organic compounds

Ethyl 4-hydroxy-1-(2-morpholinopropanoyl)-2,6-diphenyl-1,2,5,6-tetrahydropyridin-3-carboxylate

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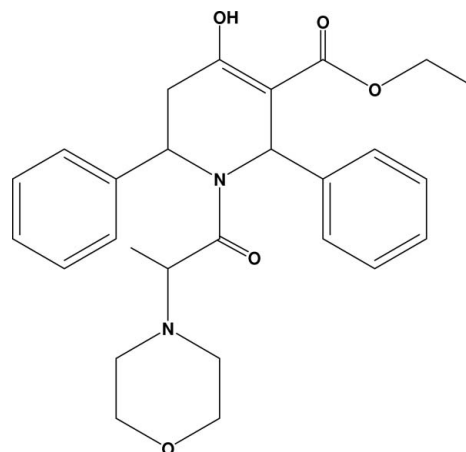Correspondence e-mail: ytjeong@pknu.ac.kr

In the title compound, $C_{27}H_{32}N_2O_5$, the morpholine ring adopts a chair conformation with two C atoms deviating by -0.656 (4) and 0.679 (3) Å from the least-squares plane defined by the rest of atoms in the ring. The tetrahydropyridine ring adopts a half-chair conformation. The molecular structure is stabilized by a strong intramolecular O—H···O interaction, generating an $S(6)$ motif. The crystal packing is stabilized by intermolecular C—H···O interactions, generating a $C(7)$ chain along the a axis, and $R_2^2(20)$ and $R_4^4(20)$ graph-set motifs.

Related literature

For related structures, see: Aridoss et al. (2009a,b); Gayathri et al. (2008); Kavitha et al. (2007); Ramachandran et al. (2008); Subha Nandhini et al. (2003). For ring conformational analysis, see: Cremer & Pople (1975); Nardelli (1983).

Experimental

Crystal data

$C_{27}H_{32}N_2O_5$	V = 2505.66 (14) Å^3
M_r = 464.55	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 8.2251 (2) Å	μ = 0.09 mm^{-1}
b = 10.6219 (4) Å	T = 293 K
c = 28.7046 (10) Å	$0.30 \times 0.20 \times 0.20$ mm
β = 92.375 (2)°	

Data collection

Bruker Kappa APEXII CCD diffractometer	22895 measured reflections
	4850 independent reflections
Absorption correction: multi-scan (SADABS; Bruker 1999)	3353 reflections with $I > 2\sigma(I)$
T_{min} = 0.975, T_{max} = 0.983	R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052	308 parameters
$wR(F^2)$ = 0.145	H-atom parameters constrained
S = 1.02	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
4850 reflections	$\Delta\rho_{min}$ = -0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O4	0.82	1.83	2.542 (2)	145
C10—H10A···O1[i]	0.97	2.51	3.311 (3)	140
C11—H11A···O2[ii]	0.97	2.54	3.222 (3)	127
C26—H26B···O3[iii]	0.97	2.53	3.470 (4)	163

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SIR92 (Altomare et al., 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2497).

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supporting information

Ethyl 4-hydroxy-1-(2-morpholinopropanoyl)-2,6-diphenyl-1,2,5,6-tetrahydro-pyridin-3-carboxylate

G. Aridoss, D. Gayathri, R. Ramachandran, Kwon Taek Lim and Yeon Tae Jeong

S1. Comment

It has been reported earlier that 2,6-diarylpiperidin-4-ones are in rigid chair conformation with equatorial orientation of the two aryl groups (Gayathri *et al.* 2008; Kavitha *et al.* 2007). Upon chloroacetylation (Aridoss *et al.* 2009*b*) or bromo-acetylation (Ramachandran *et al.* 2008) of the 2,6-diarylpiperidin-4-one, the normal chair conformation of the piperidone ring was changed into non-chair conformation of its preference. Similarly, bromopropionylation of ethyl 4-oxo-2,6-di-phenyl-4-piperidin-3-carboxylate gave ethyl 1-(2-bromopropanoyl)-4-hydroxy-2,6-diphenyl- 1,2,5,6-tetrahydropyridin-3-carboxylate as the product (Aridoss *et al.* 2009*a*) wherein the normal chair conformation of the piperidone ring in starting material (Subha Nandhini *et al.* 2003) was changed into a non-chair conformation. In continuation of this, we report here the crystal structure of the title compound.

