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N-(2,5-Dimethoxyphenyl)-6-nitroquinazolin-4-amine

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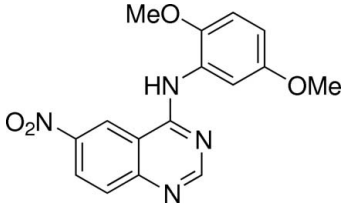
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.120; data-to-parameter ratio = 12.5.

In the title molecule, $C_{16}H_{14}N_4O_4$, the quinazoline ring is substantially planar (r.m.s. deviation = 0.0129 Å) and forms a dihedral angle of 2.73 (8)° with the benzene ring. The conformation of the molecule is stabilized by an intramolecular C—H···N hydrogen bond. In the crystal, molecules are linked into chains running parallel to the b axis by C—H···O hydrogen bonds. In addition, π–π stacking is observed between dimethoxy-substituted and nitro-substituted benzene rings, with centroid–centroid distances in the range 3.6438 (10)–3.7148 (10) Å.

Related literature

For the biological activity of quinazoline derivatives, see: Arfan *et al.* (2008); Sheng-Li *et al.* (2005); Kung *et al.* (1999); Ram *et al.* (1990); Misra *et al.* (1981); Hess *et al.* (1968). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{16}H_{14}N_4O_4$
M_r = 326.31
Triclinic, $P\overline{1}$
a = 7.2440 (7) Å
b = 10.2832 (10) Å
c = 11.1622 (11) Å
α = 72.475 (2)°
β = 83.663 (2)°
γ = 70.429 (2)°
V = 747.05 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 K
0.29 × 0.19 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.970, T_{max} = 0.984
8510 measured reflections
2792 independent reflections
2249 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.120
S = 1.05
2792 reflections
224 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···N2	0.93	2.22	2.833 (2)	123
C8—H8A···O3^{i}	0.93	2.60	3.490 (2)	161

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5029).

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supplementary materials

Acta Cryst. (2013). E**69**, o8 [doi:10.1107/S1600536812048878]

N-(2,5-Dimethoxyphenyl)-6-nitroquinazolin-4-amine

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Comment

Quinazoline derivatives are the aromatic bicyclic compounds obtained upon the fusion of benzene and pyrimidine rings. Quinazoline analogs are found to be biologically active rendering a variety of therapeutic effects such as anti-inflammatory (Misra *et al.*, 1981), anticancer (Sheng-Li *et al.*, 2005), antihypertensive (Hess *et al.*, 1968), antibacterial (Kung *et al.*, 1999), leishmanicidal (Ram *et al.*, 1990) and antimicrobial (Arfan *et al.*, 2008) activities. The title compound is a quiazoline derivative synthesized as a part of our ongoing project in order to evaluate the biological potential of new derivatives of this important class of organic compounds.

The molecule of the title compound (Fig. 1) is composed of a phenyl (C1–C6) and a nearly planar quinazoline ring (N2–N3/C7–C14; r.m.s. deviation 0.0129 Å) linked through a C6—N1—C7 amino linkage. The bond lengths (Allen *et al.*, 1987) and angles were found to be in normal range. The molecular conformation is stabilized by an intramolecular C5—H5A···N2 hydrogen bond (Table 1). In the crystal, molecules form chains by intermolecular C8—H8A···O3 interactions (symmetry codes as in Table 1, Fig. 2) running parallel to the *b* axis. The crystal structure is further strengthened by significant π–π stackings: *Cg*(1)···*Cg*(2)^{i}, 3.7148 (10) Å; *Cg*(1)···*Cg*(3)^{i}, 3.7099 (10) Å; *Cg*(1)··· *Cg*(3)^{ii}, 3.6438 (10) Å; *Cg*(1), *Cg*(2) and *Cg*(3) are the centroids of the C1–C6, N2/C7/C11/C9/N3/C8 and C9–C14 rings, respectively; symmetry codes: (i) 1-x, 2-y, -z; (ii) -x, 2-y, -z.

