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tert-Butyl N-[4-methyl-3-[4-(3-pyridyl)-pyrimidin-2-yloxy]phenyl]carbamate

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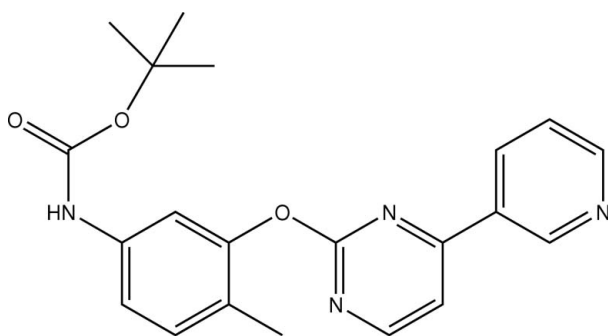
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 Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.058; wR factor = 0.184; data-to-parameter ratio = 14.4.

In the molecule of the title compound, $\text{C}_{21}\text{H}_{22}\text{N}_4\text{O}_3$, the pyrimidine ring is oriented at dihedral angles of 0.51 (3) and 50.76 (3)° to the pyridine and benzene rings, respectively. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds link the molecules into centrosymmetric dimers, forming $R_2^2(24)$ ring motifs; the dimers are linked by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds into a two-dimensional network. $\pi-\pi$ contacts between the benzene rings and between the pyrimidine and pyridine rings [centroid-centroid distances = 3.891 (1) and 3.646 (1) Å, respectively] may further stabilize the structure. Two weak $\text{C}-\text{H}\cdots\pi$ interactions are also present.

Related literature

For bond-length data, see: Allen *et al.* (1987). For ring-motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

 $\text{C}_{21}\text{H}_{22}\text{N}_4\text{O}_3$
 $M_r = 378.43$

 Triclinic, $P\bar{1}$
 $a = 9.951$ (2) Å

 $b = 10.733$ (2) Å
 $c = 11.577$ (2) Å
 $\alpha = 114.74$ (3)°
 $\beta = 107.14$ (3)°
 $\gamma = 99.97$ (3)°
 $V = 1008.6$ (6) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 294$ K
 $0.30 \times 0.20 \times 0.10$ mm

Data collection

 Enraf-Nonius CAD-4
 diffractometer
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.975$, $T_{\max} = 0.992$
 3882 measured reflections

 3652 independent reflections
 2333 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 3 standard reflections
 frequency: 120 min
 intensity decay: 1%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.184$
 $S = 1.01$
 3652 reflections

 254 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{N4}^i$	0.86	2.10	2.944 (4)	165
$\text{C15}-\text{H15A}\cdots\text{O2}^{ii}$	0.93	2.45	3.382 (4)	177
$\text{C18}-\text{H18A}\cdots\text{O2}^{ii}$	0.93	2.39	3.319 (4)	174
$\text{C3}-\text{H3B}\cdots\text{Cg1}^i$	0.96	2.86	3.560 (3)	131
$\text{C12}-\text{H12B}\cdots\text{Cg2}^{iii}$	0.96	2.90	3.788 (3)	154

Symmetry codes: (i) $-x, -y + 2, -z + 1$; (ii) $-x, -y + 1, -z + 1$; (iii) $-x + 1, -y + 2, -z + 2$. Cg1 and Cg2 are the centroids of the $\text{C6}-\text{C11}$ and $\text{N2}/\text{N3}/\text{C13}-\text{C16}$ rings, respectively.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2725).

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supporting information

Acta Cryst. (2009). E65, o1849 [doi:10.1107/S1600536809025604]

tert*-Butyl *N*-{4-methyl-3-[4-(3-pyridyl)pyrimidin-2-yloxy]phenyl}carbamate*Shi-Gui Tang, Jian-Qiang Wang and Cheng Guo****S1. Comment**

Some derivatives of phenol are important chemical materials. We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Rings A (C6-C11), B (N2/N3/C13-C16) and C (N4/C17-C21) are, of course, planar and the dihedral angles between them are A/B = 50.76 (3), A/C = 50.58 (3) and B/C = 0.51 (3) °.