The sum of the angles at N1 [359.5 (6)°] and N2 [337.6 (6)°] are in accordance with *sp²* and *sp³* hybridization. The dihedral angle between the two phenyl rings is 35.0 (1)°. The morpholine ring adopts a chair conformation with atoms C9 and C11 deviating by -0.656 (4) and 0.679 (3) Å, respectively, from the least squares plane defined by N2/C8/O2/C10. The tetrahydropyridine ring adopts a half chair conformation. The puckering parameters (Cremer & Pople, 1975) and the smallest displacement asymmetry parameters (Nardelli, 1983) for the morpholine and tetrahydropyridine rings are q_2 = 0.010 (3), 0.324 (2) Å, q_3 = -0.572 (3), -0.287 (2) Å; Q_T = 0.573 (3), 0.433 (2) Å and θ = 177.8 (3), 131.5 (3)°, respectively.

The molecule is stabilized by a strong O—H⋯O intramolecular interaction, wherein, atom O3 acts as a donor to O4, generating an S(6) motif. The crystal packing is stabilized by C—H⋯O intermolecular interactions. Atoms C10 and C26 act as donors to O1 and O3, respectively, each generating a chain of C(7) running along the *a* axis, which in turn generates an $R_2^2(20)$ graph set motif. Atom C11 acts as a donor to O2 at (1 - *x*, 1/2 + *y*, 1/2 - *z*), generating an $R_4^4(20)$ graph set motif together with a C10—H10A⋯O1 intermolecular interaction.

S2. Experimental

To a solution of morpholine (1 equiv.) and dry K₂CO₃ in benzene, ethyl 1-(2-bromopropanoyl)-4-hydroxy-2,6-di-phenyl-1,2,5,6-tetrahydropyridin-3- carboxylate (1 equiv.) in benzene (Aridoss *et al.*, 2009*a*) was added slowly over a period of 15 minutes. Later the contents were refluxed over night. After the completion of reaction, the contents were poured into water and extracted twice with ethyl acetate. The combined organic extracts were then washed well with brine and dried over anhydrous sodium sulfate. This upon evaporation, column purification and subsequent recrystallization in distilled ethanol afforded fine white crystals suitable for X-ray diffraction study.

S3. Refinement

C-bound H atoms were refined using a riding model, with d(C—H) = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C) for aromatic, 0.98 Å and U_{iso}(H) = $1.2U_{eq}$(C) for CH, 0.97 Å and U_{iso}(H) = $1.2U_{eq}$(C) for CH$_2$, and 0.96 Å and U_{iso}(H) = $1.5U_{eq}$(C) for CH$_3$. The H atom of the OH group was also refined using a riding model, with d(O—H) = 0.82 Å, but the U_{iso}(H) was refiend freely.
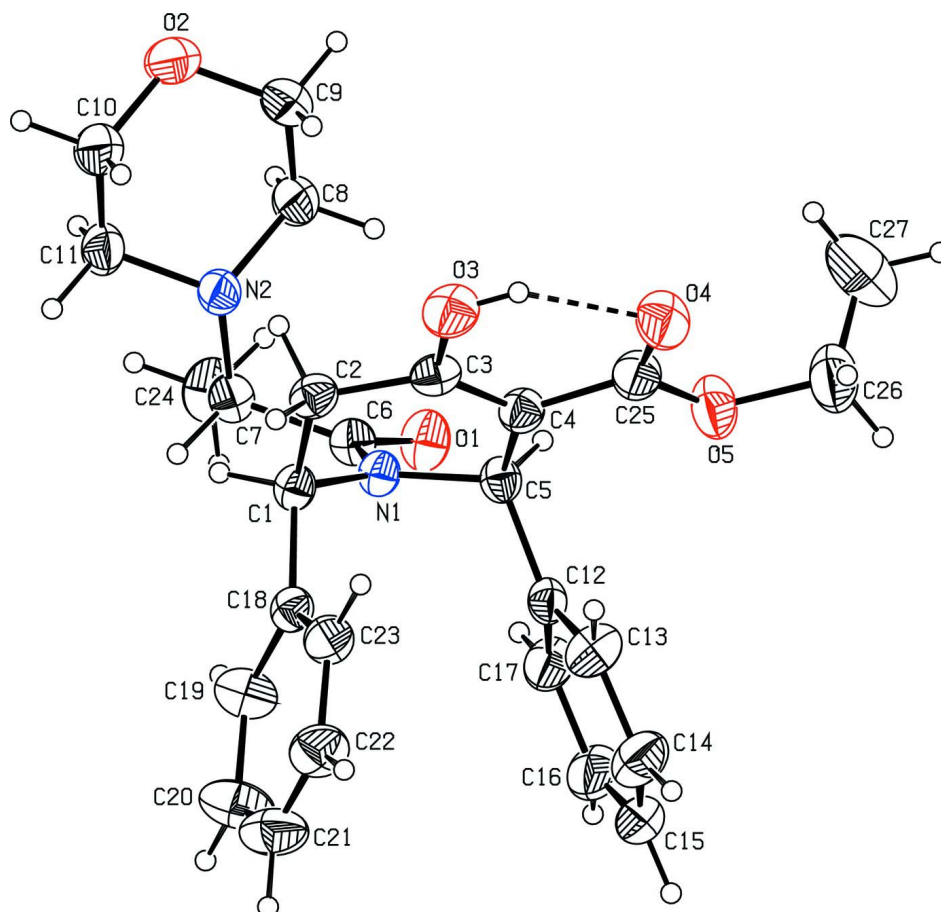
Figure 1