Experimental

A mixture of (*E*)-*N*′-(2-cyano-4-nitrophenyl)-*N*,*N*-dimethylformimidamide (0.436 g, 2 mmol) and 2,5-dimethoxyaniline (0.35 g, 2 mmol) was refluxed in acetic acid (12 ml) at 75 °C for 2 h. Progress of the reaction was monitored by thin layer chromatography. After completion of the reaction, the mixture was cooled to room temperature and neutralized by adding a saturated aqueous solution of sodium bicarbonate until the evolution of CO_2 gas ceased. The reaction mixture yielded brown crystals on standing at room temperature, which were filtered and washed with water. The crystals were re-grown using ethanol and collected in 50.2% yield (0.3273 g). All chemicals were purchased by sigma Aldrich Germany.

Refinement

H atoms on aromatic rings and methyl carbons were positioned geomatrically with 0.93–0.96 Å and constrained to ride on their parent atoms with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(C) for methyl H atoms. The H atoms of the nitrogen atom (N–H = 0.868 (19) Å) was located in a difference Fourier map and refined isotropically. A rotating group model was applied to the methyl groups.

Computing details

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* (Bruker, 2000); 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 (Sheldrick, 2008), *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

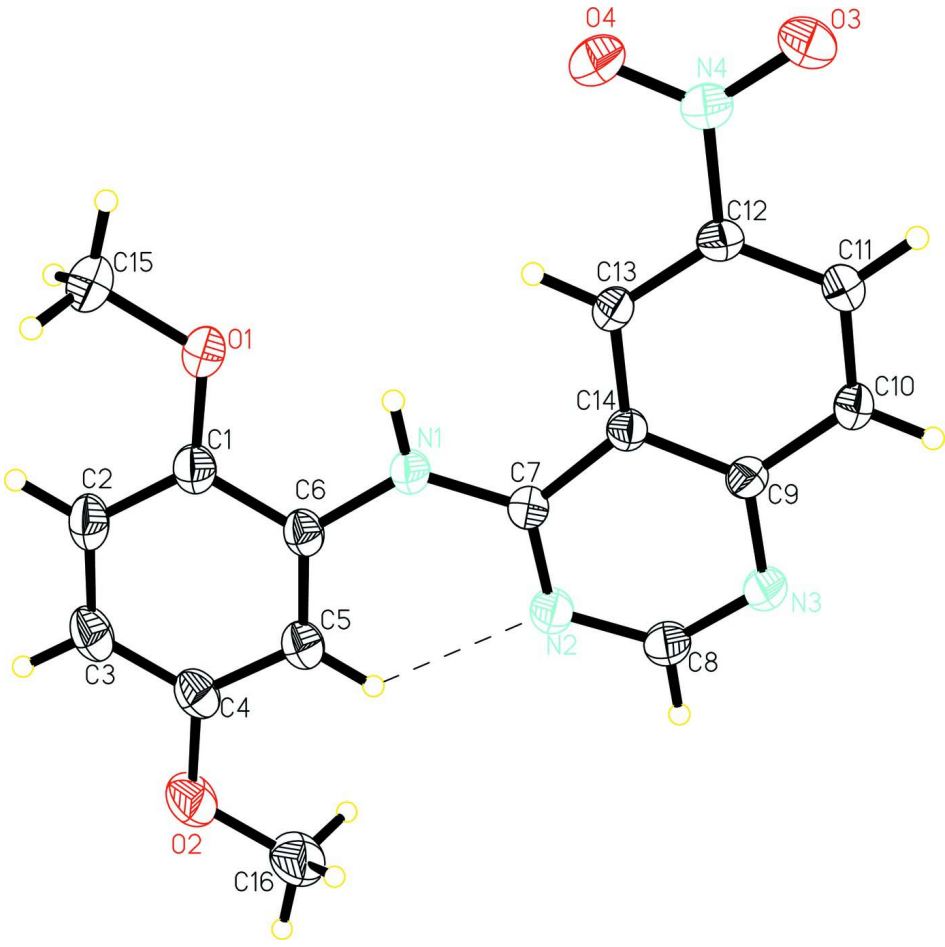

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level. An intramolecular hydrogen bond is shown as a dashed line.

