95 (6)	1.96 (5)	2.735 (5)	137 (4)
N6—H6*N*···N1	0.95 (6)	2.31 (5)	2.813 (5)	112 (4)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2761).

[1] Fused heterocyclic systems with *s*-triazine ring. Part 17. For part 16, see Dolzhenko *et al.* (2011).
§ Thomson Reuters ResearcherID: B-1130-2008.

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supplementary materials

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2-Phenyl-7-(4-pyridylmethylamino)-1,2,4-triazolo[1,5-*a*][1,3,5]triazin-5(4*H*)-one

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Comment

The 1,2,4-triazolo[1,5-*a*]triazines are 5-azaisosters of the purine heterocyclic system that carries a bridge nitrogen atom. They have been shown to possess a variety of promising biological effects (Dolzhenko *et al.*, 2006). In continuation of our works on the synthesis and structural investigations of 1,2,4-triazolo[1,5-*a*][1,3,5]triazines (Dolzhenko *et al.*, 2007*a*,*b*; Dolzhenko *et al.*, 2008), we report herein molecular and crystal structure of 2-phenyl-7-(4-pyridylmethylamino)-1,2,4-triazolo[1,5-*a*][1,3,5]triazin-5-one, $C_{16}H_{13}N_7O$. (Fig. 1 & 2).

The 1,2,4-triazolo[1,5-*a*][1,3,5]triazine heterocyclic system is essentially planar with a r.m.s. deviation of 0.0375 Å. The phenyl ring lies practically in the plane of the 1,2,4-triazolo[1,5-*a*][1,3,5]triazine core (with a small dihedral angle of 1.36 (23)° between the mean planes). The amino group nitrogen atom N6 is located 0.2246 (50) Å above the 1,2,4-triazolo[1,5-*a*][1,3,5]triazine mean plane. The pyridine ring is turned out of this plane by twisting of the aminomethyl bridge [C3—N6—C11—C14 torsion angle is 118.50 (40)°]. This results in a dihedral angle of 69.22 (9)° between the 1,2,4-triazolo[1,5-*a*][1,3,5]triazine and pyridine mean planes. The amino group N6H hydrogen atom acts as a hydrogen donor in the NH···N intramolecular hydrogen bonding with the triazole N1 atom.

In the crystal, molecules form a three dimensional network of chains. The *C*(11) chains (Bernstein *et al.*, 1995) parallel to a [100] axis consist of the molecules linked *via* the CONH···N hydrogen bonds between the triazine N6H atom and the N7 atom of pyridine ring. The *C*(6) chains running along [011] and [01$\bar{1}$] directions are made of the molecules connected *via* the NH···O═C contacts between the N6—H amino group acting as a hydrogen donor and the carbonyl group O1 atom in the role of a hydrogen acceptor.

Experimental

7-Methylthio-2-phenyl-1,2,4-triazole[1,5-*a*][1,3,5]triazin-5-one (0.52 g, 2 mmol) was added to a solution of 4-pyridylmethylamine (0.32 g, 3 mmol) in DMF (5 ml) and the mixture was heated at 70–80°C with stirring for 6 h. After cooling, ice cold water (40 ml) was added and the product was filtered and recrystalized from methanol. Yield: 0.56 g (87%), m.p. 567 K.

Refinement

All C-bound H atoms were positioned geometrically and included in the refinement in riding-motion approximation [0.95 Å for aromatic CH and 0.99 Å for methylenic protons; $U_{iso}(H) = 1.2U_{eq}(C_{Ar})$ and $U_{iso}(H)= 1.2U_{eq}(C_{methylenic})$] while the N-bound H atoms were located in a difference map and refined freely. 1221 Friedel pairs were merged.

Figures

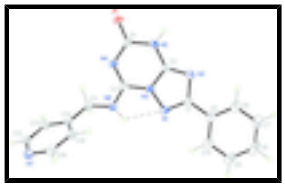

Fig. 1. The molecular structure of 2-phenyl-7-(4-pyridylmethylamino)-1,2,4-triazolo[1,5-*a*][1,3,5]triazin-5-one showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

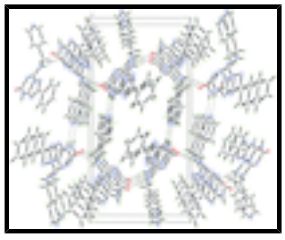

Fig. 2. Crystal packing in the cell (view along axis *c*).