The molecular structure of title compound, showing 30% probability displacement ellipsoids.
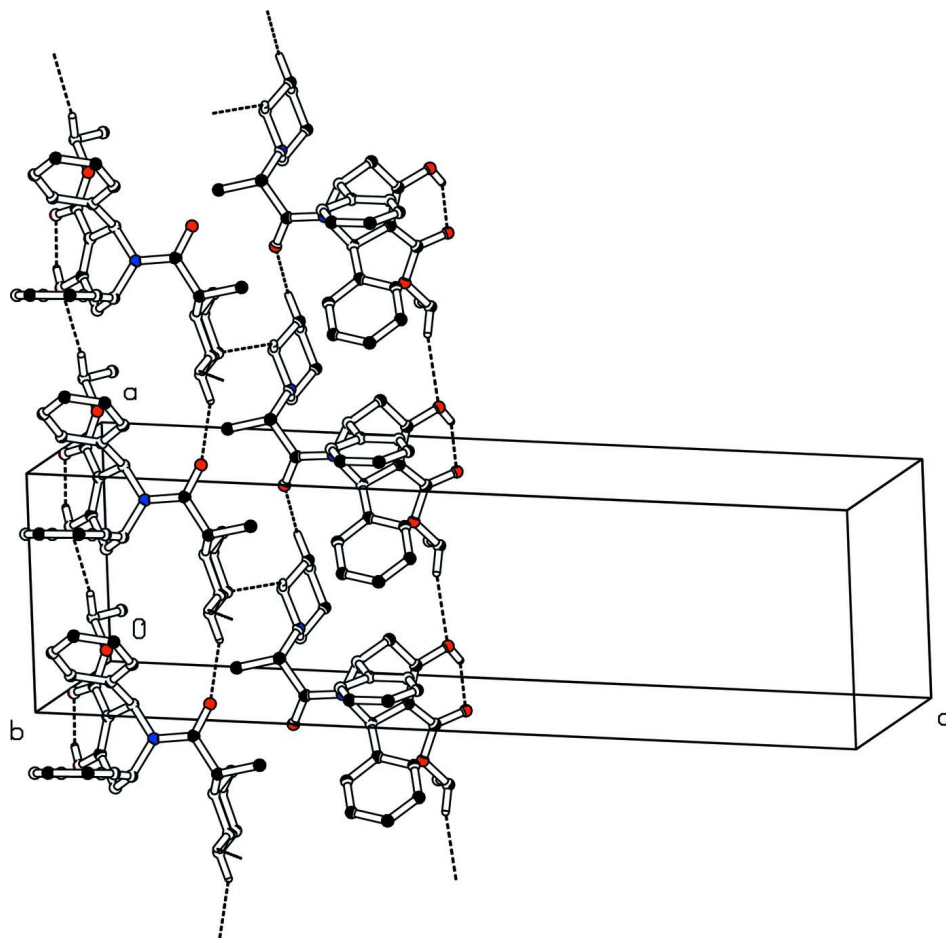
Figure 2

The molecular packing of (I). For clarity, hydrogen atoms which are not involved in hydrogen bonding are omitted.