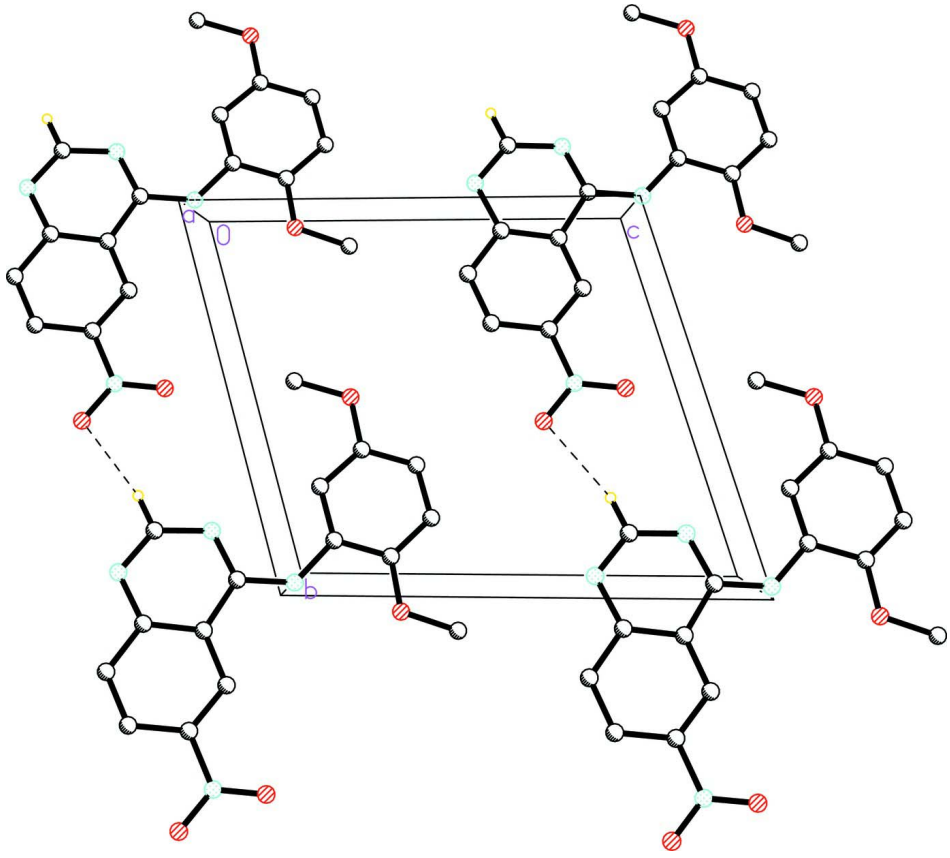

Figure 2

The crystal packing of the title compound. Only hydrogen atoms involved in hydrogen bonding (dashed lines) are shown.

N-(2,5-Dimethoxyphenyl)-6-nitroquinazolin-4-amine

Crystal data

$C_{16}H_{14}N_4O_4$
$M_r = 326.31$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.2440\ (7)$ Å
$b = 10.2832\ (10)$ Å
$c = 11.1622\ (11)$ Å
$\alpha = 72.475\ (2)°$
$\beta = 83.663\ (2)°$
$\gamma = 70.429\ (2)°$
$V = 747.05\ (13)$ Å^3
$Z = 2$
$F(000) = 340$
$D_x = 1.451$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2914 reflections
$\theta = 2.2–28.2°$
$\mu = 0.11$ mm^{-1}
$T = 298$ K
Block, brown
0.29 × 0.19 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.970$, $T_{max} = 0.984$
8510 measured reflections
2792 independent reflections
2249 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.9°$
$h = -8\rightarrow8$
$k = -12\rightarrow12$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.120$
$S = 1.05$
2792 reflections
224 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 0.1096P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.012 (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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.32912 (17)	0.94268 (12)	−0.22927 (10)	0.0562 (3)
O2	0.3236 (2)	1.48679 (13)	−0.24856 (12)	0.0691 (4)
O3	0.1791 (2)	0.42539 (13)	0.34841 (13)	0.0830 (5)
O4	0.2239 (2)	0.50964 (14)	0.15126 (12)	0.0760 (4)
N1	0.25382 (19)	1.01670 (14)	−0.02167 (11)	0.0433 (3)
H1A	0.271 (2)	0.936 (2)	−0.0378 (16)	0.057 (5)*
N2	0.1798 (2)	1.14710 (13)	0.12319 (12)	0.0509 (4)
N3	0.1201 (2)	1.04595 (13)	0.34070 (12)	0.0490 (3)
N4	0.1950 (2)	0.52243 (14)	0.25729 (13)	0.0527 (4)
C1	0.3302 (2)	1.07924 (17)	−0.23984 (14)	0.0458 (4)
C2	0.3659 (2)	1.1756 (2)	−0.34973 (15)	0.0538 (4)
H2B	0.3923	1.1489	−0.4239	0.065*
C3	0.3625 (2)	1.31047 (19)	−0.35023 (15)	0.0553 (4)
H3B	0.3870	1.3742	−0.4244	0.066*
C4	0.3231 (2)	1.35085 (17)	−0.24107 (15)	0.0498 (4)
C5	0.2860 (2)	1.25646 (16)	−0.12990 (15)	0.0470 (4)
H5A	0.2590	1.2843	−0.0563	0.056*
C6	0.2894 (2)	1.12074 (16)	−0.12903 (13)	0.0413 (3)
C7	0.2062 (2)	1.02516 (15)	0.09734 (13)	0.0383 (3)
C8	0.1392 (3)	1.14894 (17)	0.24328 (15)	0.0543 (4)
H8A	0.1223	1.2361	0.2589	0.065*
C9	0.1398 (2)	0.91960 (15)	0.31559 (13)	0.0388 (3)
C10	0.1148 (2)	0.80460 (16)	0.41591 (14)	0.0444 (4)
H10A	0.0859	0.8167	0.4959	0.053*