2-Phenyl-7-(4-pyridylmethylamino)-1,2,4- triazolo[1,5-*a*][1,3,5]triazin-5(4*H*)-one

Crystal data

$C_{16}H_{13}N_7O$	D_x = 1.451 Mg m^{-3}
M_r = 319.33	Melting point: 567 K
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 569 reflections
a = 22.142 (8) Å	θ = 2.6–21.1°
b = 11.016 (4) Å	μ = 0.10 mm^{-1}
c = 5.992 (2) Å	*T* = 100 K
V = 1461.5 (9) Å^3	Thin plate, colourless
Z = 4	0.58 × 0.36 × 0.04 mm
F(000) = 664	

Data collection

Bruker SMART APEX CCD diffractometer	1830 independent reflections
Radiation source: fine-focus sealed tube	1530 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.088
φ and ω scans	θ_{max} = 27.5°, θ_{min} = 2.1°
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)	*h* = −25→28
T_{min} = 0.945, T_{max} = 0.996	*k* = −14→14
9607 measured reflections	*l* = −7→7

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.067$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.145$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.19$	$w = 1/[\sigma^2(F_o^2) + (0.0695P)^2 + 0.135P]$ where $P = (F_o^2 + 2F_c^2)/3$
1830 reflections	$(\Delta/\sigma)_{max} < 0.001$
225 parameters	$\Delta\rho_{max} = 0.35$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.27$ e Å^{-3}

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.

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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.83275 (13)	0.3791 (3)	0.1382 (6)	0.0251 (8)
N1	0.78903 (15)	0.0671 (3)	0.7906 (7)	0.0191 (8)
N2	0.88088 (15)	0.1634 (3)	0.7854 (7)	0.0186 (8)
N3	0.79295 (15)	0.1475 (3)	0.6125 (6)	0.0174 (8)
N4	0.76558 (15)	0.2401 (3)	0.2791 (7)	0.0187 (8)
N5	0.86084 (16)	0.2819 (3)	0.4502 (6)	0.0186 (8)
H5N	0.900 (2)	0.301 (4)	0.429 (8)	0.018 (12)*
N6	0.70697 (15)	0.0862 (3)	0.4338 (6)	0.0201 (8)
H6N	0.712 (2)	0.025 (5)	0.544 (10)	0.039 (15)*
N7	0.48227 (17)	0.1748 (3)	0.3615 (7)	0.0236 (8)
C1	0.84184 (19)	0.0814 (4)	0.8851 (8)	0.0177 (9)
C2	0.84876 (18)	0.2014 (3)	0.6159 (7)	0.0166 (9)
C3	0.75455 (18)	0.1596 (3)	0.4347 (7)	0.0175 (9)
C4	0.81929 (18)	0.3037 (4)	0.2826 (8)	0.0183 (9)
C5	0.85949 (19)	0.0149 (4)	1.0875 (7)	0.0199 (9)
C6	0.9147 (2)	0.0359 (4)	1.1868 (8)	0.0264 (10)
H6	0.9422	0.0910	1.1197	0.032*
C7	0.9305 (2)	−0.0226 (4)	1.3837 (9)	0.0329 (12)
H7	0.9687	−0.0080	1.4504	0.040*
C8	0.8899 (3)	−0.1029 (4)	1.4827 (9)	0.0358 (13)
H8	0.9001	−0.1420	1.6190	0.043*
C9	0.8347 (2)	−0.1258 (4)	1.3827 (9)	0.0317 (11)
H9	0.8075	−0.1820	1.4492	0.038*

