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3-*tert*-Butyl-4-(4-nitrophenyl)-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine

Rodrigo Abonia,[a] Emerson Rengifo,[a] Justo Cobo,[b] John N. Low[c] and Christopher Glidewell[d]*

[a]Grupo de Investigación de Compuestos Heterocíclicos, Departamento de Química, Universidad de Valle, AA 25360 Cali, Colombia, [b]Departamento de Química Inorgánica y Orgánica, Universidad de Jaén, 23071 Jaén, Spain, [c]Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB24 3UE, Scotland, and [d]School of Chemistry, University of St Andrews, St Andrews, Fife KY16 9ST, Scotland

Correspondence e-mail: cg@st-andrews.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.057
wR factor = 0.137
Data-to-parameter ratio = 16.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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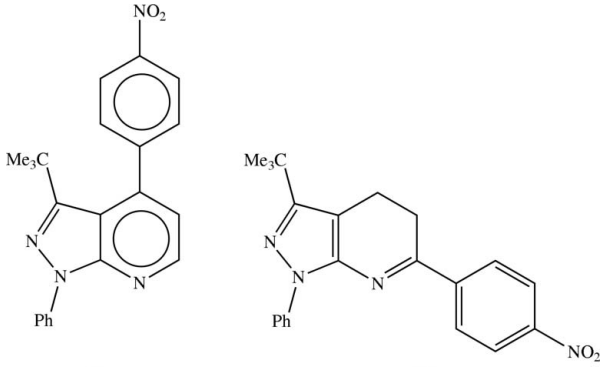
Molecules of the title compound, $C_{22}H_{20}N_4O_2$, are linked by paired C—H···O hydrogen bonds into centrosymmetric $R_2^2(18)$ dimers and these dimers are linked into chains by paired C—H···π(arene) hydrogen bonds.

Comment

We have recently described the preparation of pyrazolo[3,4-*b*]pyridines from 5-aminopyrazoles in solution with different reactants (Low *et al.*, 2002, and references therein), and we have reported the crystal structure of the fully aromatized 3-methyl-1,4-diphenyl-1*H*-pyrazolo[3,4-*b*]pyridine (Low *et al.*, 2002). We report here an analogous structure, that of 3-*tert*-butyl-4-(4-nitrophenyl)-1-phenyl-1*H*-pyrazolo[3,4-*b*]pyridine, (I), obtained from the solvent-free reaction of the corresponding 5-aminopyrazole and the Mannich adduct β-dimethylamino-4-nitropropiophenone hydrochloride, under microwave irradiation. The title compound, (I), was obtained along with the reduced 6-(4-nitrophenyl) analogue, (II); however, in pyridine solution under reflux, a similar reaction yielded regioselectively the isomeric 6-arylpyrazolo[3,4-*b*]pyridine (Quiroga *et al.*, 1998).



(I) (II)

Neither of the aryl rings in compound (I) (Fig. 1) is coplanar with the pyrazolopyridine system; unsubstituted phenyl ring C11–C16 makes a dihedral angle of 25.3 (2)° with the adjacent pyrazole ring, while substituted ring C41–C46 is nearly orthogonal to the pyridine ring, with a dihedral angle between these ring planes of 85.1 (2)°; in addition, the nitro group makes a dihedral angle of 11.6 (2)° with the adjacent aryl ring. The bond distances within the fused heterocyclic ring system (Table 1) are consistent with electronic delocalization in the pyridine ring and strong bond fixation in the pyrazole ring.

The molecules of compound (I) are linked into chains of fused rings by a combination of one C—H···O hydrogen bond and one C—H···π(arene) hydrogen bond (Table 2). Pyridine

