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Ethyl 1-benzoyl-4-hydroxy-2,6-diphenyl-1,2,5,6-tetrahydropyridine-3-carboxylate

G. Aridoss,[a] S. Sundaramoorthy,[b] D. Velmurugan[b] and Y. T. Jeong[a]*

[a]Department of Image Science and Engineering, Pukyong National University, Busan 608-739, Republic of Korea, and [b]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India
Correspondence e-mail: ytjeong@pknu.ac.kr

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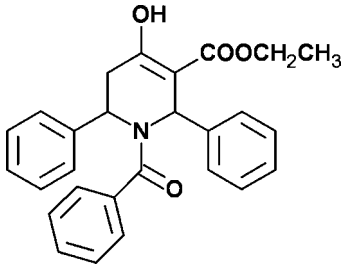
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.120; data-to-parameter ratio = 19.1.

In the title compound, $C_{27}H_{25}NO_4$, the tetrahydropyridine ring adopts a half-chair conformation. The three phenyl rings form dihedral angles of 66.33 (7), 87.36 (8) and 36.90 (7)° with the least-squares plane through the tetrahydropyridine ring. The molecular conformation is stabilized by an intramolecular O—H···O hydrogen bond, generating an S(6) motif.

Related literature

For related structures, see: Subha Nandhini *et al.* (2003); Nithya *et al.* (2009); Aravindhan *et al.* (2009); Aridoss *et al.* (2009, 2010). For ring conformational analysis, see: Cremer & Pople (1975); Nardelli (1983).



Experimental

Crystal data

$C_{27}H_{25}NO_4$
M_r = 427.48
Triclinic, $P\overline{1}$
a = 8.2784 (7) Å
b = 10.6116 (9) Å
c = 12.7572 (11) Å
α = 85.681 (4)°
β = 89.963 (4)°
γ = 82.508 (5)°
V = 1107.91 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.25 × 0.23 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.979, T_{max} = 0.983
20295 measured reflections
5526 independent reflections
4179 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.120
S = 1.04
5526 reflections
290 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O2	0.82	1.85	2.570 (2)	146

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (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: IS2669).

References

Aravindhan, S., Ponnuswamy, S., Umamaheswari, J., Ramesh, P. & Ponnuswamy, M. N. (2009). *Acta Cryst.* E**65**, o1975.
Aridoss, G., Gayathri, D., Velmurugan, D., Kim, M. S. & Jeong, Y. T. (2009). *Acta Cryst.* E**65**, o1708–o1709.
Aridoss, G., Sundaramoorthy, S., Velmurugan, D., Park, K. S. & Jeong, Y. T. (2010). *Acta Cryst.* E**66**, o1982.
Bruker (2008). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Nardelli, M. (1983). *Acta Cryst.* C**39**, 1141–1142.
Nithya, P., Hathwar, V. R., Kone, S., Malathi, N. & Khan, F. N. (2009). *Acta Cryst.* E**65**, 1692–1693.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Subha Nandhini, M., Vijayakumar, V., Mostad, A., Sundaravadivelu, M. & Natarajan, S. (2003). *Acta Cryst.* E**59**, o1672–o1674.

supporting information

Acta Cryst. (2011). E**67**, o540 [doi:10.1107/S1600536811003266]

Ethyl 1-benzoyl-4-hydroxy-2,6-diphenyl-1,2,5,6-tetrahydropyridine-3-carboxylate

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S1. Comment

Owing to the relevance of piperidine-containing bioactive compounds, the development of new piperidine based derivatives continues to be a subject of considerable interest. The pharmacological effects of potential new drugs depend entirely on the stereochemistry and ring conformations of the compounds and hence the crystallographic study of the title compound has been carried out.

The *ORTEP* diagram of the title compound is shown in Fig. 1. The tetrahydropyridine ring adopts a half-chair conformation. The puckering parameters (Cremer & Pople, 1975) and the smallest displacement asymmetry parameters (Nardelli, 1983) for this ring are q_2 = 0.344 (1) Å, q_3 = -0.288 (1) Å; Q_T = 0.4485 Å and θ = 130.02 (2)°, φ_2 = 205.6 (2)°, respectively. The three phenyl rings are twisted away from the best plane of the tetrahydropyridine ring by 66.33 (7), 87.36 (8) and 36.90 (7)°, respectively. The sum of the bond angles around the atom N1 [360.09 (10)°] of the tetrahydropyridine ring in the molecule is in accordance with sp^2 hybridization. The ethyl acetate group shows an extended conformation [C18—O3—C19—C20 = 90.67 (2)°]. The molecular structure is stabilized by a strong O—H···O hydrogen bond, wherein, atom O1 acts as a donor to O2, generating an *S*(6) motif.