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Crystal data

$C_{27}H_{32}N_2O_5$	$F(000) = 992$
$M_r = 464.55$	$D_x = 1.231$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 5113 reflections
$a = 8.2251$ (2) Å	$\theta = 2.4$–23.3°
$b = 10.6219$ (4) Å	$\mu = 0.09$ mm^{-1}
$c = 28.7046$ (10) Å	$T = 293$ K
$\beta = 92.375$ (2)°	Block, colourless
$V = 2505.66$ (14) Å^3	$0.30 \times 0.20 \times 0.20$ mm
$Z = 4$	

Data collection

Bruker Kappa APEXII CCD diffractometer	Absorption correction: multi-scan (*SADABS*; Bruker 1999)
Radiation source: fine-focus sealed tube	$T_{min} = 0.975$, $T_{max} = 0.983$
Graphite monochromator	22895 measured reflections
ω and φ scan	4850 independent reflections
	3353 reflections with $I > 2\sigma(I)$

$R_{int} = 0.036$

$\theta_{max} = 25.9°$, $\theta_{min} = 2.0°$

$h = -10 \rightarrow 9$

$k = -13 \rightarrow 12$

$l = -35 \rightarrow 35$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.052$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.145$	
$S = 1.02$	H-atom parameters constrained
4850 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 1.1339P]$
308 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.29$ e Å^{-3}
	$\Delta\rho_{min} = -0.21$ 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	−0.09176 (19)	0.60293 (18)	0.27695 (5)	0.0644 (5)
N2	0.2969 (2)	0.54061 (17)	0.28207 (6)	0.0498 (5)
C1	0.2028 (2)	0.6983 (2)	0.36715 (7)	0.0444 (5)
H1A	0.2803	0.7179	0.3432	0.053*
C2	0.2787 (3)	0.5948 (2)	0.39704 (8)	0.0509 (5)
H2A	0.3412	0.5401	0.3775	0.061*
H2B	0.3535	0.6323	0.4201	0.061*
O2	0.4987 (2)	0.32639 (18)	0.27766 (9)	0.0972 (7)
O3	0.2277 (2)	0.44389 (18)	0.45418 (6)	0.0688 (5)
H3A	0.1594	0.3950	0.4637	0.118 (15)*
C3	0.1586 (3)	0.5184 (2)	0.42121 (7)	0.0502 (5)
O4	−0.0581 (2)	0.36103 (18)	0.46520 (6)	0.0758 (5)
C4	−0.0018 (3)	0.5187 (2)	0.40991 (7)	0.0491 (5)
O5	−0.2586 (2)	0.43166 (18)	0.41704 (7)	0.0763 (5)
C5	−0.0748 (2)	0.6014 (2)	0.37157 (7)	0.0445 (5)
H5A	−0.1409	0.5455	0.3513	0.053*
N1	0.05448 (19)	0.65010 (16)	0.34259 (5)	0.0433 (4)
C6	0.0380 (3)	0.6339 (2)	0.29554 (7)	0.0486 (5)
C7	0.1903 (3)	0.6443 (2)	0.26673 (7)	0.0509 (5)
H7A	0.2453	0.7233	0.2753	0.061*
C8	0.2302 (3)	0.4162 (2)	0.27172 (10)	0.0669 (7)
H8A	0.2218	0.4036	0.2382	0.080*