C11	0.1322 (2)	0.67639 (16)	0.39744 (14)	0.0440 (4)
H11A	0.1156	0.6007	0.4638	0.053*
C12	0.1754 (2)	0.66082 (14)	0.27654 (14)	0.0399 (3)
C13	0.2004 (2)	0.76883 (15)	0.17581 (13)	0.0388 (3)
H13A	0.2281	0.7546	0.0965	0.047*
C14	0.18346 (19)	0.90156 (14)	0.19406 (13)	0.0358 (3)
C15	0.3816 (3)	0.8934 (2)	−0.33839 (17)	0.0663 (5)
H15A	0.3811	0.7959	−0.3187	0.099*
H15B	0.5102	0.8974	−0.3664	0.099*
H15C	0.2889	0.9534	−0.4036	0.099*
C16	0.2820 (3)	1.5289 (2)	−0.1356 (2)	0.0781 (6)
H16A	0.2891	1.6242	−0.1515	0.117*
H16B	0.3760	1.4631	−0.0730	0.117*
H16C	0.1528	1.5278	−0.1061	0.117*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0745 (8)	0.0609 (7)	0.0399 (6)	−0.0283 (6)	0.0097 (5)	−0.0198 (5)
O2	0.0911 (9)	0.0502 (7)	0.0614 (8)	−0.0316 (7)	0.0063 (7)	−0.0012 (6)
O3	0.1479 (14)	0.0451 (7)	0.0626 (8)	−0.0462 (8)	0.0084 (8)	−0.0107 (6)
O4	0.1248 (12)	0.0602 (8)	0.0589 (8)	−0.0407 (8)	0.0150 (8)	−0.0326 (6)
N1	0.0579 (8)	0.0396 (7)	0.0338 (7)	−0.0191 (6)	0.0037 (5)	−0.0098 (5)
N2	0.0736 (9)	0.0398 (7)	0.0417 (7)	−0.0227 (6)	0.0058 (6)	−0.0123 (6)
N3	0.0688 (9)	0.0436 (7)	0.0419 (7)	−0.0235 (6)	0.0078 (6)	−0.0189 (6)
N4	0.0701 (9)	0.0434 (7)	0.0505 (8)	−0.0224 (7)	0.0030 (7)	−0.0181 (6)
C1	0.0430 (8)	0.0549 (9)	0.0386 (8)	−0.0169 (7)	0.0003 (6)	−0.0105 (7)
C2	0.0529 (9)	0.0717 (11)	0.0335 (8)	−0.0209 (8)	0.0025 (7)	−0.0098 (7)
C3	0.0542 (10)	0.0614 (10)	0.0399 (9)	−0.0218 (8)	−0.0014 (7)	0.0048 (7)
C4	0.0484 (9)	0.0474 (9)	0.0461 (9)	−0.0165 (7)	−0.0019 (7)	−0.0003 (7)
C5	0.0495 (9)	0.0470 (8)	0.0405 (8)	−0.0164 (7)	0.0007 (7)	−0.0060 (7)
C6	0.0394 (8)	0.0469 (8)	0.0336 (8)	−0.0143 (6)	−0.0016 (6)	−0.0048 (6)
C7	0.0402 (8)	0.0403 (8)	0.0349 (7)	−0.0138 (6)	0.0008 (6)	−0.0109 (6)
C8	0.0794 (12)	0.0412 (8)	0.0498 (9)	−0.0251 (8)	0.0078 (8)	−0.0199 (7)
C9	0.0414 (8)	0.0414 (8)	0.0374 (8)	−0.0154 (6)	0.0023 (6)	−0.0152 (6)
C10	0.0564 (9)	0.0474 (8)	0.0331 (7)	−0.0210 (7)	0.0079 (6)	−0.0146 (6)
C11	0.0518 (9)	0.0432 (8)	0.0375 (8)	−0.0204 (7)	0.0040 (6)	−0.0078 (6)
C12	0.0441 (8)	0.0357 (7)	0.0430 (8)	−0.0140 (6)	0.0001 (6)	−0.0140 (6)
C13	0.0444 (8)	0.0410 (8)	0.0334 (7)	−0.0137 (6)	0.0012 (6)	−0.0142 (6)
C14	0.0359 (7)	0.0377 (7)	0.0341 (7)	−0.0119 (6)	0.0007 (6)	−0.0105 (6)
C15	0.0800 (13)	0.0786 (12)	0.0517 (10)	−0.0321 (10)	0.0150 (9)	−0.0323 (9)
C16	0.1048 (16)	0.0540 (11)	0.0800 (14)	−0.0356 (11)	0.0166 (12)	−0.0196 (10)