In the crystal structure, intermolecular N-H...N hydrogen bonds (Table 1) link the molecules into centrosymmetric dimers forming $R_2^2(24)$ ring motifs (Bernstein *et al.*, 1995), and then intermolecular C-H...O hydrogen bonds (Table 1) link them into a two dimensional network (Fig. 2), in which they may be effective in the stabilization of the structure. The π - π contacts between the phenyl rings and between the pyrimidine and the pyridine rings, Cg1—Cg1ⁱ and Cg2—Cg3ⁱⁱ [symmetry codes: (i) 1 - x, 2 - y, 1 - z, (ii) -x, 1 - y, 1 - z, where Cg1, Cg2 and Cg3 are centroids of the rings A (C6-C11), B (N2/N3/C13-C16) and C (N4/C17-C21), respectively] may further stabilize the structure, with centroid-centroid distances of 3.891 (1) and 3.646 (1) Å, respectively. There also exist two weak C—H... π interactions (Table 1).

S2. Experimental

To a mixture of 2-(methylsulfonyl)-4-(pyridin-3-yl)pyrimidine (47.1 g, 0.2 mol) in DMF (75 ml) and *tert*-butyl-3-hydroxy-4-methylphenylcarbamate (44.7 g, 0.2 mol) in DMF (150 ml) was added sodium hydride (44.4 g) slowly and was stirred for 18 h at room temperature. After acidified with citric acid the reaction mixture was poured into ice-water (2000 ml). The precipitate was filtered, washed with water and was extracted with dichloromethane. The dichloromethane layer was dried over anhydrous magnesium sulfate and evaporated *in vacuo*. The residue was recrystallized from ethyl ether to give the title compound (yield; 73.4 g). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

S3. Refinement

H atoms were positioned geometrically with N-H = 0.86 Å (for NH) and C-H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C,N})$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H atoms.

