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7-Amino-1,3-dimethyl-5-(4-nitrophenyl)-2,4-dioxo-1,2,3,4-tetrahydropyrido-[2,3-*d*]pyrimidine-6-carbonitrile

Jie-Xing Zhou, Li-Hui Niu, Xiao-Yue Li and Da-Qing Shi*

Department of Chemistry, Xuzhou Normal University, Xuzhou 221116, People's Republic of China
Correspondence e-mail: dqshi@263.net

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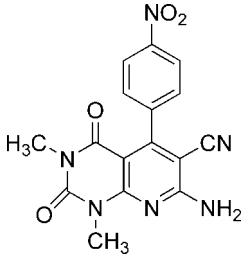
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.122; data-to-parameter ratio = 14.6.

The title compound, $C_{16}H_{12}N_6O_4$, was synthesized by the reaction of 6-amino-1,3-dimethylpyrimidine-2,4(1*H*,3*H*)-dione and 4-nitrobenzaldehyde with malononitrile in water in the presence of triethylbenzylammonium chloride at 363 K. X-ray analysis reveals that the pyrimidine ring adopts a flattened envelope conformation. The dihedral angle between the pyridine and benzene rings is 81.83 (3)°. Molecules are linked by N—H···O, C—H···O and C—H···N hydrogen bonds, forming a three-dimensional network.

Related literature

For general background, see: Bhuyan *et al.* (1999); Clercq (1986); Gangjee *et al.* (1999); Griengl *et al.* (1987); Hirota *et al.* (1981); Jones *et al.* (1979); Nasr & Gineinah (2002); Pontikis & Monneret (1994); Sasaki *et al.* (1980).



Experimental

Crystal data

$C_{16}H_{12}N_6O_4$
M_r = 352.32
Monoclinic, $P2_1/n$
a = 9.6209 (9) Å
b = 11.7064 (12) Å
c = 14.5493 (16) Å
β = 106.939 (3)°
V = 1567.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 193 (2) K
0.60 × 0.40 × 0.32 mm

Data collection

Rigaku Mercury diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.936, T_{max} = 0.965
17123 measured reflections
3595 independent reflections
3259 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.122
S = 1.11
3595 reflections
246 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5A···O1^{i}	0.84 (2)	2.06 (2)	2.8912 (15)	171 (2)
N5—H5B···O1^{ii}	0.96 (2)	2.53 (2)	3.4463 (17)	160 (2)
C9—H9···O2^{iii}	0.95	2.52	3.4275 (16)	160
C10—H10···N4^{iv}	0.95	2.58	3.5275 (18)	174
C13—H13···O3^{i}	0.95	2.60	3.4547 (17)	151
C15—H15C···O4^{v}	0.98	2.52	3.464 (2)	162

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2368).

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supplementary materials

Acta Cryst. (2007). E**63**, o2667 [**doi:10.1107/S1600536807019356**]

7-Amino-1,3-dimethyl-5-(4-nitrophenyl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-*d*]pyrimidine-6-carbonitrile

J.-X. Zhou, L.-H. Niu, X.-Y. Li and D.-Q. Shi

Comment

The importance of uracil and its annelated derivatives is well recognized in synthetic (Sasaki *et al.*, 1980; Bhuyan *et al.*, 1999) as well as biological (Griengl *et al.*, 1987; Pontikis *et al.*, 1994) chemistry. With the development of clinically useful anticancer and antiviral drugs (Clercq *et al.*, 1986; Jones *et al.*, 1979), there has recently been remarkable interest in the synthetic manipulations of uracils (Hirota *et al.*, 1981). Pyrido[2,3-d]pyrimidines represent a heterocyclic ring system of considerable interest because of several biological activities associated with this scaffold. Some analogues have been found to act as anticancer agents inhibiting dihydrofolate reductases or tyrosine kinases (Gangjee *et al.*, 1999), while others are known antiviral agents (Nasr *et al.*, 2002). We report here the crystal structure of the title compound, (I).

The pyrimidine ring adopts a flattened envelope conformation, with atom C6 deviating from the C1/C2/C7/N2/N3 plane by 0.144 (2) Å (Fig. 1). The dihedral angle between the C1—C5/N1 and C1/C2/C7/N2/N3 planes is 0.56 (7)°. The dihedral angle between the pyridine and benzene rings is 81.83 (3)°. The nitro group is coplanar with the attached benzene ring.