Geometric parameters (Å, º)

O1—C1	1.3761 (19)	C4—C5	1.389 (2)
O1—C15	1.4234 (19)	C5—C6	1.385 (2)
O2—C4	1.376 (2)	C5—H5A	0.9300
O2—C16	1.423 (2)	C7—C14	1.4430 (19)
O3—N4	1.2179 (17)	C8—H8A	0.9300

O4—N4	1.2176 (17)	C9—C10	1.409 (2)
N1—C7	1.3564 (18)	C9—C14	1.4115 (19)
N1—C6	1.4112 (18)	C10—C11	1.358 (2)
N1—H1A	0.868 (19)	C10—H10A	0.9300
N2—C7	1.3182 (19)	C11—C12	1.396 (2)
N2—C8	1.345 (2)	C11—H11A	0.9300
N3—C8	1.302 (2)	C12—C13	1.367 (2)
N3—C9	1.3687 (18)	C13—C14	1.4033 (19)
N4—C12	1.4608 (18)	C13—H13A	0.9300
C1—C2	1.387 (2)	C15—H15A	0.9600
C1—C6	1.397 (2)	C15—H15B	0.9600
C2—C3	1.377 (2)	C15—H15C	0.9600
C2—H2B	0.9300	C16—H16A	0.9600
C3—C4	1.374 (2)	C16—H16B	0.9600
C3—H3B	0.9300	C16—H16C	0.9600