S2. Experimental

To a mixture of 3-carboxyethyl-2,6-diphenylpiperidin-4-one (1 equiv.) and triethylamine (1.5 equiv.) in benzene, freshly distilled benzoyl chloride in benzene was added dropwise and stirred well at room temperature until completion. The crude mass obtained by the base work upon purification and recrystallization in distilled ethanol gave fine white crystals suitable for X-ray study.

S3. Refinement

The C bound H atoms positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with 1.5U_{eq}(C) for methyl H and 1.2U_{eq}(C) for other H atoms.

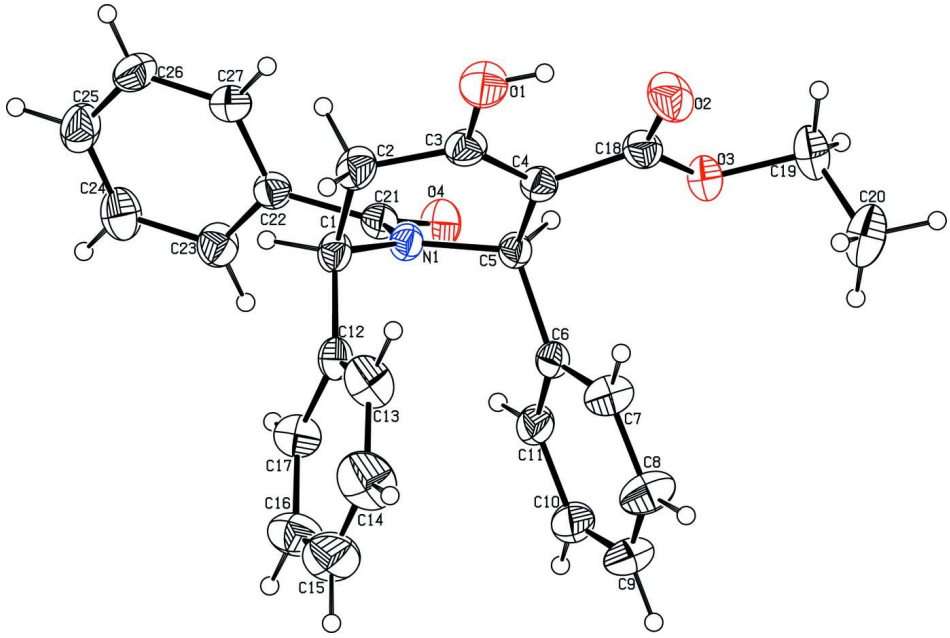

Figure 1

Perspective view of the title compound, showing displacement ellipsoids drawn at the 30% probability level.