H8B	0.1219	0.4096	0.2837	0.080*
C9	0.3375 (3)	0.3183 (3)	0.29354 (13)	0.0853 (9)
H9A	0.3400	0.3282	0.3272	0.102*
H9B	0.2933	0.2356	0.2861	0.102*
C10	0.5629 (3)	0.4474 (3)	0.28766 (12)	0.0811 (9)
H10A	0.6724	0.4527	0.2765	0.097*
H10B	0.5690	0.4600	0.3212	0.097*
C11	0.4610 (3)	0.5486 (2)	0.26541 (9)	0.0634 (7)
H11A	0.5074	0.6303	0.2731	0.076*
H11B	0.4584	0.5390	0.2318	0.076*
C12	−0.1901 (2)	0.7031 (2)	0.38781 (7)	0.0454 (5)
C13	−0.2138 (3)	0.7287 (3)	0.43393 (8)	0.0654 (7)
H13A	−0.1534	0.6855	0.4569	0.078*
C14	−0.3262 (3)	0.8179 (3)	0.44672 (11)	0.0777 (8)
H14A	−0.3411	0.8335	0.4781	0.093*
C15	−0.4147 (3)	0.8827 (3)	0.41383 (12)	0.0761 (8)
H15A	−0.4900	0.9427	0.4225	0.091*
C16	−0.3922 (3)	0.8588 (3)	0.36786 (12)	0.0791 (8)
H16A	−0.4518	0.9034	0.3451	0.095*
C17	−0.2821 (3)	0.7691 (3)	0.35491 (9)	0.0647 (7)
H17A	−0.2696	0.7528	0.3234	0.078*
C18	0.1703 (2)	0.8208 (2)	0.39239 (7)	0.0456 (5)
C19	0.1431 (3)	0.9284 (2)	0.36661 (9)	0.0683 (7)
H19A	0.1400	0.9239	0.3342	0.082*
C20	0.1205 (4)	1.0428 (3)	0.38800 (12)	0.0894 (10)
H20A	0.1021	1.1148	0.3701	0.107*
C21	0.1254 (4)	1.0502 (3)	0.43555 (12)	0.0841 (9)
H21A	0.1099	1.1274	0.4500	0.101*
C22	0.1524 (3)	0.9460 (3)	0.46159 (9)	0.0727 (8)
H22A	0.1563	0.9515	0.4940	0.087*
C23	0.1744 (3)	0.8312 (2)	0.44022 (8)	0.0577 (6)
H23A	0.1923	0.7598	0.4584	0.069*
C24	0.1449 (3)	0.6501 (3)	0.21484 (8)	0.0750 (8)
H24A	0.2419	0.6567	0.1976	0.113*
H24B	0.0771	0.7222	0.2086	0.113*
H24C	0.0870	0.5750	0.2057	0.113*
C25	−0.1051 (3)	0.4311 (2)	0.43333 (9)	0.0593 (6)
C26	−0.3741 (4)	0.3489 (3)	0.43944 (13)	0.0938 (10)
H26A	−0.3403	0.3369	0.4719	0.113*
H26B	−0.4810	0.3875	0.4383	0.113*
C27	−0.3819 (6)	0.2296 (4)	0.41630 (19)	0.1500 (18)
H27A	−0.4578	0.1761	0.4313	0.225*
H27B	−0.2762	0.1912	0.4177	0.225*
H27C	−0.4169	0.2416	0.3843	0.225*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0516 (9)	0.0898 (13)	0.0509 (9)	−0.0112 (9)	−0.0078 (7)	−0.0060 (8)
N2	0.0478 (10)	0.0492 (11)	0.0528 (10)	−0.0081 (8)	0.0058 (8)	−0.0110 (8)
C1	0.0400 (11)	0.0524 (13)	0.0408 (10)	−0.0027 (9)	0.0002 (8)	−0.0027 (9)
C2	0.0457 (12)	0.0547 (13)	0.0518 (12)	0.0047 (10)	−0.0029 (9)	−0.0057 (10)
O2	0.0619 (12)	0.0616 (12)	0.169 (2)	0.0010 (9)	0.0195 (12)	−0.0312 (13)