In the crystal structure, the molecules are linked to form a three-dimensional network (Fig. 2) by N—H···O, C—H···O and C—H···N type hydrogen bonds (Table 1).

Experimental

Compound (I) was prepared by the reaction of 6-amino-1,3-dimethylpyrimidine-2,4(1*H*,3H)-dione (2 mmol) and 4-nitrobenzaldehyde (2 mmol) with malononitrile (2 mmol) in water (10 ml) in the presence of triethylbenzylammonium chloride (0.15 g) at 363 K. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Refinement

Amino H atoms were located in a difference map and refined freely. C-bound H atoms were placed in calculated positions, with C—H = 0.95 or 0.98 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2-1.5(methyl)U_{eq}(C).

Figures

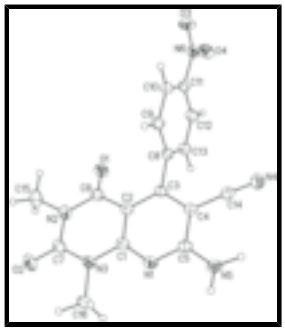

Fig. 1. The molecular structure of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme.

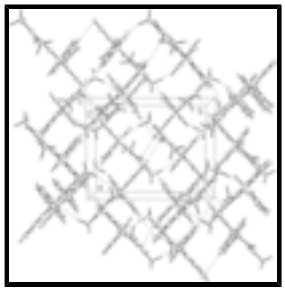

Fig. 2. The crystal packing of (I). Hydrogen bonds are shown as dashed lines.

7-Amino-1,3-dimethyl-5-(4-nitrophenyl)-2,4-dioxo-1,2,3,4- tetrahydropyrido[2,3-*d*]pyrimidine-6-carbonitrile

Crystal data

$C_{16}H_{12}N_6O_4$	F_{000} = 728
M_r = 352.32	D_x = 1.493 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71070 Å
Hall symbol: -P 2yn	Cell parameters from 6117 reflections
a = 9.6209 (9) Å	θ = 3.1–27.5º
b = 11.7064 (12) Å	μ = 0.11 mm^{-1}
c = 14.5493 (16) Å	T = 193 (2) K
β = 106.939 (3)º	Block, gold
V = 1567.5 (3) Å^3	0.60 × 0.40 × 0.32 mm
Z = 4	

Data collection

Rigaku Mercury diffractometer	3595 independent reflections
Radiation source: fine-focus sealed tube	3259 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 193(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.4º
Absorption correction: multi-scan (Jacobson, 1998)	h = −12→10
T_{min} = 0.936, T_{max} = 0.965	k = −15→14

17123 measured reflections

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.122$

$S = 1.11$

3595 reflections

246 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 0.3577P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.24$ e Å^{-3}

$\Delta\rho_{min} = -0.25$ e Å^{-3}

Extinction correction: none

Special details

Experimental. ^{1}H NMR (DMSO-d_6, δ): 3.08 (3*H*, s, CH_3), 3.51 (3*H*, s, CH_3), 7.57 (2*H*, d, J = 8.8 Hz, ArH), 8.02 (2*H*, s, NH_2), 8.32 (2*H*, d, J = 8.8 Hz, ArH).

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.40040 (11)	0.58289 (9)	0.61943 (7)	0.0371 (3)
O2	0.27711 (11)	0.53458 (9)	0.89364 (8)	0.0408 (3)
O3	0.40782 (12)	0.88345 (11)	0.25427 (7)	0.0449 (3)
O4	0.58170 (12)	0.76386 (10)	0.26221 (7)	0.0434 (3)
N1	0.62792 (11)	0.80081 (9)	0.90036 (7)	0.0271 (2)
N2	0.32494 (12)	0.57102 (9)	0.75276 (8)	0.0297 (3)
N3	0.45263 (12)	0.66590 (10)	0.89615 (7)	0.0293 (3)
N4	0.86032 (13)	0.96383 (11)	0.68190 (8)	0.0362 (3)
N5	0.81041 (13)	0.93043 (10)	0.91201 (8)	0.0324 (3)
N6	0.50203 (12)	0.81687 (10)	0.29905 (8)	0.0314 (3)
C1	0.53176 (13)	0.72749 (11)	0.84755 (9)	0.0254 (3)
C2	0.50682 (13)	0.70913 (11)	0.74838 (9)	0.0250 (3)