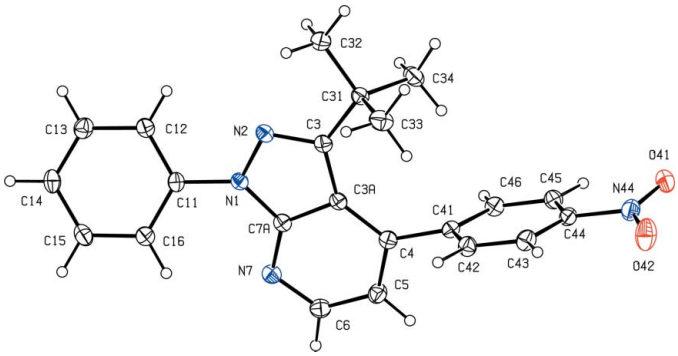


Figure 1
The molecule of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

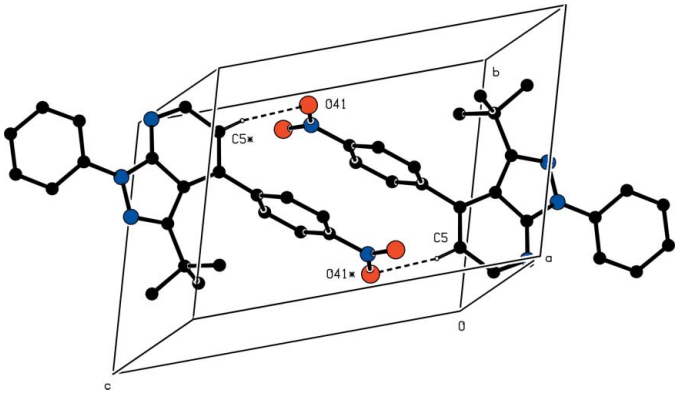


Figure 2
Part of the crystal structure of (I), showing the formation of a centrosymmetric $R_2^2(18)$ dimer. For the sake of clarity, the H atoms not involved in the motif shown have been omitted. Atoms marked with an asterisk (*) are at the symmetry position $(1-x, 1-y, 1-z)$. Dashed lines indicate hydrogen bonds.

atom C5 in the molecule at (x, y, z) acts as hydrogen-bond donor to nitro atom O41 in the molecule at $(1-x, 1-y, 1-z)$, generating a centrosymmetric $R_2^2(18)$ dimer centred at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (Fig. 2). In addition, aryl atoms C43 in the molecules at (x, y, z) and $(1-x, 1-y, 1-z)$, which are both components of the $R_2^2(18)$ dimer centred at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, act as donors respectively to aryl rings C11–C16 in the molecules at $(-x, 1-y, -z)$ and $(1+x, y, 1+z)$, which themselves are components of the $R_2^2(18)$ dimers centred at $(-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$ and $(\frac{3}{2}, \frac{1}{2}, \frac{3}{2})$. Propagation by inversion of these two interactions thus generates a chain of edge-fused rings running parallel to the [101] direction, rings built from paired C—H···O hydrogen bonds centred at $(n+\frac{1}{2}, \frac{1}{2}, n+\frac{1}{2})$ (n = zero or integer) and rings built from paired C—H···π(arene) hydrogen bonds centred at $(n, \frac{1}{2}, n)$ (n = zero or integer) (Fig. 3).

Experimental

Equimolar quantities (0.465 mmol) of 5-amino-3-*tert*-butyl-1-phenyl-1*H*-pyrazole and β-dimethylamino-4-nitropropiophenone hydrochloride were placed in open Pyrex-glass vessels and irradiated in a domestic microwave oven for 15 s (at 600 W). The reaction mixture was extracted with ethyl acetate and the product was purified by column chromatography on silica gel, using hexane/ethyl acetate (15:1 (*v*/*v*) as eluent. Evaporation of the eluate yielded colourless crystals of compound (I) (yield 45%; m.p. 448–450 K) suitable for single-crystal X-ray diffraction, accompanied by a small quantity of the reduced 6-(4-nitrophenyl) derivative, (II). MS (EI 30 eV), *m*/*z* (%): 372 (M^+, 10), 357, (17), 149 (58), 57 (100).