O3	0.0628 (10)	0.0734 (12)	0.0696 (11)	0.0181 (10)	−0.0053 (9)	0.0206 (9)
C3	0.0548 (13)	0.0490 (13)	0.0466 (12)	0.0115 (10)	−0.0001 (10)	−0.0004 (10)
O4	0.0742 (12)	0.0752 (12)	0.0780 (12)	0.0057 (10)	0.0046 (9)	0.0336 (10)
C4	0.0472 (12)	0.0507 (13)	0.0493 (12)	0.0049 (10)	0.0022 (9)	0.0051 (10)
O5	0.0573 (10)	0.0811 (13)	0.0902 (13)	−0.0100 (9)	0.0009 (9)	0.0335 (10)
C5	0.0411 (11)	0.0482 (12)	0.0438 (11)	−0.0037 (9)	−0.0013 (9)	0.0040 (9)
N1	0.0397 (9)	0.0502 (10)	0.0399 (9)	−0.0025 (8)	−0.0006 (7)	−0.0016 (8)
C6	0.0494 (12)	0.0520 (13)	0.0439 (11)	−0.0026 (10)	−0.0020 (9)	−0.0026 (10)
C7	0.0557 (13)	0.0551 (14)	0.0420 (11)	−0.0060 (11)	0.0029 (9)	−0.0028 (10)
C8	0.0549 (14)	0.0582 (15)	0.0883 (18)	−0.0127 (12)	0.0102 (13)	−0.0190 (14)
C9	0.0709 (18)	0.0493 (16)	0.137 (3)	−0.0089 (13)	0.0176 (18)	−0.0140 (17)
C10	0.0524 (15)	0.0664 (18)	0.125 (3)	−0.0077 (13)	0.0122 (15)	−0.0193 (17)
C11	0.0523 (13)	0.0639 (16)	0.0748 (16)	−0.0151 (12)	0.0146 (12)	−0.0146 (13)
C12	0.0364 (10)	0.0493 (12)	0.0505 (12)	−0.0039 (9)	0.0012 (9)	0.0070 (10)
C13	0.0607 (14)	0.0823 (18)	0.0530 (13)	0.0145 (13)	−0.0005 (11)	−0.0028 (13)
C14	0.0641 (16)	0.093 (2)	0.0767 (18)	0.0074 (16)	0.0106 (14)	−0.0208 (16)
C15	0.0513 (15)	0.0607 (17)	0.117 (3)	0.0051 (12)	0.0178 (15)	−0.0037 (17)
C16	0.0612 (16)	0.078 (2)	0.099 (2)	0.0209 (14)	0.0122 (15)	0.0306 (17)
C17	0.0573 (14)	0.0737 (17)	0.0636 (15)	0.0108 (13)	0.0070 (11)	0.0185 (13)
C18	0.0378 (11)	0.0509 (13)	0.0476 (12)	−0.0014 (9)	−0.0027 (9)	−0.0040 (10)
C19	0.0879 (19)	0.0577 (16)	0.0577 (14)	0.0038 (13)	−0.0153 (13)	−0.0019 (12)
C20	0.118 (3)	0.0547 (17)	0.093 (2)	0.0152 (16)	−0.0289 (19)	−0.0008 (16)
C21	0.091 (2)	0.0642 (19)	0.095 (2)	0.0138 (16)	−0.0131 (17)	−0.0268 (17)
C22	0.0827 (19)	0.075 (2)	0.0602 (15)	0.0021 (15)	0.0043 (13)	−0.0204 (15)
C23	0.0636 (14)	0.0596 (15)	0.0502 (13)	−0.0008 (12)	0.0064 (11)	−0.0055 (11)
C24	0.0797 (18)	0.101 (2)	0.0441 (13)	−0.0055 (16)	0.0046 (12)	0.0004 (14)
C25	0.0559 (14)	0.0597 (15)	0.0625 (14)	0.0066 (12)	0.0047 (11)	0.0135 (12)
C26	0.0666 (18)	0.096 (3)	0.119 (3)	−0.0084 (17)	0.0110 (17)	0.041 (2)
C27	0.161 (4)	0.083 (3)	0.206 (5)	−0.035 (3)	0.016 (4)	0.014 (3)