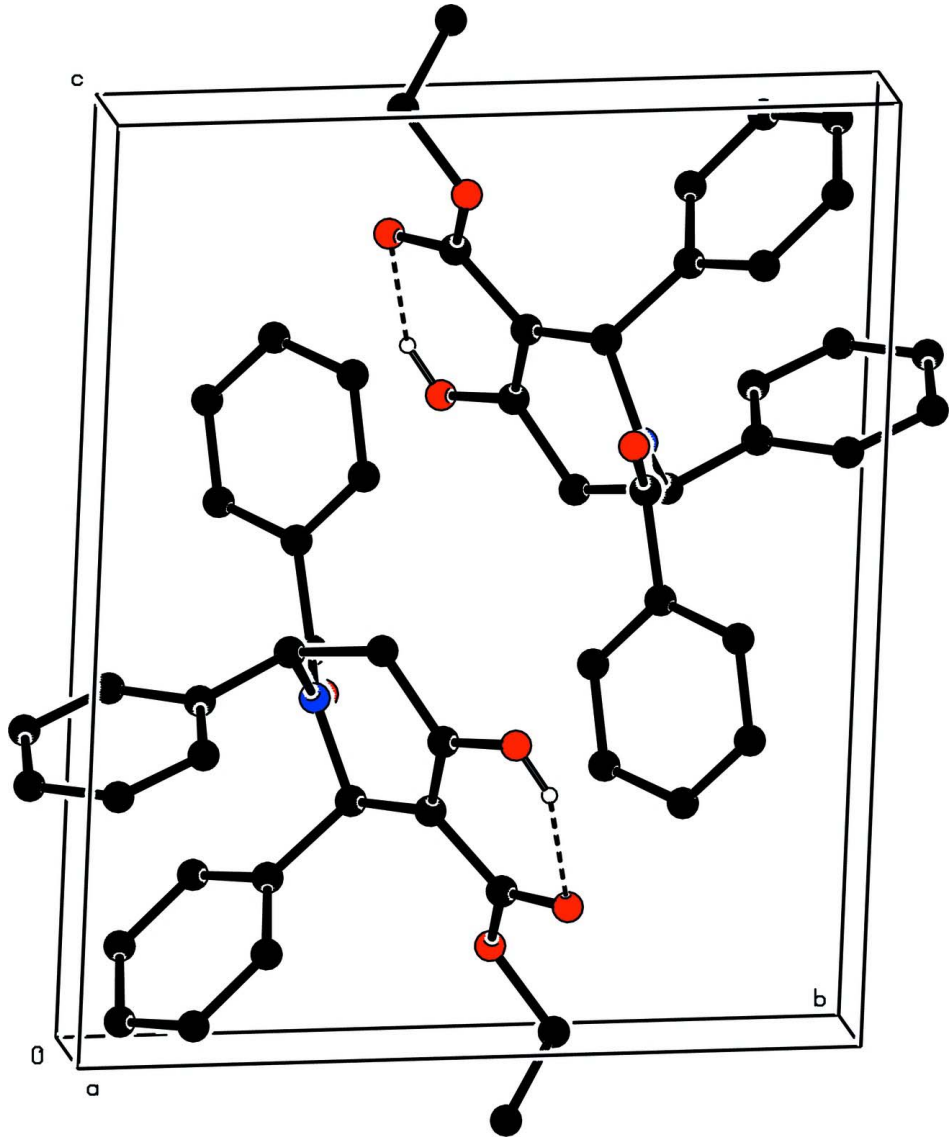

Figure 2

Crystal packing of the title compound, viewed down the *a* axis. For clarity, hydrogen atoms not involved in hydrogen bonding have been omitted.

Ethyl 1-benzoyl-4-hydroxy-2,6-diphenyl-1,2,5,6-tetrahydropyridine-3-carboxylate

Crystal data

$C_{27}H_{25}NO_4$
$M_r = 427.48$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.2784\ (7)$ Å
$b = 10.6116\ (9)$ Å
$c = 12.7572\ (11)$ Å
$\alpha = 85.681\ (4)°$
$\beta = 89.963\ (4)°$
$\gamma = 82.508\ (5)°$
$V = 1107.91\ (16)$ Å^3
$Z = 2$
$F(000) = 452$
$D_x = 1.281$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1225 reflections
$\theta = 1.6–28.4°$
$\mu = 0.09$ mm^{-1}

T = 293 K
Block, white

0.25 × 0.23 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.979, T_{max} = 0.983

20295 measured reflections
5526 independent reflections
4179 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 28.4°, θ_{min} = 1.6°
h = −11→11
k = −14→14
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.120
S = 1.04
5526 reflections
290 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
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.2116P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.35152 (15)	0.26735 (12)	0.41384 (9)	0.0431 (3)
H1	0.3276	0.2416	0.4870	0.052*
C2	0.44264 (18)	0.38303 (14)	0.41541 (11)	0.0551 (3)
H2A	0.4025	0.4326	0.4731	0.066*
H2B	0.5573	0.3539	0.4285	0.066*
C3	0.42551 (17)	0.46663 (12)	0.31645 (11)	0.0483 (3)
C4	0.31584 (15)	0.45704 (11)	0.23982 (9)	0.0421 (3)
C5	0.19897 (14)	0.35828 (11)	0.24886 (9)	0.0382 (2)
H5	0.0906	0.4048	0.2328	0.046*
C6	0.22569 (15)	0.25498 (11)	0.17071 (9)	0.0410 (3)
C7	0.34280 (18)	0.25430 (15)	0.09352 (12)	0.0585 (4)
H7	0.4142	0.3152	0.0911	0.070*
C8	0.3555 (2)	0.16428 (18)	0.01975 (15)	0.0758 (5)
H8	0.4340	0.1660	−0.0324	0.091*