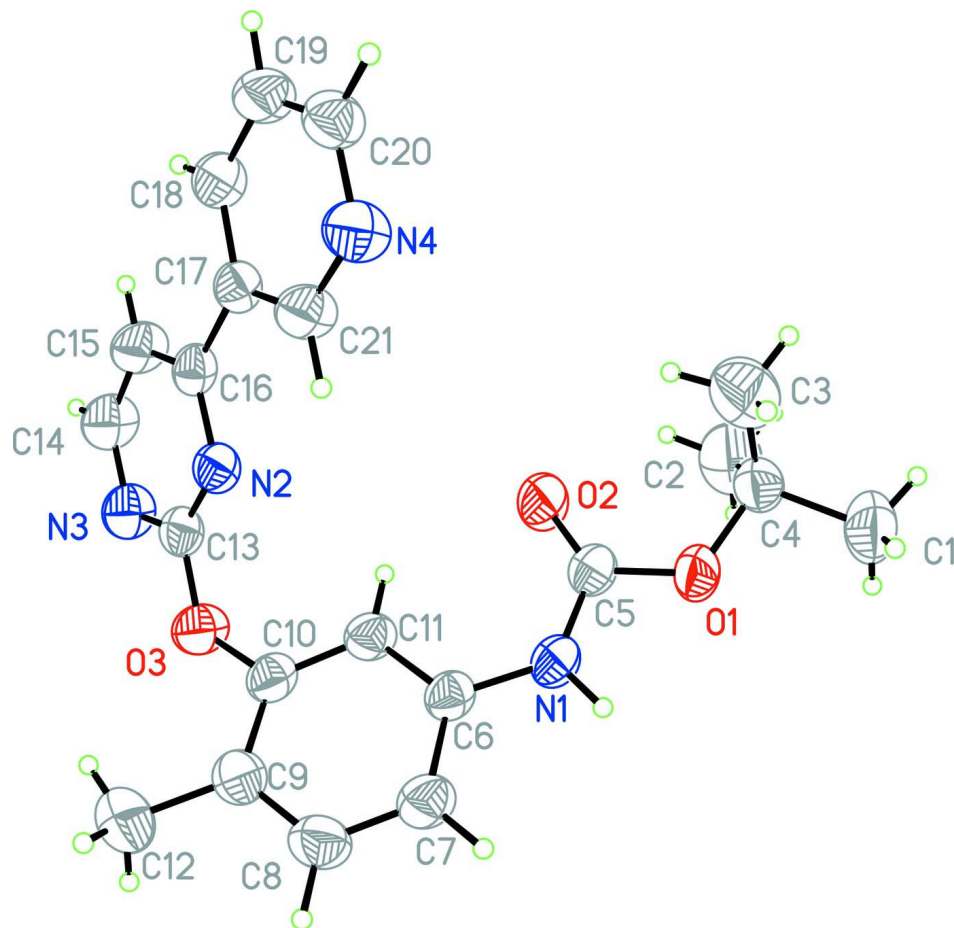
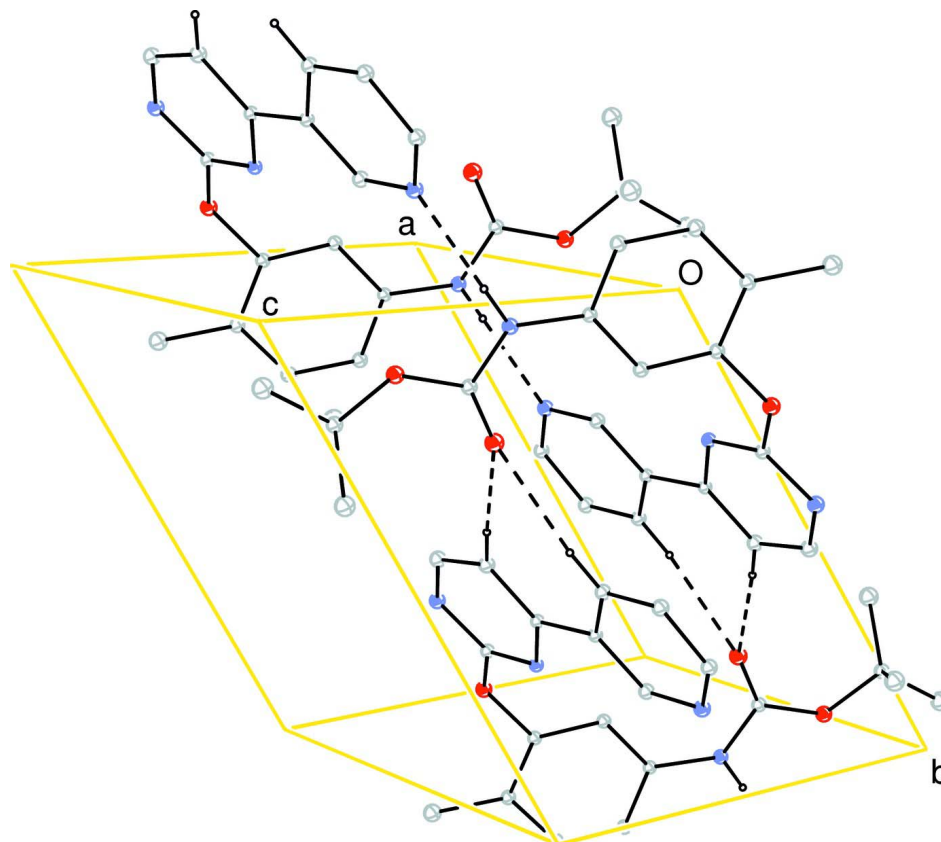


Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

**Figure 2**

A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

***tert*-Butyl *N*-{4-methyl-3-[4-(3-pyridyl)pyrimidin-2-yloxy]phenyl}carbamate**

Crystal data

$C_{21}H_{22}N_4O_3$

$M_r = 378.43$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 9.951\ (2)\ \text{\AA}$

$b = 10.733\ (2)\ \text{\AA}$

$c = 11.577\ (2)\ \text{\AA}$

$\alpha = 114.74\ (3)^\circ$

$\beta = 107.14\ (3)^\circ$

$\gamma = 99.97\ (3)^\circ$

$V = 1008.6\ (6)\ \text{\AA}^3$

$Z = 2$

$F(000) = 400$

$D_x = 1.246\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 25 reflections

$\theta = 9\text{--}13^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 294\ \text{K}$

Block, colorless

$0.30 \times 0.20 \times 0.10\ \text{mm}$

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega/2\theta$ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{\min} = 0.975$, $T_{\max} = 0.992$