C3	0.58756 (13)	0.77512 (10)	0.70202 (8)	0.0232 (3)
C4	0.69181 (13)	0.84923 (10)	0.75676 (8)	0.0252 (3)
C5	0.71081 (13)	0.85990 (11)	0.85729 (8)	0.0255 (3)
C6	0.40912 (14)	0.61853 (11)	0.70021 (9)	0.0273 (3)
C7	0.34766 (14)	0.58771 (12)	0.85086 (10)	0.0306 (3)
C8	0.56079 (13)	0.77645 (10)	0.59552 (8)	0.0233 (3)
C9	0.44885 (14)	0.84520 (11)	0.54105 (9)	0.0276 (3)
H9	0.3861	0.8832	0.5708	0.033*
C10	0.42892 (14)	0.85827 (11)	0.44323 (9)	0.0279 (3)
H10	0.3536	0.9057	0.4055	0.033*
C11	0.52071 (14)	0.80098 (11)	0.40213 (8)	0.0260 (3)
C12	0.63132 (14)	0.73093 (11)	0.45431 (9)	0.0291 (3)
H12	0.6916	0.6912	0.4236	0.035*
C13	0.65246 (14)	0.71979 (11)	0.55214 (9)	0.0277 (3)
H13	0.7293	0.6736	0.5896	0.033*
C14	0.78334 (13)	0.91355 (11)	0.71367 (9)	0.0267 (3)
C15	0.21570 (17)	0.48538 (13)	0.70592 (12)	0.0409 (4)
H15A	0.1877	0.4965	0.6362	0.061*
H15B	0.1299	0.4938	0.7288	0.061*
H15C	0.2565	0.4087	0.7216	0.061*
C16	0.48811 (17)	0.67789 (15)	1.00141 (10)	0.0394 (3)
H16A	0.4223	0.6301	1.0251	0.059*
H16B	0.4769	0.7579	1.0177	0.059*
H16C	0.5887	0.6537	1.0313	0.059*
H5A	0.8264 (18)	0.9259 (15)	0.9718 (13)	0.038 (4)*
H5B	0.877 (2)	0.9721 (17)	0.8866 (14)	0.056 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0469 (6)	0.0400 (6)	0.0246 (5)	−0.0109 (4)	0.0107 (4)	−0.0044 (4)
O2	0.0414 (6)	0.0428 (6)	0.0466 (6)	−0.0009 (5)	0.0259 (5)	0.0087 (5)
O3	0.0447 (6)	0.0592 (7)	0.0266 (5)	0.0033 (5)	0.0037 (4)	0.0130 (5)
O4	0.0593 (7)	0.0475 (6)	0.0273 (5)	−0.0024 (5)	0.0185 (5)	−0.0043 (4)
N1	0.0302 (6)	0.0302 (6)	0.0209 (5)	0.0041 (4)	0.0072 (4)	0.0007 (4)
N2	0.0285 (6)	0.0288 (6)	0.0345 (6)	−0.0009 (4)	0.0135 (5)	−0.0006 (4)
N3	0.0314 (6)	0.0353 (6)	0.0244 (5)	0.0033 (4)	0.0132 (4)	0.0039 (4)
N4	0.0368 (6)	0.0375 (7)	0.0351 (6)	−0.0069 (5)	0.0116 (5)	−0.0008 (5)
N5	0.0383 (6)	0.0349 (6)	0.0211 (5)	−0.0030 (5)	0.0040 (5)	−0.0015 (5)
N6	0.0360 (6)	0.0352 (6)	0.0225 (5)	−0.0102 (5)	0.0077 (4)	0.0001 (4)
C1	0.0266 (6)	0.0273 (6)	0.0241 (6)	0.0063 (5)	0.0100 (5)	0.0037 (5)
C2	0.0271 (6)	0.0254 (6)	0.0231 (6)	0.0026 (5)	0.0084 (5)	0.0017 (5)
C3	0.0251 (6)	0.0236 (6)	0.0208 (5)	0.0047 (4)	0.0064 (4)	0.0017 (4)
C4	0.0283 (6)	0.0249 (6)	0.0224 (6)	0.0027 (5)	0.0072 (5)	0.0015 (5)
C5	0.0274 (6)	0.0254 (6)	0.0226 (6)	0.0062 (5)	0.0054 (5)	0.0012 (4)
C6	0.0272 (6)	0.0284 (6)	0.0264 (6)	0.0019 (5)	0.0079 (5)	0.0035 (5)
C7	0.0288 (7)	0.0318 (7)	0.0358 (7)	0.0060 (5)	0.0164 (5)	0.0048 (5)
C8	0.0262 (6)	0.0229 (6)	0.0205 (6)	−0.0030 (4)	0.0065 (4)	0.0009 (4)