Geometric parameters (Å, º)

O1—C6	1.219 (2)	C10—H10B	0.9700
N2—C11	1.453 (3)	C11—H11A	0.9700
N2—C8	1.457 (3)	C11—H11B	0.9700
N2—C7	1.464 (3)	C12—C13	1.373 (3)
C1—N1	1.475 (2)	C12—C17	1.377 (3)
C1—C2	1.513 (3)	C13—C14	1.384 (4)
C1—C18	1.518 (3)	C13—H13A	0.9300
C1—H1A	0.9800	C14—C15	1.356 (4)

C2—C3	1.474 (3)	C14—H14A	0.9300
C2—H2A	0.9700	C15—C16	1.364 (4)
C2—H2B	0.9700	C15—H15A	0.9300
O2—C10	1.414 (3)	C16—C17	1.376 (4)
O2—C9	1.423 (3)	C16—H16A	0.9300
O3—C3	1.342 (3)	C17—H17A	0.9300
O3—H3A	0.8200	C18—C19	1.375 (3)
C3—C4	1.345 (3)	C18—C23	1.376 (3)
O4—C25	1.229 (3)	C19—C20	1.378 (4)
C4—C25	1.445 (3)	C19—H19A	0.9300
C4—C5	1.513 (3)	C20—C21	1.366 (4)
O5—C25	1.328 (3)	C20—H20A	0.9300
O5—C26	1.463 (3)	C21—C22	1.349 (4)
C5—N1	1.471 (2)	C21—H21A	0.9300
C5—C12	1.524 (3)	C22—C23	1.380 (3)
C5—H5A	0.9800	C22—H22A	0.9300
N1—C6	1.363 (3)	C23—H23A	0.9300
C6—C7	1.533 (3)	C24—H24A	0.9600
C7—C24	1.522 (3)	C24—H24B	0.9600
C7—H7A	0.9800	C24—H24C	0.9600
C8—C9	1.486 (4)	C26—C27	1.430 (5)
C8—H8A	0.9700	C26—H26A	0.9700
C8—H8B	0.9700	C26—H26B	0.9700
C9—H9A	0.9700	C27—H27A	0.9600
C9—H9B	0.9700	C27—H27B	0.9600
C10—C11	1.491 (4)	C27—H27C	0.9600
C10—H10A	0.9700		
C11—N2—C8	109.46 (18)	C10—C11—H11A	109.8
C11—N2—C7	114.22 (18)	N2—C11—H11B	109.8
C8—N2—C7	113.89 (18)	C10—C11—H11B	109.8
N1—C1—C2	109.42 (17)	H11A—C11—H11B	108.3
N1—C1—C18	111.54 (16)	C13—C12—C17	117.7 (2)
C2—C1—C18	115.37 (17)	C13—C12—C5	123.4 (2)
N1—C1—H1A	106.7	C17—C12—C5	118.8 (2)
C2—C1—H1A	106.7	C12—C13—C14	120.9 (2)
C18—C1—H1A	106.7	C12—C13—H13A	119.5
C3—C2—C1	113.42 (17)	C14—C13—H13A	119.5
C3—C2—H2A	108.9	C15—C14—C13	120.6 (3)
C1—C2—H2A	108.9	C15—C14—H14A	119.7
C3—C2—H2B	108.9	C13—C14—H14A	119.7
C1—C2—H2B	108.9	C14—C15—C16	119.3 (3)
H2A—C2—H2B	107.7	C14—C15—H15A	120.4
C10—O2—C9	109.6 (2)	C16—C15—H15A	120.4
C3—O3—H3A	109.5	C15—C16—C17	120.5 (3)
O3—C3—C4	123.6 (2)	C15—C16—H16A	119.8
O3—C3—C2	112.59 (19)	C17—C16—H16A	119.8
C4—C3—C2	123.7 (2)	C12—C17—C16	121.1 (2)

C3—C4—C25	118.4 (2)	C12—C17—H17A	119.5
C3—C4—C5	122.17 (19)	C16—C17—H17A	119.5
C25—C4—C5	119.27 (19)	C19—C18—C23	117.8 (2)
C25—O5—C26	117.9 (2)	C19—C18—C1	118.91 (19)
N1—C5—C4	109.94 (16)	C23—C18—C1	123.2 (2)
N1—C5—C12	113.43 (17)	C18—C19—C20	121.0 (2)
C4—C5—C12	114.99 (17)	C18—C19—H19A	119.5
N1—C5—H5A	105.9	C20—C19—H19A	119.5
C4—C5—H5A	105.9	C21—C20—C19	119.8 (3)
C12—C5—H5A	105.9	C21—C20—H20A	120.1
C6—N1—C5	118.14 (16)	C19—C20—H20A	120.1
C6—N1—C1	124.31 (17)	C22—C21—C20	120.2 (3)
C5—N1—C1	117.05 (15)	C22—C21—H21A	119.9
O1—C6—N1	121.15 (19)	C20—C21—H21A	119.9
O1—C6—C7	120.23 (19)	C21—C22—C23	120.0 (3)
N1—C6—C7	118.41 (18)	C21—C22—H22A	120.0
N2—C7—C24	116.4 (2)	C23—C22—H22A	120.0
N2—C7—C6	106.06 (17)	C18—C23—C22	121.1 (2)
C24—C7—C6	110.97 (18)	C18—C23—H23A	119.5
N2—C7—H7A	107.7	C22—C23—H23A	119.5
C24—C7—H7A	107.7	C7—C24—H24A	109.5
C6—C7—H7A	107.7	C7—C24—H24B	109.5
N2—C8—C9	109.7 (2)	H24A—C24—H24B	109.5
N2—C8—H8A	109.7	C7—C24—H24C	109.5
C9—C8—H8A	109.7	H24A—C24—H24C	109.5
N2—C8—H8B	109.7	H24B—C24—H24C	109.5
C9—C8—H8B	109.7	O4—C25—O5	122.0 (2)
H8A—C8—H8B	108.2	O4—C25—C4	124.3 (2)
O2—C9—C8	111.6 (2)	O5—C25—C4	113.7 (2)
O2—C9—H9A	109.3	C27—C26—O5	110.2 (3)
C8—C9—H9A	109.3	C27—C26—H26A	109.6
O2—C9—H9B	109.3	O5—C26—H26A	109.6
C8—C9—H9B	109.3	C27—C26—H26B	109.6
H9A—C9—H9B	108.0	O5—C26—H26B	109.6
O2—C10—C11	111.7 (2)	H26A—C26—H26B	108.1
O2—C10—H10A	109.3	C26—C27—H27A	109.5
C11—C10—H10A	109.3	C26—C27—H27B	109.5
O2—C10—H10B	109.3	H27A—C27—H27B	109.5
C11—C10—H10B	109.3	C26—C27—H27C	109.5
H10A—C10—H10B	107.9	H27A—C27—H27C	109.5
N2—C11—C10	109.3 (2)	H27B—C27—H27C	109.5
N2—C11—H11A	109.8		
N1—C1—C2—C3	−40.7 (2)	C9—O2—C10—C11	−58.4 (3)
C18—C1—C2—C3	86.0 (2)	C8—N2—C11—C10	−57.6 (3)
C1—C2—C3—O3	−167.93 (18)	O2—C10—C11—N2	58.9 (3)
C1—C2—C3—C4	15.2 (3)	N1—C5—C12—C13	−120.7 (2)
O3—C3—C4—C25	−2.2 (3)		