3882 measured reflections

3652 independent reflections

2333 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 25.3^\circ$, $\theta_{\min} = 2.1^\circ$

$h = 0 \rightarrow 11$

$k = -12 \rightarrow 12$
 $l = -13 \rightarrow 13$

3 standard reflections every 120 min
 intensity decay: 1%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.184$
 $S = 1.01$
 3652 reflections
 254 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
 $w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.07P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.033 (5)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.0153 (2)	0.8866 (2)	0.2102 (2)	0.0600 (6)
O2	0.0613 (2)	0.7528 (2)	0.3167 (2)	0.0719 (7)
O3	0.4840 (2)	0.8449 (2)	0.7311 (2)	0.0594 (6)
N1	0.2087 (2)	0.9880 (2)	0.4085 (2)	0.0498 (6)
H1A	0.2141	1.0599	0.3929	0.060*
N2	0.2426 (2)	0.7463 (2)	0.7031 (2)	0.0429 (5)
N3	0.4351 (3)	0.6437 (3)	0.7463 (3)	0.0574 (7)
N4	-0.1874 (3)	0.7568 (2)	0.6228 (3)	0.0567 (7)
C1	-0.1644 (4)	0.8538 (4)	0.0096 (4)	0.0910 (12)
H1B	-0.1731	0.9458	0.0640	0.136*
H1C	-0.2570	0.7920	-0.0708	0.136*
H1D	-0.0855	0.8694	-0.0200	0.136*
C2	-0.1138 (4)	0.6358 (4)	0.0150 (4)	0.0862 (11)
H2B	-0.0922	0.5919	0.0724	0.129*
H2C	-0.0339	0.6503	-0.0136	0.129*
H2D	-0.2057	0.5727	-0.0659	0.129*
C3	-0.2421 (4)	0.7685 (5)	0.1575 (4)	0.0929 (12)
H3B	-0.2485	0.8630	0.2080	0.139*
H3C	-0.2119	0.7312	0.2196	0.139*
H3D	-0.3381	0.7032	0.0834	0.139*
C4	-0.1288 (3)	0.7813 (3)	0.0971 (3)	0.0550 (8)