C9	0.0287 (6)	0.0297 (6)	0.0252 (6)	0.0025 (5)	0.0091 (5)	0.0011 (5)
C10	0.0274 (6)	0.0291 (6)	0.0249 (6)	0.0010 (5)	0.0041 (5)	0.0046 (5)
C11	0.0294 (6)	0.0286 (6)	0.0194 (5)	−0.0078 (5)	0.0060 (5)	0.0007 (5)
C12	0.0320 (7)	0.0317 (7)	0.0256 (6)	0.0011 (5)	0.0116 (5)	−0.0016 (5)
C13	0.0297 (6)	0.0282 (6)	0.0248 (6)	0.0041 (5)	0.0074 (5)	0.0025 (5)
C14	0.0281 (6)	0.0264 (6)	0.0234 (6)	0.0009 (5)	0.0042 (5)	−0.0015 (5)
C15	0.0391 (8)	0.0370 (8)	0.0514 (9)	−0.0099 (6)	0.0205 (7)	−0.0088 (6)
C16	0.0392 (8)	0.0573 (9)	0.0248 (6)	0.0031 (7)	0.0139 (6)	0.0078 (6)

Geometric parameters (Å, °)

O1—C6	1.2267 (16)	C3—C4	1.3883 (17)
O2—C7	1.2169 (16)	C3—C8	1.4950 (16)
O3—N6	1.2285 (16)	C4—C5	1.4257 (16)
O4—N6	1.2245 (15)	C4—C14	1.4343 (17)
N1—C1	1.3300 (17)	C8—C9	1.3922 (17)
N1—C5	1.3411 (17)	C8—C13	1.3930 (17)
N2—C6	1.3823 (16)	C9—C10	1.3881 (17)
N2—C7	1.3933 (17)	C9—H9	0.95
N2—C15	1.4686 (18)	C10—C11	1.3766 (18)
N3—C7	1.3799 (18)	C10—H10	0.95
N3—C1	1.3830 (16)	C11—C12	1.3822 (18)
N3—C16	1.4755 (17)	C12—C13	1.3841 (17)
N4—C14	1.1437 (17)	C12—H12	0.95
N5—C5	1.3376 (17)	C13—H13	0.95
N5—H5A	0.84 (2)	C15—H15A	0.98
N5—H5B	0.96 (2)	C15—H15B	0.98
N6—C11	1.4694 (15)	C15—H15C	0.98
C1—C2	1.4085 (17)	C16—H16A	0.98
C2—C3	1.4001 (17)	C16—H16B	0.98
C2—C6	1.4546 (18)	C16—H16C	0.98
C1—N1—C5	118.12 (10)	N3—C7—N2	117.17 (11)
C6—N2—C7	124.61 (11)	C9—C8—C13	120.28 (11)
C6—N2—C15	118.25 (11)	C9—C8—C3	117.85 (11)
C7—N2—C15	116.65 (11)	C13—C8—C3	121.60 (11)
C7—N3—C1	122.48 (11)	C10—C9—C8	120.02 (12)
C7—N3—C16	118.33 (11)	C10—C9—H9	120.0
C1—N3—C16	119.06 (11)	C8—C9—H9	120.0
C5—N5—H5A	117.4 (12)	C11—C10—C9	118.50 (11)
C5—N5—H5B	121.8 (12)	C11—C10—H10	120.7
H5A—N5—H5B	119.3 (17)	C9—C10—H10	120.7
O4—N6—O3	123.27 (11)	C10—C11—C12	122.63 (11)
O4—N6—C11	118.46 (11)	C10—C11—N6	118.58 (11)
O3—N6—C11	118.27 (11)	C12—C11—N6	118.78 (11)
N1—C1—N3	115.79 (11)	C11—C12—C13	118.66 (11)
N1—C1—C2	124.92 (11)	C11—C12—H12	120.7
N3—C1—C2	119.30 (12)	C13—C12—H12	120.7
C3—C2—C1	117.16 (11)	C12—C13—C8	119.89 (11)
C3—C2—C6	122.79 (11)	C12—C13—H13	120.1