C10	0.8187 (2)	−0.0678 (4)	1.1872 (7)	0.0241 (10)
H10	0.7806	−0.0832	1.1201	0.029*
C11	0.66773 (18)	0.0743 (4)	0.2433 (7)	0.0206 (10)
H11A	0.6682	−0.0112	0.1928	0.025*
H11B	0.6838	0.1248	0.1202	0.025*
C12	0.49957 (19)	0.1204 (4)	0.1724 (8)	0.0242 (10)
H12	0.4698	0.1032	0.0627	0.029*
C13	0.55916 (19)	0.0879 (4)	0.1287 (8)	0.0218 (10)
H13	0.5698	0.0500	−0.0082	0.026*
C14	0.60260 (19)	0.1119 (4)	0.2896 (8)	0.0187 (9)
C15	0.58514 (19)	0.1699 (4)	0.4811 (8)	0.0211 (9)
H15	0.6141	0.1894	0.5923	0.025*
C16	0.5247 (2)	0.2002 (4)	0.5120 (8)	0.0245 (10)
H16	0.5133	0.2406	0.6456	0.029*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0245 (16)	0.0180 (14)	0.0328 (19)	0.0027 (12)	0.0069 (15)	0.0101 (15)
N1	0.0230 (18)	0.0146 (17)	0.0196 (17)	−0.0022 (14)	0.0025 (17)	0.0034 (15)
N2	0.0180 (18)	0.0137 (16)	0.0240 (18)	0.0024 (13)	0.0013 (16)	−0.0026 (16)
N3	0.0192 (17)	0.0115 (16)	0.022 (2)	−0.0018 (13)	0.0019 (15)	0.0038 (15)
N4	0.0214 (18)	0.0105 (16)	0.0241 (19)	0.0029 (13)	0.0030 (16)	0.0038 (16)
N5	0.0176 (18)	0.0123 (17)	0.026 (2)	−0.0018 (13)	0.0039 (16)	0.0019 (16)
N6	0.0173 (18)	0.0153 (17)	0.028 (2)	0.0014 (13)	−0.0002 (17)	0.0088 (17)
N7	0.0244 (19)	0.0164 (17)	0.030 (2)	0.0040 (15)	0.0003 (17)	0.0025 (17)
C1	0.020 (2)	0.0154 (19)	0.018 (2)	0.0020 (16)	0.0032 (18)	−0.0025 (18)
C2	0.018 (2)	0.0092 (17)	0.023 (2)	0.0000 (15)	0.0027 (18)	−0.0024 (18)
C3	0.0169 (19)	0.0130 (19)	0.023 (2)	0.0054 (15)	0.0042 (18)	−0.0031 (18)
C4	0.020 (2)	0.0132 (19)	0.021 (2)	0.0056 (15)	0.0000 (19)	0.0011 (19)
C5	0.025 (2)	0.0156 (19)	0.019 (2)	0.0070 (17)	0.0032 (19)	−0.0046 (18)
C6	0.035 (3)	0.022 (2)	0.023 (2)	0.0087 (19)	−0.003 (2)	−0.005 (2)
C7	0.044 (3)	0.024 (2)	0.031 (3)	0.014 (2)	−0.013 (2)	−0.004 (2)
C8	0.062 (4)	0.027 (2)	0.018 (2)	0.022 (2)	−0.006 (2)	−0.002 (2)
C9	0.049 (3)	0.020 (2)	0.026 (2)	0.012 (2)	0.006 (2)	0.004 (2)
C10	0.031 (2)	0.017 (2)	0.024 (2)	0.0049 (17)	0.005 (2)	−0.002 (2)
C11	0.023 (2)	0.0137 (18)	0.025 (3)	0.0005 (17)	0.0012 (19)	−0.0021 (19)
C12	0.022 (2)	0.022 (2)	0.028 (3)	−0.0003 (18)	0.003 (2)	0.000 (2)
C13	0.024 (2)	0.016 (2)	0.025 (2)	−0.0008 (17)	−0.001 (2)	−0.0008 (19)
C14	0.023 (2)	0.0082 (17)	0.025 (2)	0.0013 (15)	0.003 (2)	0.0068 (18)
C15	0.024 (2)	0.015 (2)	0.025 (2)	−0.0018 (17)	−0.004 (2)	−0.0004 (19)
C16	0.034 (3)	0.0121 (19)	0.028 (2)	0.0022 (18)	0.003 (2)	−0.0026 (19)

Geometric parameters (Å, °)

O1—C4	1.236 (5)	C6—C7	1.389 (7)
N1—C1	1.309 (5)	C6—H6	0.9500
N1—N3	1.389 (5)	C7—C8	1.394 (8)
N2—C2	1.308 (6)	C7—H7	0.9500