C5	0.0919 (3)	0.8649 (3)	0.3128 (3)	0.0490 (7)
C6	0.3229 (3)	1.0147 (3)	0.5304 (3)	0.0417 (6)
C7	0.4275 (3)	1.1551 (3)	0.6155 (3)	0.0515 (7)
H7A	0.4202	1.2258	0.5898	0.062*
C8	0.5415 (3)	1.1899 (3)	0.7372 (3)	0.0573 (8)
H8A	0.6102	1.2844	0.7926	0.069*
C9	0.5577 (3)	1.0880 (3)	0.7807 (3)	0.0505 (7)
C10	0.4535 (3)	0.9502 (3)	0.6937 (3)	0.0449 (6)
C11	0.3367 (3)	0.9096 (3)	0.5703 (3)	0.0459 (7)
H11A	0.2689	0.8147	0.5150	0.055*
C12	0.6828 (4)	1.1258 (4)	0.9146 (3)	0.0766 (10)
H12A	0.6742	1.0413	0.9256	0.115*
H12B	0.6764	1.2028	0.9920	0.115*
H12C	0.7773	1.1573	0.9114	0.115*
C13	0.3789 (3)	0.7420 (3)	0.7256 (3)	0.0446 (6)
C14	0.3369 (3)	0.5396 (3)	0.7410 (3)	0.0610 (8)
H14A	0.3692	0.4692	0.7562	0.073*
C15	0.1907 (3)	0.5281 (3)	0.7147 (3)	0.0569 (8)
H15A	0.1244	0.4510	0.7090	0.068*
C16	0.1453 (3)	0.6373 (3)	0.6967 (2)	0.0404 (6)
C17	-0.0094 (3)	0.6389 (3)	0.6684 (3)	0.0404 (6)
C18	-0.1188 (3)	0.5330 (3)	0.6602 (3)	0.0507 (7)
H18A	-0.0970	0.4574	0.6725	0.061*
C19	-0.2597 (3)	0.5405 (3)	0.6339 (3)	0.0571 (8)
H19A	-0.3347	0.4697	0.6277	0.068*
C20	-0.2896 (3)	0.6538 (3)	0.6167 (3)	0.0525 (7)
H20A	-0.3854	0.6584	0.6000	0.063*
C21	-0.0505 (3)	0.7479 (3)	0.6477 (3)	0.0519 (7)
H21A	0.0217	0.8189	0.6514	0.062*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0613 (12)	0.0482 (11)	0.0602 (12)	0.0112 (10)	0.0039 (10)	0.0353 (10)
O2	0.0703 (14)	0.0469 (12)	0.0834 (15)	0.0087 (10)	0.0013 (12)	0.0443 (11)
O3	0.0419 (11)	0.0666 (13)	0.0880 (15)	0.0232 (10)	0.0201 (10)	0.0567 (12)
N1	0.0556 (14)	0.0365 (12)	0.0589 (14)	0.0166 (11)	0.0147 (12)	0.0307 (11)
N2	0.0440 (13)	0.0406 (12)	0.0466 (13)	0.0166 (10)	0.0146 (10)	0.0258 (10)
N3	0.0573 (15)	0.0581 (15)	0.0733 (17)	0.0319 (13)	0.0248 (13)	0.0435 (14)
N4	0.0489 (14)	0.0506 (14)	0.0806 (18)	0.0231 (12)	0.0241 (13)	0.0406 (14)
C1	0.089 (3)	0.086 (3)	0.079 (2)	0.018 (2)	0.000 (2)	0.053 (2)
C2	0.101 (3)	0.064 (2)	0.071 (2)	0.030 (2)	0.023 (2)	0.0216 (19)
C3	0.068 (2)	0.119 (3)	0.106 (3)	0.039 (2)	0.037 (2)	0.066 (3)
C4	0.0508 (17)	0.0516 (17)	0.0580 (18)	0.0161 (14)	0.0135 (15)	0.0299 (15)
C5	0.0509 (16)	0.0428 (15)	0.0578 (17)	0.0181 (13)	0.0175 (14)	0.0313 (14)
C6	0.0423 (14)	0.0407 (14)	0.0512 (16)	0.0192 (12)	0.0210 (13)	0.0275 (13)
C7	0.0546 (17)	0.0417 (15)	0.0616 (18)	0.0178 (13)	0.0215 (15)	0.0296 (14)
C8	0.0544 (17)	0.0427 (16)	0.0601 (18)	0.0088 (13)	0.0149 (15)	0.0219 (14)

C9	0.0457 (15)	0.0533 (17)	0.0540 (17)	0.0176 (14)	0.0182 (13)	0.0293 (14)
C10	0.0398 (14)	0.0521 (16)	0.0591 (17)	0.0218 (13)	0.0230 (13)	0.0375 (14)
C11	0.0455 (15)	0.0396 (14)	0.0556 (17)	0.0150 (12)	0.0194 (13)	0.0271 (13)
C12	0.066 (2)	0.079 (2)	0.065 (2)	0.0115 (18)	0.0066 (17)	0.0370 (19)
C13	0.0442 (15)	0.0469 (15)	0.0458 (15)	0.0180 (12)	0.0138 (12)	0.0278 (13)
C14	0.064 (2)	0.0559 (18)	0.086 (2)	0.0355 (16)	0.0306 (17)	0.0495 (18)
C15	0.0608 (19)	0.0468 (16)	0.078 (2)	0.0229 (14)	0.0281 (16)	0.0424 (16)
C16	0.0502 (15)	0.0341 (13)	0.0380 (14)	0.0169 (12)	0.0157 (12)	0.0193 (11)
C17	0.0445 (15)	0.0343 (13)	0.0423 (14)	0.0150 (11)	0.0142 (12)	0.0210 (11)
C18	0.0527 (17)	0.0448 (15)	0.0610 (18)	0.0179 (13)	0.0187 (14)	0.0343 (14)
C19	0.0512 (17)	0.0516 (17)	0.072 (2)	0.0109 (14)	0.0213 (15)	0.0392 (16)
C20	0.0439 (15)	0.0542 (17)	0.0623 (18)	0.0186 (13)	0.0200 (14)	0.0321 (15)
C21	0.0466 (16)	0.0412 (15)	0.073 (2)	0.0157 (12)	0.0196 (14)	0.0363 (15)