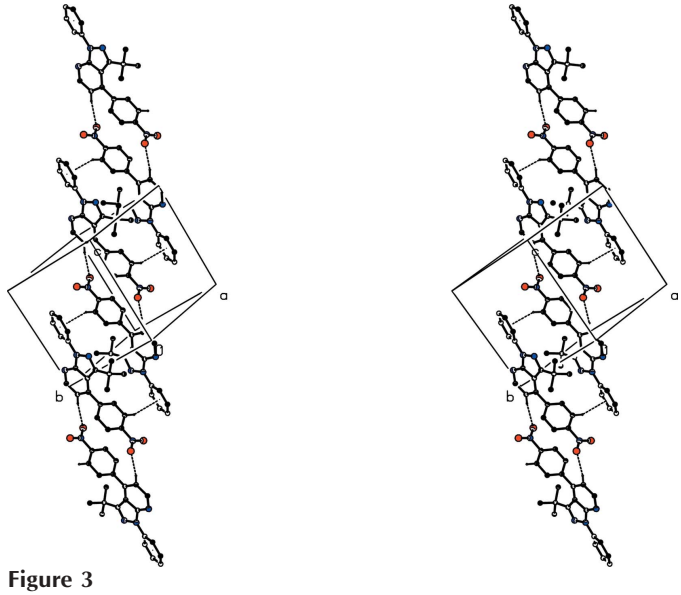


Figure 3
Stereoview of part of the crystal structure of (I), showing the formation of a [101] chain of edge-fused rings. For the sake of clarity, the H atoms not involved in the motifs shown have been omitted. Dashed lines indicate hydrogen bonds.

Crystal data

$C_{22}H_{20}N_4O_2$	$Z = 2$
$M_r = 372.42$	$D_x = 1.311$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 9.5877$ (5) Å	Cell parameters from 4338 reflections
$b = 9.8541$ (5) Å	$\theta = 3.2$–$27.7°$
$c = 11.7050$ (4) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 105.982$ (2)°	$T = 120$ (2) K
$\beta = 103.570$ (2)°	Plate, colourless
$\gamma = 108.433$ (2)°	0.19 × 0.08 × 0.05 mm
$V = 943.75$ (8) Å^3	

Data collection

Bruker–Nonius KappaCCD diffractometer	4338 independent reflections
φ and ω scans	2724 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$R_{int} = 0.070$
$T_{min} = 0.980$, $T_{max} = 0.996$	$\theta_{max} = 27.7°$
23240 measured reflections	$h = -12 \rightarrow 12$
	$k = -12 \rightarrow 12$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2 + 0.1475P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.057$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.137$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.34$ e Å^{-3}
4338 reflections	
256 parameters	
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

N1—N2	1.371 (2)	C5—C6	1.394 (3)
N2—C3	1.327 (2)	C6—N7	1.332 (2)
C3—C3*A*	1.447 (3)	N7—C7*A*	1.340 (2)
C3*A*—C4	1.415 (3)	C7*A*—N1	1.363 (2)
C4—C5	1.386 (3)	C3*A*—C7*A*	1.419 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O41^{i}	0.95	2.46	3.399 (2)	169
C43—H43···*Cg*^{ii}	0.95	2.65	3.501 (2)	149

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

All H atoms were located in difference maps and then treated as riding atoms, with C—H distances of 0.95 (aromatic) or 0.98 Å (methyl), and with $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}(C)$ for the methyl groups.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. JC thanks the Consejería de Innovación, Ciencia y Empresa (Junta de Andalucía, Spain) and the Universidad de Jaén for financial support. RA and ER thank COLCIENCIAS and UNIVALLE (Universidad del Valle, Colombia) for financial support.

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supporting information

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Hall symbol: -P 1
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$\alpha = 105.982$ (2)°
$\beta = 103.570$ (2)°
$\gamma = 108.433$ (2)°
$V = 943.75$ (8) Å^3
$Z = 2$
$F(000) = 392$
$D_x = 1.311$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4338 reflections
$\theta = 3.2$–27.7°
$\mu = 0.09$ mm^{-1}
$T = 120$ K
Plate, colourless
0.19 × 0.08 × 0.05 mm

Data collection

Bruker–Nonius 95mm CCD camera on κ goniostat diffractometer
Radiation source: Bruker–Nonius FR91 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.980$, $T_{max} = 0.996$
23240 measured reflections
4338 independent reflections
2724 reflections with $I > 2\sigma(I)$
$R_{int} = 0.070$
$\theta_{max} = 27.7°$, $\theta_{min} = 3.2°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.137$
$S = 1.02$
4338 reflections
256 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2 + 0.1475P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O41	0.69225 (17)	0.83405 (17)	0.65880 (13)	0.0458 (4)