N2—C1	1.386 (5)	C8—C9	1.384 (8)
N3—C3	1.370 (5)	C8—H8	0.9500
N3—C2	1.371 (5)	C9—C10	1.381 (7)
N4—C3	1.310 (5)	C9—H9	0.9500
N4—C4	1.380 (5)	C10—H10	0.9500
N5—C2	1.358 (5)	C11—C14	1.526 (6)
N5—C4	1.383 (6)	C11—H11A	0.9900
N5—H5N	0.90 (4)	C11—H11B	0.9900
N6—C3	1.328 (5)	C12—C13	1.392 (6)
N6—C11	1.441 (5)	C12—H12	0.9500
N6—H6N	0.95 (6)	C13—C14	1.387 (6)
N7—C16	1.332 (6)	C13—H13	0.9500
N7—C12	1.338 (6)	C14—C15	1.369 (7)
C1—C5	1.470 (6)	C15—C16	1.392 (6)
C5—C6	1.379 (6)	C15—H15	0.9500
C5—C10	1.415 (6)	C16—H16	0.9500
C1—N1—N3	101.5 (3)	C6—C7—H7	120.2
C2—N2—C1	101.8 (3)	C8—C7—H7	120.2
C3—N3—C2	121.9 (4)	C9—C8—C7	120.0 (5)
C3—N3—N1	128.4 (3)	C9—C8—H8	120.0
C2—N3—N1	108.7 (3)	C7—C8—H8	120.0
C3—N4—C4	119.6 (4)	C10—C9—C8	120.6 (5)
C2—N5—C4	120.9 (4)	C10—C9—H9	119.7
C2—N5—H5N	116 (3)	C8—C9—H9	119.7
C4—N5—H5N	120 (3)	C9—C10—C5	119.5 (4)
C3—N6—C11	122.5 (4)	C9—C10—H10	120.2
C3—N6—H6N	110 (3)	C5—C10—H10	120.2
C11—N6—H6N	123 (3)	N6—C11—C14	113.7 (4)
C16—N7—C12	117.7 (4)	N6—C11—H11A	108.8
N1—C1—N2	116.7 (4)	C14—C11—H11A	108.8
N1—C1—C5	122.3 (4)	N6—C11—H11B	108.8
N2—C1—C5	121.0 (4)	C14—C11—H11B	108.8
N2—C2—N5	132.0 (4)	H11A—C11—H11B	107.7
N2—C2—N3	111.3 (4)	N7—C12—C13	123.1 (4)
N5—C2—N3	116.7 (4)	N7—C12—H12	118.5
N4—C3—N6	123.9 (4)	C13—C12—H12	118.5
N4—C3—N3	120.3 (4)	C14—C13—C12	118.5 (4)
N6—C3—N3	115.9 (4)	C14—C13—H13	120.7
O1—C4—N4	122.6 (4)	C12—C13—H13	120.7
O1—C4—N5	117.7 (4)	C15—C14—C13	118.4 (4)
N4—C4—N5	119.7 (4)	C15—C14—C11	123.1 (4)
C6—C5—C10	119.5 (4)	C13—C14—C11	118.5 (4)
C6—C5—C1	120.5 (4)	C14—C15—C16	119.7 (4)
C10—C5—C1	120.0 (4)	C14—C15—H15	120.2
C5—C6—C7	120.8 (5)	C16—C15—H15	120.2
C5—C6—H6	119.6	N7—C16—C15	122.6 (4)
C7—C6—H6	119.6	N7—C16—H16	118.7
C6—C7—C8	119.6 (5)	C15—C16—H16	118.7