C9	0.2530 (2)	0.07296 (16)	0.02343 (14)	0.0739 (5)
H9	0.2626	0.0117	−0.0255	0.089*
C10	0.1359 (2)	0.07199 (15)	0.09956 (12)	0.0663 (4)
H10	0.0657	0.0102	0.1020	0.080*
C11	0.12177 (19)	0.16256 (13)	0.17261 (11)	0.0528 (3)
H11	0.0416	0.1614	0.2236	0.063*
C12	0.44595 (15)	0.15211 (13)	0.36780 (10)	0.0447 (3)
C13	0.59156 (19)	0.15546 (17)	0.31517 (14)	0.0692 (4)
H13	0.6367	0.2313	0.3062	0.083*
C14	0.6700 (2)	0.0462 (2)	0.27598 (19)	0.0929 (7)
H14	0.7676	0.0494	0.2403	0.112*
C15	0.6072 (2)	−0.0660 (2)	0.28857 (17)	0.0873 (6)
H15	0.6602	−0.1385	0.2606	0.105*
C16	0.4653 (2)	−0.07137 (17)	0.34282 (16)	0.0748 (5)
H16	0.4226	−0.1482	0.3531	0.090*
C17	0.38547 (18)	0.03709 (14)	0.38216 (12)	0.0573 (4)
H17	0.2892	0.0326	0.4190	0.069*
C18	0.29783 (17)	0.55330 (12)	0.15177 (10)	0.0477 (3)
C19	0.1465 (2)	0.63209 (17)	−0.00422 (12)	0.0685 (4)
H19A	0.1880	0.7112	0.0078	0.082*
H19B	0.0311	0.6514	−0.0203	0.082*
C20	0.2327 (2)	0.5731 (2)	−0.09393 (13)	0.0832 (6)
H20A	0.3479	0.5599	−0.0799	0.125*
H20B	0.2108	0.6286	−0.1567	0.125*
H20C	0.1954	0.4927	−0.1033	0.125*
C21	0.04496 (15)	0.30444 (11)	0.40464 (10)	0.0416 (3)
C22	0.03654 (15)	0.27946 (12)	0.52150 (10)	0.0433 (3)
C23	−0.04315 (18)	0.18014 (14)	0.56215 (11)	0.0549 (3)
H23	−0.0836	0.1265	0.5172	0.066*
C24	−0.0628 (2)	0.16050 (17)	0.66984 (12)	0.0655 (4)
H24	−0.1142	0.0925	0.6971	0.079*
C25	−0.0065 (2)	0.24121 (17)	0.73612 (12)	0.0643 (4)
H25	−0.0203	0.2280	0.8083	0.077*
C26	0.0700 (2)	0.34139 (15)	0.69651 (12)	0.0620 (4)
H26	0.1068	0.3965	0.7417	0.074*
C27	0.09253 (18)	0.36049 (13)	0.58943 (11)	0.0531 (3)
H27	0.1454	0.4280	0.5628	0.064*
N1	0.19330 (12)	0.30648 (9)	0.35920 (7)	0.0388 (2)
O1	0.52511 (14)	0.55669 (10)	0.31367 (9)	0.0663 (3)
H1A	0.5089	0.6028	0.2592	0.099*
O2	0.38767 (14)	0.63583 (10)	0.13602 (9)	0.0687 (3)
O3	0.17091 (12)	0.54509 (9)	0.08975 (7)	0.0530 (2)
O4	−0.08244 (11)	0.32515 (10)	0.35338 (8)	0.0563 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0447 (6)	0.0496 (7)	0.0359 (6)	−0.0114 (5)	−0.0075 (5)	−0.0002 (5)