O42	0.46382 (19)	0.7917 (2)	0.67528 (13)	0.0557 (5)
N1	0.11065 (16)	0.35207 (17)	−0.22947 (13)	0.0253 (4)
N2	0.17138 (16)	0.51029 (17)	−0.17602 (13)	0.0267 (4)
N7	0.09648 (17)	0.14201 (17)	−0.16190 (14)	0.0294 (4)
N44	0.5484 (2)	0.77491 (19)	0.61333 (15)	0.0361 (4)
C3	0.23820 (19)	0.5540 (2)	−0.05157 (16)	0.0250 (4)
C3A	0.22141 (19)	0.4193 (2)	−0.01952 (16)	0.0245 (4)
C4	0.2566 (2)	0.3797 (2)	0.08789 (17)	0.0266 (4)
C5	0.2111 (2)	0.2236 (2)	0.06525 (18)	0.0328 (5)
C6	0.1342 (2)	0.1116 (2)	−0.05761 (17)	0.0324 (5)
C7A	0.14011 (19)	0.2932 (2)	−0.13833 (16)	0.0249 (4)
C11	0.0266 (2)	0.2763 (2)	−0.36273 (16)	0.0258 (4)
C12	0.0587 (2)	0.3567 (2)	−0.44065 (17)	0.0289 (4)
C13	−0.0246 (2)	0.2847 (2)	−0.57028 (18)	0.0337 (5)
C14	−0.1388 (2)	0.1357 (2)	−0.62257 (18)	0.0350 (5)
C15	−0.1704 (2)	0.0575 (2)	−0.54349 (18)	0.0368 (5)
C16	−0.0891 (2)	0.1262 (2)	−0.41376 (18)	0.0331 (5)
C31	0.3120 (2)	0.7265 (2)	0.02705 (16)	0.0264 (4)
C32	0.3095 (2)	0.8158 (2)	−0.06107 (18)	0.0358 (5)
C33	0.2145 (3)	0.7647 (2)	0.10799 (19)	0.0406 (5)
C34	0.4821 (2)	0.7785 (2)	0.1107 (2)	0.0400 (5)
C41	0.3343 (2)	0.4888 (2)	0.22334 (16)	0.0261 (4)
C42	0.2448 (2)	0.5348 (2)	0.29180 (17)	0.0311 (4)
C43	0.3139 (2)	0.6283 (2)	0.41949 (17)	0.0329 (5)
C44	0.4730 (2)	0.6759 (2)	0.47773 (16)	0.0282 (4)
C45	0.5651 (2)	0.6324 (2)	0.41341 (17)	0.0305 (4)
C46	0.4945 (2)	0.5371 (2)	0.28592 (17)	0.0296 (4)
H5	0.2327	0.1924	0.1349	0.039*
H6	0.1070	0.0065	−0.0676	0.039*
H12	0.1367	0.4596	−0.4056	0.035*
H13	−0.0026	0.3390	−0.6240	0.040*
H14	−0.1950	0.0874	−0.7115	0.042*
H15	−0.2492	−0.0450	−0.5789	0.044*
H16	−0.1118	0.0718	−0.3603	0.040*
H32A	0.3549	0.9269	−0.0101	0.054*
H32B	0.2008	0.7838	−0.1154	0.054*
H32C	0.3711	0.7940	−0.1141	0.054*
H33A	0.1066	0.7333	0.0524	0.061*
H33B	0.2610	0.8761	0.1577	0.061*
H33C	0.2137	0.7089	0.1656	0.061*
H34A	0.5295	0.8911	0.1553	0.060*
H34B	0.5411	0.7487	0.0577	0.060*
H34C	0.4850	0.7292	0.1729	0.060*
H42	0.1353	0.5015	0.2501	0.037*
H43	0.2528	0.6590	0.4660	0.040*
H45	0.6748	0.6670	0.4557	0.037*