Geometric parameters (Å, °)

O1—C4	1.463 (3)	C6—C7	1.391 (4)
O1—C5	1.344 (3)	C6—C11	1.399 (3)
O2—C5	1.211 (3)	C7—C8	1.373 (4)
O3—C10	1.418 (3)	C7—H7A	0.9300
O3—C13	1.349 (3)	C8—C9	1.396 (4)
N1—C5	1.345 (3)	C8—H8A	0.9300
N1—C6	1.403 (3)	C9—C10	1.372 (4)
N1—H1A	0.8600	C9—C12	1.509 (4)
N3—C13	1.349 (3)	C10—C11	1.380 (4)
N3—C14	1.318 (4)	C11—H11A	0.9300
N4—C20	1.327 (3)	C12—H12A	0.9600
N4—C21	1.336 (3)	C12—H12B	0.9600
C1—C4	1.518 (4)	C12—H12C	0.9600
C1—H1B	0.9600	C14—C15	1.367 (4)
C1—H1C	0.9600	C14—H14A	0.9300
C1—H1D	0.9600	C15—C16	1.397 (3)
N2—C13	1.317 (3)	C15—H15A	0.9300
N2—C16	1.344 (3)	C16—C17	1.482 (4)
C2—C4	1.512 (4)	C17—C18	1.380 (4)
C2—H2B	0.9600	C17—C21	1.391 (3)
C2—H2C	0.9600	C18—C19	1.368 (4)
C2—H2D	0.9600	C18—H18A	0.9300
C3—C4	1.507 (5)	C19—C20	1.379 (4)
C3—H3B	0.9600	C19—H19A	0.9300
C3—H3C	0.9600	C20—H20A	0.9300
C3—H3D	0.9600	C21—H21A	0.9300
C5—O1—C4	122.7 (2)	C9—C8—H8A	118.9
C13—O3—C10	123.90 (19)	C10—C9—C8	116.0 (3)
C5—N1—C6	128.6 (2)	C10—C9—C12	121.7 (3)
C5—N1—H1A	115.7	C8—C9—C12	122.3 (3)
C6—N1—H1A	115.7	C9—C10—C11	124.2 (2)