C2—C3—C4—C25	174.4 (2)	C4—C5—C12—C13	7.0 (3)
O3—C3—C4—C5	−178.2 (2)	N1—C5—C12—C17	62.6 (3)
C2—C3—C4—C5	−1.6 (3)	C4—C5—C12—C17	−169.6 (2)
C3—C4—C5—N1	14.9 (3)	C17—C12—C13—C14	0.0 (4)
C25—C4—C5—N1	−161.11 (19)	C5—C12—C13—C14	−176.7 (2)
C3—C4—C5—C12	−114.6 (2)	C12—C13—C14—C15	−0.5 (4)
C25—C4—C5—C12	69.4 (3)	C13—C14—C15—C16	0.2 (4)
C4—C5—N1—C6	127.7 (2)	C14—C15—C16—C17	0.6 (4)
C12—C5—N1—C6	−102.0 (2)	C13—C12—C17—C16	0.9 (4)
C4—C5—N1—C1	−44.5 (2)	C5—C12—C17—C16	177.7 (2)
C12—C5—N1—C1	85.8 (2)	C15—C16—C17—C12	−1.2 (4)
C2—C1—N1—C6	−113.0 (2)	N1—C1—C18—C19	−71.5 (2)
C18—C1—N1—C6	118.1 (2)	C2—C1—C18—C19	162.9 (2)
C2—C1—N1—C5	58.7 (2)	N1—C1—C18—C23	111.8 (2)
C18—C1—N1—C5	−70.1 (2)	C2—C1—C18—C23	−13.8 (3)
C5—N1—C6—O1	14.1 (3)	C23—C18—C19—C20	−0.1 (4)
C1—N1—C6—O1	−174.3 (2)	C1—C18—C19—C20	−177.0 (3)
C5—N1—C6—C7	−160.63 (18)	C18—C19—C20—C21	0.2 (5)
C1—N1—C6—C7	11.0 (3)	C19—C20—C21—C22	0.1 (5)
C11—N2—C7—C24	67.5 (3)	C20—C21—C22—C23	−0.4 (5)
C8—N2—C7—C24	−59.3 (3)	C19—C18—C23—C22	−0.1 (3)
C11—N2—C7—C6	−168.57 (18)	C1—C18—C23—C22	176.6 (2)
C8—N2—C7—C6	64.6 (2)	C21—C22—C23—C18	0.4 (4)
O1—C6—C7—N2	−110.6 (2)	C26—O5—C25—O4	2.3 (4)
N1—C6—C7—N2	64.2 (2)	C26—O5—C25—C4	−178.2 (2)
O1—C6—C7—C24	16.7 (3)	C3—C4—C25—O4	4.8 (4)
N1—C6—C7—C24	−168.6 (2)	C5—C4—C25—O4	−179.1 (2)
C11—N2—C8—C9	57.5 (3)	C3—C4—C25—O5	−174.8 (2)
C7—N2—C8—C9	−173.2 (2)	C5—C4—C25—O5	1.4 (3)
C10—O2—C9—C8	58.0 (3)	C25—O5—C26—C27	−91.5 (4)
N2—C8—C9—O2	−58.1 (3)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O4	0.82	1.83	2.542 (2)	145
C10—H10A···O1[i]	0.97	2.51	3.311 (3)	140
C11—H11A···O2[ii]	0.97	2.54	3.222 (3)	127
C26—H26B···O3[iii]	0.97	2.53	3.470 (4)	163

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