H46	0.5559	0.5043	0.2408	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O41	0.0379 (9)	0.0472 (9)	0.0333 (8)	0.0042 (7)	0.0039 (6)	0.0107 (7)
O42	0.0562 (10)	0.0796 (12)	0.0316 (8)	0.0369 (9)	0.0180 (7)	0.0084 (8)
N1	0.0255 (8)	0.0228 (8)	0.0254 (8)	0.0090 (6)	0.0085 (6)	0.0073 (7)
N2	0.0232 (8)	0.0255 (9)	0.0280 (8)	0.0081 (7)	0.0084 (6)	0.0078 (7)
N7	0.0299 (8)	0.0266 (9)	0.0322 (9)	0.0134 (7)	0.0108 (7)	0.0100 (7)
N44	0.0426 (11)	0.0359 (10)	0.0282 (9)	0.0167 (8)	0.0098 (8)	0.0117 (8)
C3	0.0188 (9)	0.0294 (10)	0.0283 (10)	0.0102 (8)	0.0109 (7)	0.0105 (8)
C3A	0.0192 (8)	0.0267 (10)	0.0272 (9)	0.0094 (7)	0.0092 (7)	0.0088 (8)
C4	0.0218 (9)	0.0308 (11)	0.0291 (10)	0.0117 (8)	0.0107 (7)	0.0115 (8)
C5	0.0369 (11)	0.0340 (12)	0.0299 (10)	0.0166 (9)	0.0103 (8)	0.0144 (9)
C6	0.0360 (11)	0.0276 (11)	0.0368 (11)	0.0154 (9)	0.0139 (9)	0.0131 (9)
C7A	0.0207 (9)	0.0276 (10)	0.0278 (10)	0.0112 (8)	0.0103 (7)	0.0096 (8)
C11	0.0256 (9)	0.0284 (10)	0.0229 (9)	0.0136 (8)	0.0082 (7)	0.0065 (8)
C12	0.0246 (9)	0.0322 (11)	0.0273 (10)	0.0103 (8)	0.0107 (8)	0.0079 (8)
C13	0.0343 (11)	0.0406 (12)	0.0299 (10)	0.0167 (9)	0.0158 (8)	0.0133 (9)
C14	0.0383 (11)	0.0370 (12)	0.0235 (10)	0.0175 (10)	0.0071 (8)	0.0035 (9)
C15	0.0330 (11)	0.0299 (11)	0.0339 (11)	0.0088 (9)	0.0029 (9)	0.0048 (9)
C16	0.0334 (11)	0.0300 (11)	0.0315 (10)	0.0103 (9)	0.0079 (8)	0.0113 (9)
C31	0.0249 (9)	0.0253 (10)	0.0270 (10)	0.0087 (8)	0.0094 (7)	0.0086 (8)
C32	0.0402 (12)	0.0286 (11)	0.0351 (11)	0.0113 (9)	0.0110 (9)	0.0123 (9)
C33	0.0475 (13)	0.0306 (11)	0.0436 (12)	0.0143 (10)	0.0250 (10)	0.0082 (10)
C34	0.0311 (11)	0.0308 (11)	0.0437 (12)	0.0048 (9)	0.0017 (9)	0.0120 (9)
C41	0.0282 (10)	0.0263 (10)	0.0265 (9)	0.0120 (8)	0.0103 (8)	0.0122 (8)
C42	0.0254 (10)	0.0382 (11)	0.0300 (10)	0.0135 (9)	0.0093 (8)	0.0130 (9)
C43	0.0341 (11)	0.0403 (12)	0.0309 (10)	0.0189 (9)	0.0168 (9)	0.0141 (9)
C44	0.0322 (10)	0.0282 (10)	0.0253 (10)	0.0130 (8)	0.0094 (8)	0.0115 (8)
C45	0.0248 (10)	0.0334 (11)	0.0321 (10)	0.0109 (8)	0.0082 (8)	0.0133 (9)
C46	0.0279 (10)	0.0339 (11)	0.0312 (10)	0.0151 (9)	0.0127 (8)	0.0132 (9)