C1—O1—C15	117.06 (13)	N3—C8—H8A	115.4
C4—O2—C16	116.73 (13)	N2—C8—H8A	115.4
C7—N1—C6	129.76 (13)	N3—C9—C10	117.95 (13)
C7—N1—H1A	118.8 (12)	N3—C9—C14	122.40 (13)
C6—N1—H1A	111.4 (12)	C10—C9—C14	119.65 (12)
C7—N2—C8	117.26 (13)	C11—C10—C9	120.95 (13)
C8—N3—C9	114.77 (13)	C11—C10—H10A	119.5
O4—N4—O3	123.00 (13)	C9—C10—H10A	119.5
O4—N4—C12	118.81 (13)	C10—C11—C12	118.47 (13)
O3—N4—C12	118.18 (13)	C10—C11—H11A	120.8
O1—C1—C2	125.36 (14)	C12—C11—H11A	120.8
O1—C1—C6	115.44 (13)	C13—C12—C11	123.04 (13)
C2—C1—C6	119.20 (15)	C13—C12—N4	118.71 (13)
C3—C2—C1	120.74 (15)	C11—C12—N4	118.25 (13)
C3—C2—H2B	119.6	C12—C13—C14	118.91 (13)
C1—C2—H2B	119.6	C12—C13—H13A	120.5
C4—C3—C2	119.96 (14)	C14—C13—H13A	120.5
C4—C3—H3B	120.0	C13—C14—C9	118.98 (12)
C2—C3—H3B	120.0	C13—C14—C7	125.30 (12)
C3—C4—O2	116.71 (14)	C9—C14—C7	115.72 (12)
C3—C4—C5	120.38 (15)	O1—C15—H15A	109.5
O2—C4—C5	122.91 (15)	O1—C15—H15B	109.5
C6—C5—C4	119.81 (15)	H15A—C15—H15B	109.5
C6—C5—H5A	120.1	O1—C15—H15C	109.5
C4—C5—H5A	120.1	H15A—C15—H15C	109.5
C5—C6—C1	119.91 (13)	H15B—C15—H15C	109.5
C5—C6—N1	124.48 (13)	O2—C16—H16A	109.5
C1—C6—N1	115.61 (13)	O2—C16—H16B	109.5
N2—C7—N1	119.40 (13)	H16A—C16—H16B	109.5
N2—C7—C14	120.64 (13)	O2—C16—H16C	109.5
N1—C7—C14	119.95 (12)	H16A—C16—H16C	109.5
N3—C8—N2	129.14 (14)	H16B—C16—H16C	109.5

C15—O1—C1—C2	4.4 (2)	C7—N2—C8—N3	−0.5 (3)
C15—O1—C1—C6	−176.33 (14)	C8—N3—C9—C10	−178.01 (14)
O1—C1—C2—C3	179.65 (14)	C8—N3—C9—C14	1.9 (2)
C6—C1—C2—C3	0.4 (2)	N3—C9—C10—C11	179.96 (14)
C1—C2—C3—C4	−0.2 (2)	C14—C9—C10—C11	0.0 (2)
C2—C3—C4—O2	179.56 (14)	C9—C10—C11—C12	0.0 (2)
C2—C3—C4—C5	−0.1 (2)	C10—C11—C12—C13	−0.2 (2)
C16—O2—C4—C3	179.79 (16)	C10—C11—C12—N4	179.70 (13)
C16—O2—C4—C5	−0.6 (2)	O4—N4—C12—C13	−3.3 (2)
C3—C4—C5—C6	0.2 (2)	O3—N4—C12—C13	177.54 (14)
O2—C4—C5—C6	−179.49 (14)	O4—N4—C12—C11	176.73 (14)
C4—C5—C6—C1	0.1 (2)	O3—N4—C12—C11	−2.4 (2)
C4—C5—C6—N1	−179.94 (13)	C11—C12—C13—C14	0.5 (2)
O1—C1—C6—C5	−179.67 (13)	N4—C12—C13—C14	−179.45 (12)
C2—C1—C6—C5	−0.4 (2)	C12—C13—C14—C9	−0.5 (2)
O1—C1—C6—N1	0.34 (19)	C12—C13—C14—C7	179.88 (13)
C2—C1—C6—N1	179.66 (13)	N3—C9—C14—C13	−179.70 (13)
C7—N1—C6—C5	1.8 (2)	C10—C9—C14—C13	0.2 (2)
C7—N1—C6—C1	−178.23 (14)	N3—C9—C14—C7	0.0 (2)
C8—N2—C7—N1	−177.84 (14)	C10—C9—C14—C7	179.89 (12)
C8—N2—C7—C14	2.6 (2)	N2—C7—C14—C13	177.34 (13)
C6—N1—C7—N2	2.7 (2)	N1—C7—C14—C13	−2.2 (2)
C6—N1—C7—C14	−177.71 (13)	N2—C7—C14—C9	−2.3 (2)
C9—N3—C8—N2	−1.8 (3)	N1—C7—C14—C9	178.10 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*A*···N2	0.93	2.22	2.833 (2)	123
C8—H8*A*···O3^{i}	0.93	2.60	3.490 (2)	161

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