C1—C2—C6	119.88 (11)	C8—C13—H13	120.1
C4—C3—C2	118.55 (11)	N4—C14—C4	177.66 (14)
C4—C3—C8	117.74 (10)	N2—C15—H15A	109.5
C2—C3—C8	123.56 (11)	N2—C15—H15B	109.5
C3—C4—C5	119.90 (11)	H15A—C15—H15B	109.5
C3—C4—C14	120.69 (11)	N2—C15—H15C	109.5
C5—C4—C14	119.40 (11)	H15A—C15—H15C	109.5
N5—C5—N1	117.43 (11)	H15B—C15—H15C	109.5
N5—C5—C4	121.35 (12)	N3—C16—H16A	109.5
N1—C5—C4	121.21 (11)	N3—C16—H16B	109.5
O1—C6—N2	120.37 (12)	H16A—C16—H16B	109.5
O1—C6—C2	124.32 (11)	N3—C16—H16C	109.5
N2—C6—C2	115.30 (11)	H16A—C16—H16C	109.5
O2—C7—N3	122.31 (13)	H16B—C16—H16C	109.5
O2—C7—N2	120.52 (13)		
C5—N1—C1—N3	177.84 (10)	C1—C2—C6—O1	−166.42 (12)
C5—N1—C1—C2	−1.95 (18)	C3—C2—C6—N2	−172.61 (11)
C7—N3—C1—N1	179.16 (11)	C1—C2—C6—N2	12.36 (17)
C16—N3—C1—N1	−5.18 (17)	C1—N3—C7—O2	−179.17 (12)
C7—N3—C1—C2	−1.03 (18)	C16—N3—C7—O2	5.15 (19)
C16—N3—C1—C2	174.63 (11)	C1—N3—C7—N2	1.01 (18)
N1—C1—C2—C3	−1.43 (18)	C16—N3—C7—N2	−174.68 (11)
N3—C1—C2—C3	178.78 (10)	C6—N2—C7—O2	−173.21 (12)
N1—C1—C2—C6	173.87 (11)	C15—N2—C7—O2	−1.41 (19)
N3—C1—C2—C6	−5.92 (18)	C6—N2—C7—N3	6.62 (19)
C1—C2—C3—C4	3.48 (17)	C15—N2—C7—N3	178.41 (11)
C6—C2—C3—C4	−171.68 (11)	C4—C3—C8—C9	−94.22 (14)
C1—C2—C3—C8	−172.06 (11)	C2—C3—C8—C9	81.35 (15)
C6—C2—C3—C8	12.79 (18)	C4—C3—C8—C13	79.81 (15)
C2—C3—C4—C5	−2.33 (17)	C2—C3—C8—C13	−104.62 (15)
C8—C3—C4—C5	173.46 (10)	C13—C8—C9—C10	−0.53 (19)
C2—C3—C4—C14	176.22 (11)	C3—C8—C9—C10	173.59 (11)
C8—C3—C4—C14	−7.98 (17)	C8—C9—C10—C11	0.76 (19)
C1—N1—C5—N5	−177.77 (11)	C9—C10—C11—C12	0.19 (19)
C1—N1—C5—C4	3.20 (17)	C9—C10—C11—N6	−178.55 (11)
C3—C4—C5—N5	179.91 (11)	O4—N6—C11—C10	−178.40 (11)
C14—C4—C5—N5	1.34 (18)	O3—N6—C11—C10	2.14 (17)
C3—C4—C5—N1	−1.10 (18)	O4—N6—C11—C12	2.81 (18)
C14—C4—C5—N1	−179.67 (11)	O3—N6—C11—C12	−176.64 (12)
C7—N2—C6—O1	165.81 (12)	C10—C11—C12—C13	−1.3 (2)
C15—N2—C6—O1	−5.87 (19)	N6—C11—C12—C13	177.39 (11)
C7—N2—C6—C2	−13.03 (18)	C11—C12—C13—C8	1.55 (19)
C15—N2—C6—C2	175.30 (11)	C9—C8—C13—C12	−0.64 (19)
C3—C2—C6—O1	8.6 (2)	C3—C8—C13—C12	−174.53 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5A···O1^{i}	0.84 (2)	2.06 (2)	2.8912 (15)	171 (2)