Geometric parameters (Å, º)

N1—N2	1.371 (2)	C32—H32A	0.98
N2—C3	1.327 (2)	C32—H32B	0.98
C3—C3A	1.447 (3)	C32—H32C	0.98
C3A—C4	1.415 (3)	C33—H33A	0.98
C4—C5	1.386 (3)	C33—H33B	0.98
C5—C6	1.394 (3)	C33—H33C	0.98
C6—N7	1.332 (2)	C34—H34A	0.98
N7—C7A	1.340 (2)	C34—H34B	0.98
C7A—N1	1.363 (2)	C34—H34C	0.98
C3A—C7A	1.419 (2)	C4—C41	1.492 (2)
N1—C11	1.424 (2)	C41—C46	1.393 (3)
C11—C12	1.389 (3)	C41—C42	1.397 (2)
C11—C16	1.393 (3)	C42—C43	1.383 (3)
C12—C13	1.387 (3)	C42—H42	0.95

C12—H12	0.95	C43—C44	1.377 (3)
C13—C14	1.380 (3)	C43—H43	0.95
C13—H13	0.95	C44—C45	1.380 (2)
C14—C15	1.385 (3)	C44—N44	1.468 (2)
C14—H14	0.95	N44—O41	1.225 (2)
C15—C16	1.384 (3)	N44—O42	1.227 (2)
C15—H15	0.95	C45—C46	1.385 (2)
C16—H16	0.95	C45—H45	0.95
C3—C31	1.520 (3)	C46—H46	0.95
C31—C34	1.525 (3)	C5—H5	0.95
C31—C32	1.530 (3)	C6—H6	0.95
C31—C33	1.535 (2)		

C7A—N1—N2	110.38 (14)	C31—C34—H34A	109.5
C7A—N1—C11	130.66 (15)	C31—C34—H34B	109.5
N2—N1—C11	118.93 (14)	H34A—C34—H34B	109.5
C12—C11—C16	120.50 (17)	C31—C34—H34C	109.5
C12—C11—N1	118.72 (16)	H34A—C34—H34C	109.5
C16—C11—N1	120.75 (16)	H34B—C34—H34C	109.5
C13—C12—C11	119.10 (18)	C4—C3A—C7A	115.63 (17)
C13—C12—H12	120.4	C4—C3A—C3	140.28 (17)
C11—C12—H12	120.4	C7A—C3A—C3	104.07 (15)
C14—C13—C12	121.16 (18)	C5—C4—C3A	116.79 (17)
C14—C13—H13	119.4	C5—C4—C41	116.73 (16)
C12—C13—H13	119.4	C3A—C4—C41	126.46 (17)
C13—C14—C15	119.05 (17)	C46—C41—C42	119.02 (16)
C13—C14—H14	120.5	C46—C41—C4	120.66 (16)
C15—C14—H14	120.5	C42—C41—C4	120.15 (15)
C16—C15—C14	121.09 (19)	C43—C42—C41	120.77 (17)
C16—C15—H15	119.5	C43—C42—H42	119.6
C14—C15—H15	119.5	C41—C42—H42	119.6
C15—C16—C11	119.09 (18)	C44—C43—C42	118.61 (17)
C15—C16—H16	120.5	C44—C43—H43	120.7
C11—C16—H16	120.5	C42—C43—H43	120.7
C3—N2—N1	108.20 (15)	C43—C44—C45	122.28 (17)
N2—C3—C3A	109.76 (15)	C43—C44—N44	119.38 (16)
N2—C3—C31	116.96 (16)	C45—C44—N44	118.33 (16)
C3A—C3—C31	133.27 (16)	O41—N44—O42	123.63 (16)
C3—C31—C34	111.06 (16)	O41—N44—C44	118.17 (15)
C3—C31—C32	109.66 (14)	O42—N44—C44	118.18 (16)
C34—C31—C32	108.49 (15)	C44—C45—C46	118.68 (16)
C3—C31—C33	109.37 (14)	C44—C45—H45	120.7
C34—C31—C33	110.76 (16)	C46—C45—H45	120.7
C32—C31—C33	107.42 (16)	C45—C46—C41	120.62 (16)
C31—C32—H32A	109.5	C45—C46—H46	119.7
C31—C32—H32B	109.5	C41—C46—H46	119.7
H32A—C32—H32B	109.5	C4—C5—C6	121.42 (18)
C31—C32—H32C	109.5	C4—C5—H5	119.3