C13—N2—C16	116.2 (2)	C9—C10—O3	114.6 (2)
C14—N3—C13	113.6 (2)	C11—C10—O3	120.9 (2)
C4—C1—H1B	109.5	C10—C11—C6	118.4 (2)
C4—C1—H1C	109.5	C10—C11—H11A	120.8
H1B—C1—H1C	109.5	C6—C11—H11A	120.8
C4—C1—H1D	109.5	C9—C12—H12A	109.5
H1B—C1—H1D	109.5	C9—C12—H12B	109.5
H1C—C1—H1D	109.5	H12A—C12—H12B	109.5
C4—C2—H2B	109.5	C9—C12—H12C	109.5
C4—C2—H2C	109.5	H12A—C12—H12C	109.5
H2B—C2—H2C	109.5	H12B—C12—H12C	109.5
C4—C2—H2D	109.5	N2—C13—O3	120.7 (2)
H2B—C2—H2D	109.5	N2—C13—N3	128.4 (3)
H2C—C2—H2D	109.5	O3—C13—N3	110.9 (2)
C4—C3—H3B	109.5	N3—C14—C15	124.3 (3)
C4—C3—H3C	109.5	N3—C14—H14A	117.8
H3B—C3—H3C	109.5	C15—C14—H14A	117.8
C4—C3—H3D	109.5	C14—C15—C16	117.1 (3)
H3B—C3—H3D	109.5	C14—C15—H15A	121.4
H3C—C3—H3D	109.5	C16—C15—H15A	121.4
C20—N4—C21	117.2 (2)	N2—C16—C15	120.4 (2)
O1—C4—C3	109.0 (3)	N2—C16—C17	116.8 (2)
O1—C4—C2	110.8 (2)	C15—C16—C17	122.8 (2)
C3—C4—C2	112.3 (3)	C18—C17—C21	117.2 (2)
O1—C4—C1	102.0 (2)	C18—C17—C16	122.0 (2)
C3—C4—C1	111.1 (3)	C21—C17—C16	120.8 (2)
C2—C4—C1	111.1 (3)	C19—C18—C17	119.3 (2)
O2—C5—O1	125.6 (3)	C19—C18—H18A	120.3
O2—C5—N1	126.3 (3)	C17—C18—H18A	120.3
O1—C5—N1	108.1 (2)	C18—C19—C20	119.4 (3)
C7—C6—C11	118.9 (2)	C18—C19—H19A	120.3
C7—C6—N1	117.0 (2)	C20—C19—H19A	120.3
C11—C6—N1	124.0 (2)	N4—C20—C19	122.8 (3)
C8—C7—C6	120.3 (3)	N4—C20—H20A	118.6
C8—C7—H7A	119.8	C19—C20—H20A	118.6
C6—C7—H7A	119.8	N4—C21—C17	124.0 (2)
C7—C8—C9	122.2 (3)	N4—C21—H21A	118.0
C7—C8—H8A	118.9	C17—C21—H21A	118.0
C5—O1—C4—C3	64.0 (3)	C16—N2—C13—O3	178.7 (2)
C5—O1—C4—C2	-60.1 (4)	C16—N2—C13—N3	-1.6 (4)
C5—O1—C4—C1	-178.5 (3)	C10—O3—C13—N2	-9.7 (4)
C4—O1—C5—O2	8.5 (5)	C10—O3—C13—N3	170.6 (2)
C4—O1—C5—N1	-172.4 (2)	C14—N3—C13—N2	0.8 (4)
C6—N1—C5—O2	2.1 (5)	C14—N3—C13—O3	-179.5 (2)
C6—N1—C5—O1	-177.0 (2)	C13—N3—C14—C15	1.1 (5)
C5—N1—C6—C7	-177.0 (3)	N3—C14—C15—C16	-2.0 (5)
C5—N1—C6—C11	2.9 (4)	C13—N2—C16—C15	0.5 (4)

C11—C6—C7—C8	-0.6 (4)	C13—N2—C16—C17	-178.7 (2)
N1—C6—C7—C8	179.3 (3)	C14—C15—C16—N2	1.1 (4)
C6—C7—C8—C9	0.0 (5)	C14—C15—C16—C17	-179.7 (3)
C7—C8—C9—C10	0.6 (4)	N2—C16—C17—C18	-179.7 (2)
C7—C8—C9—C12	-179.9 (3)	C15—C16—C17—C18	1.1 (4)
C8—C9—C10—C11	-0.7 (4)	N2—C16—C17—C21	0.9 (4)
C12—C9—C10—C11	179.9 (3)	C15—C16—C17—C21	-178.3 (3)
C8—C9—C10—O3	172.1 (2)	C21—C17—C18—C19	-0.6 (4)
C12—C9—C10—O3	-7.3 (4)	C16—C17—C18—C19	180.0 (2)
C13—O3—C10—C9	138.8 (3)	C17—C18—C19—C20	-0.3 (4)
C13—O3—C10—C11	-48.2 (4)	C21—N4—C20—C19	-0.4 (4)
C9—C10—C11—C6	0.1 (4)	C18—C19—C20—N4	0.8 (5)
O3—C10—C11—C6	-172.3 (2)	C20—N4—C21—C17	-0.6 (4)
C7—C6—C11—C10	0.6 (4)	C18—C17—C21—N4	1.1 (4)
N1—C6—C11—C10	-179.3 (2)	C16—C17—C21—N4	-179.5 (3)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots N4 ⁱ	0.86	2.10	2.944 (4)	165
C15—H15A \cdots O2 ⁱⁱ	0.93	2.45	3.382 (4)	177
C18—H18A \cdots O2 ⁱⁱ	0.93	2.39	3.319 (4)	174
C3—H3B \cdots Cg1 ⁱ	0.96	2.86	3.560 (3)	131
C12—H12B \cdots Cg2 ⁱⁱⁱ	0.96	2.90	3.788 (3)	154

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $-x, -y+1, -z+1$; (iii) $-x+1, -y+2, -z+2$.