C1—N1—N3—C3	169.6 (4)	C2—N5—C4—N4	−2.1 (6)
C1—N1—N3—C2	0.9 (4)	N1—C1—C5—C6	−177.5 (4)
N3—N1—C1—N2	−0.4 (5)	N2—C1—C5—C6	2.2 (6)
N3—N1—C1—C5	179.3 (4)	N1—C1—C5—C10	−0.2 (6)
C2—N2—C1—N1	−0.2 (5)	N2—C1—C5—C10	179.5 (4)
C2—N2—C1—C5	−180.0 (4)	C10—C5—C6—C7	−0.3 (6)
C1—N2—C2—N5	−179.3 (4)	C1—C5—C6—C7	177.1 (4)
C1—N2—C2—N3	0.8 (4)	C5—C6—C7—C8	−0.4 (6)
C4—N5—C2—N2	177.7 (4)	C6—C7—C8—C9	1.3 (7)
C4—N5—C2—N3	−2.5 (6)	C7—C8—C9—C10	−1.4 (7)
C3—N3—C2—N2	−170.7 (3)	C8—C9—C10—C5	0.6 (7)
N1—N3—C2—N2	−1.1 (4)	C6—C5—C10—C9	0.2 (6)
C3—N3—C2—N5	9.4 (5)	C1—C5—C10—C9	−177.2 (4)
N1—N3—C2—N5	179.0 (3)	C3—N6—C11—C14	−118.5 (4)
C4—N4—C3—N6	−173.5 (4)	C16—N7—C12—C13	1.1 (6)
C4—N4—C3—N3	6.8 (5)	N7—C12—C13—C14	0.6 (7)
C11—N6—C3—N4	10.2 (6)	C12—C13—C14—C15	−2.0 (6)
C11—N6—C3—N3	−170.1 (3)	C12—C13—C14—C11	179.0 (4)
C2—N3—C3—N4	−11.9 (5)	N6—C11—C14—C15	10.2 (5)
N1—N3—C3—N4	−179.2 (4)	N6—C11—C14—C13	−170.8 (4)
C2—N3—C3—N6	168.4 (4)	C13—C14—C15—C16	1.6 (6)
N1—N3—C3—N6	1.0 (6)	C11—C14—C15—C16	−179.4 (4)
C3—N4—C4—O1	178.6 (4)	C12—N7—C16—C15	−1.5 (6)
C3—N4—C4—N5	0.0 (6)	C14—C15—C16—N7	0.1 (6)
C2—N5—C4—O1	179.1 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···N7^{i}	0.90 (4)	1.89 (4)	2.782 (5)	173 (4)
N6—H6N···O1^{ii}	0.95 (6)	1.96 (5)	2.735 (5)	137 (4)
N6—H6N···N1	0.95 (6)	2.31 (5)	2.813 (5)	112 (4)

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

Fig. 1

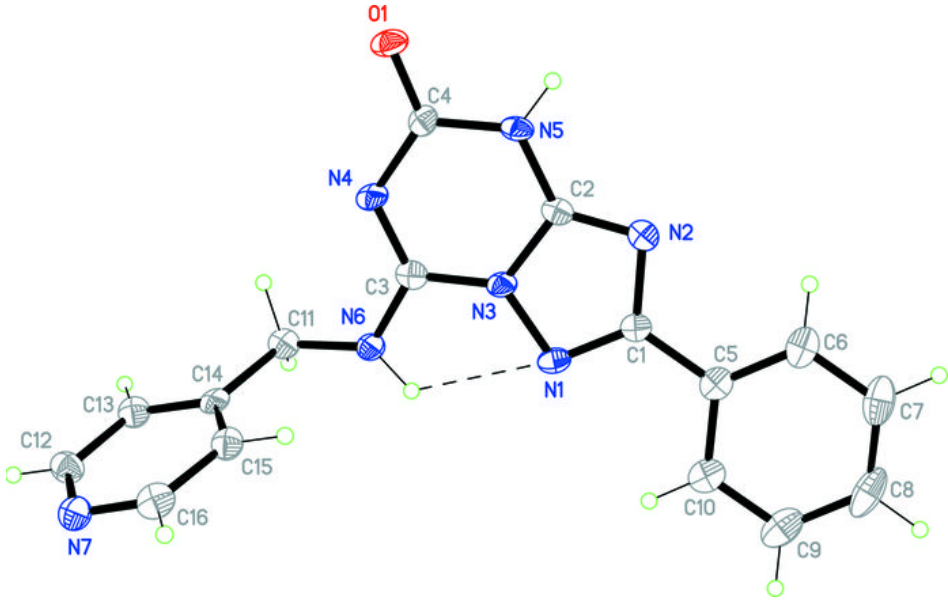
O1
C4
N5
N4
C2
N2
C3
N3
C11
N6
C1
C5
C6
C14
N1
C7
C13
C12
C15
C8
C10
C16
C9
N7

Fig. 2