H32A—C32—H32C	109.5	C6—C5—H5	119.3
H32B—C32—H32C	109.5	N7—C6—C5	124.38 (18)
C31—C33—H33A	109.5	N7—C6—H6	117.8
C31—C33—H33B	109.5	C5—C6—H6	117.8
H33A—C33—H33B	109.5	C6—N7—C7A	113.47 (16)
C31—C33—H33C	109.5	N7—C7A—N1	124.13 (16)
H33A—C33—H33C	109.5	N7—C7A—C3A	128.29 (17)
H33B—C33—H33C	109.5	N1—C7A—C3A	107.58 (16)

C7A—N1—C11—C12	−157.30 (17)	C3A—C4—C41—C46	−98.4 (2)
N2—N1—C11—C12	25.1 (2)	C5—C4—C41—C42	−92.0 (2)
C7A—N1—C11—C16	24.6 (3)	C3A—C4—C41—C42	86.5 (2)
N2—N1—C11—C16	−152.94 (16)	C46—C41—C42—C43	0.7 (3)
C16—C11—C12—C13	−0.8 (3)	C4—C41—C42—C43	175.98 (17)
N1—C11—C12—C13	−178.89 (15)	C41—C42—C43—C44	0.4 (3)
C11—C12—C13—C14	0.4 (3)	C42—C43—C44—C45	−0.6 (3)
C12—C13—C14—C15	0.1 (3)	C42—C43—C44—N44	−179.87 (17)
C13—C14—C15—C16	−0.2 (3)	C43—C44—N44—O41	−169.59 (18)
C14—C15—C16—C11	−0.2 (3)	C45—C44—N44—O41	11.1 (3)
C12—C11—C16—C15	0.7 (3)	C43—C44—N44—O42	11.6 (3)
N1—C11—C16—C15	178.75 (16)	C45—C44—N44—O42	−167.64 (18)
C7A—N1—N2—C3	−0.60 (18)	C43—C44—C45—C46	−0.2 (3)
C11—N1—N2—C3	177.44 (14)	N44—C44—C45—C46	179.05 (17)
N1—N2—C3—C3A	−0.19 (18)	C44—C45—C46—C41	1.3 (3)
N1—N2—C3—C31	−179.34 (13)	C42—C41—C46—C45	−1.6 (3)
N2—C3—C31—C34	−126.87 (17)	C4—C41—C46—C45	−176.80 (17)
C3A—C3—C31—C34	54.2 (2)	C3A—C4—C5—C6	−0.1 (3)
N2—C3—C31—C32	−7.0 (2)	C41—C4—C5—C6	178.52 (16)
C3A—C3—C31—C32	174.12 (18)	C4—C5—C6—N7	−0.8 (3)
N2—C3—C31—C33	110.58 (17)	C5—C6—N7—C7A	0.2 (3)
C3A—C3—C31—C33	−68.3 (2)	C6—N7—C7A—N1	−178.24 (16)
N2—C3—C3A—C4	−177.3 (2)	C6—N7—C7A—C3A	1.3 (3)
C31—C3—C3A—C4	1.7 (4)	N2—N1—C7A—N7	−179.27 (15)
N2—C3—C3A—C7A	0.86 (18)	C11—N1—C7A—N7	3.0 (3)
C31—C3—C3A—C7A	179.81 (17)	N2—N1—C7A—C3A	1.15 (18)
C7A—C3A—C4—C5	1.3 (2)	C11—N1—C7A—C3A	−176.59 (16)
C3—C3A—C4—C5	179.3 (2)	C4—C3A—C7A—N7	−2.1 (3)
C7A—C3A—C4—C41	−177.14 (16)	C3—C3A—C7A—N7	179.25 (16)
C3—C3A—C4—C41	0.9 (3)	C4—C3A—C7A—N1	177.51 (14)
C5—C4—C41—C46	83.2 (2)	C3—C3A—C7A—N1	−1.19 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O41^{i}	0.95	2.46	3.399 (2)	169
C43—H43···*Cg*^{ii}	0.95	2.65	3.501 (2)	149

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