N5—H5B···O1^{ii}	0.96 (2)	2.53 (2)	3.4463 (17)	160 (2)
C9—H9···O2^{iii}	0.95	2.52	3.4275 (16)	160
C10—H10···N4^{iv}	0.95	2.58	3.5275 (18)	174
C13—H13···O3^{i}	0.95	2.60	3.4547 (17)	151
C15—H15C···O4^{v}	0.98	2.52	3.464 (2)	162

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

Fig. 1

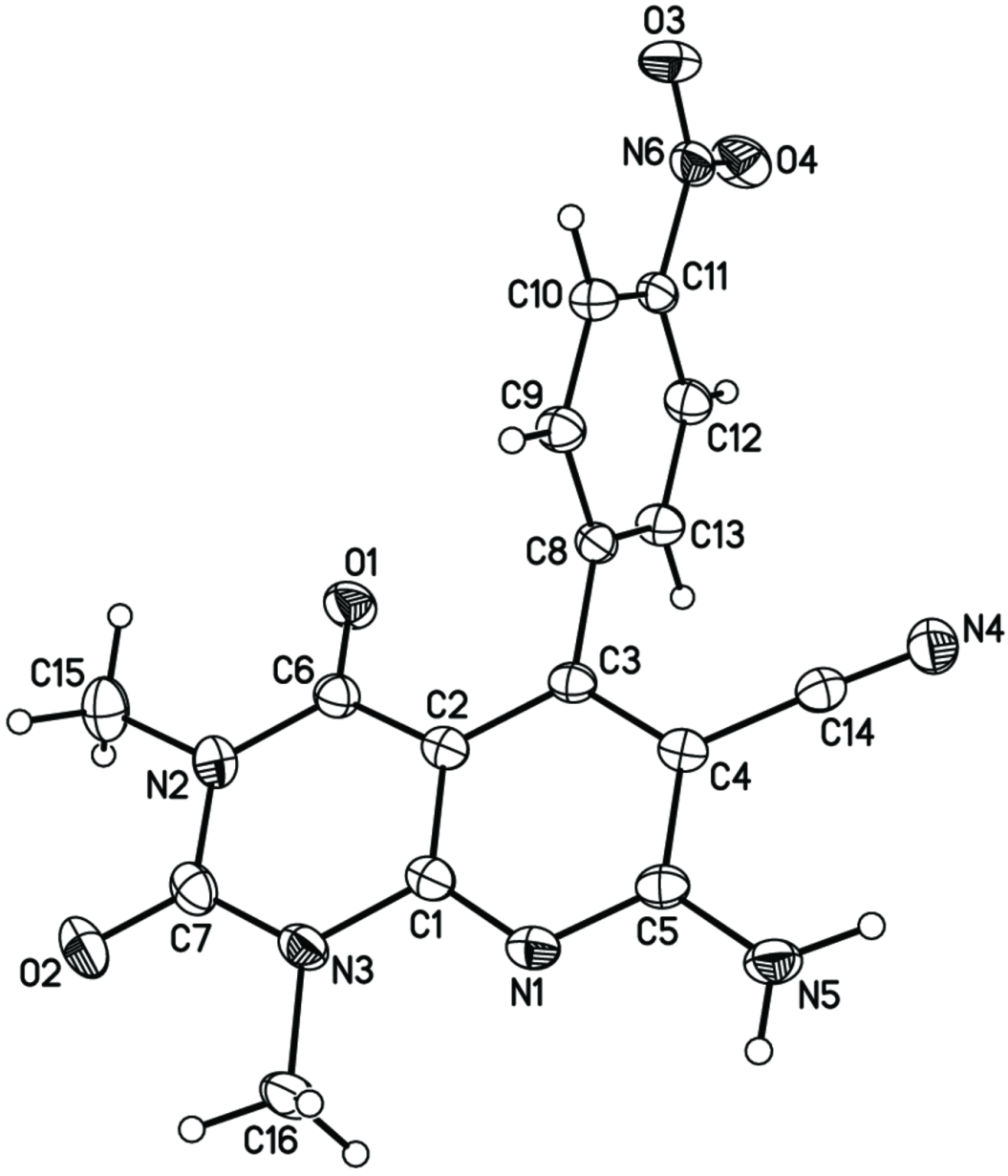
O3
N6
O4
C10
C11
C9
C12
C8
C13
O1
C15
C6
C3
N4
C2
C14
N2
C4
C7
C1
C5
O2
N3
N1
N5
C16

Fig. 2