C2	0.0608 (8)	0.0598 (8)	0.0487 (7)	−0.0218 (7)	−0.0139 (6)	−0.0056 (6)
C3	0.0527 (7)	0.0446 (7)	0.0511 (7)	−0.0167 (6)	−0.0007 (6)	−0.0096 (5)
C4	0.0474 (7)	0.0384 (6)	0.0417 (6)	−0.0098 (5)	0.0013 (5)	−0.0042 (5)
C5	0.0418 (6)	0.0381 (6)	0.0350 (6)	−0.0079 (5)	−0.0044 (5)	−0.0006 (4)
C6	0.0457 (6)	0.0398 (6)	0.0372 (6)	−0.0047 (5)	−0.0091 (5)	−0.0016 (5)
C7	0.0539 (8)	0.0606 (9)	0.0643 (9)	−0.0121 (7)	0.0074 (7)	−0.0191 (7)
C8	0.0766 (11)	0.0824 (12)	0.0721 (11)	−0.0086 (9)	0.0160 (9)	−0.0333 (9)
C9	0.0989 (13)	0.0620 (10)	0.0636 (10)	−0.0070 (9)	−0.0032 (9)	−0.0282 (8)
C10	0.0967 (12)	0.0514 (8)	0.0556 (9)	−0.0254 (8)	−0.0139 (8)	−0.0085 (7)
C11	0.0701 (9)	0.0494 (7)	0.0417 (7)	−0.0193 (6)	−0.0052 (6)	−0.0026 (5)
C12	0.0398 (6)	0.0529 (7)	0.0400 (6)	−0.0036 (5)	−0.0081 (5)	0.0025 (5)
C13	0.0483 (8)	0.0712 (10)	0.0847 (12)	−0.0031 (7)	0.0098 (8)	0.0087 (9)
C14	0.0584 (10)	0.0983 (16)	0.1135 (17)	0.0163 (10)	0.0255 (10)	0.0017 (13)
C15	0.0693 (12)	0.0831 (13)	0.1018 (15)	0.0267 (10)	−0.0038 (10)	−0.0202 (11)
C16	0.0639 (10)	0.0571 (9)	0.1021 (14)	0.0026 (8)	−0.0138 (9)	−0.0147 (9)
C17	0.0485 (8)	0.0558 (8)	0.0685 (9)	−0.0080 (6)	0.0002 (7)	−0.0080 (7)
C18	0.0531 (7)	0.0427 (7)	0.0476 (7)	−0.0077 (6)	0.0080 (6)	−0.0022 (5)
C19	0.0756 (10)	0.0728 (10)	0.0521 (8)	−0.0055 (8)	−0.0031 (7)	0.0214 (7)
C20	0.0807 (12)	0.1220 (16)	0.0467 (9)	−0.0197 (11)	0.0016 (8)	0.0062 (9)
C21	0.0462 (7)	0.0372 (6)	0.0424 (6)	−0.0089 (5)	−0.0010 (5)	−0.0027 (5)
C22	0.0443 (6)	0.0419 (6)	0.0430 (6)	−0.0025 (5)	0.0029 (5)	−0.0030 (5)
C23	0.0579 (8)	0.0568 (8)	0.0518 (8)	−0.0168 (6)	0.0020 (6)	−0.0002 (6)
C24	0.0652 (9)	0.0736 (10)	0.0566 (9)	−0.0149 (8)	0.0087 (7)	0.0130 (8)
C25	0.0656 (9)	0.0780 (11)	0.0440 (8)	0.0082 (8)	0.0107 (7)	−0.0014 (7)
C26	0.0753 (10)	0.0596 (9)	0.0489 (8)	0.0073 (7)	−0.0004 (7)	−0.0188 (7)
C27	0.0654 (9)	0.0428 (7)	0.0514 (8)	−0.0055 (6)	0.0025 (6)	−0.0085 (6)
N1	0.0415 (5)	0.0405 (5)	0.0347 (5)	−0.0073 (4)	−0.0034 (4)	−0.0013 (4)
O1	0.0744 (7)	0.0620 (6)	0.0700 (7)	−0.0369 (5)	−0.0074 (5)	−0.0056 (5)
O2	0.0769 (7)	0.0583 (6)	0.0731 (7)	−0.0273 (5)	0.0042 (6)	0.0116 (5)
O3	0.0599 (6)	0.0546 (5)	0.0427 (5)	−0.0073 (4)	−0.0006 (4)	0.0081 (4)
O4	0.0445 (5)	0.0718 (7)	0.0530 (6)	−0.0128 (5)	−0.0049 (4)	0.0030 (5)

Geometric parameters (Å, º)

C1—N1	1.4798 (15)	C14—H14	0.9300
C1—C12	1.5197 (19)	C15—C16	1.369 (3)
C1—C2	1.5237 (18)	C15—H15	0.9300
C1—H1	0.9800	C16—C17	1.379 (2)
C2—C3	1.4831 (19)	C16—H16	0.9300
C2—H2A	0.9700	C17—H17	0.9300
C2—H2B	0.9700	C18—O2	1.2263 (16)
C3—O1	1.3397 (15)	C18—O3	1.3315 (17)
C3—C4	1.3531 (18)	C19—O3	1.4545 (16)
C4—C18	1.4543 (18)	C19—C20	1.484 (2)
C4—C5	1.5145 (16)	C19—H19A	0.9700
C5—N1	1.4751 (14)	C19—H19B	0.9700
C5—C6	1.5315 (16)	C20—H20A	0.9600
C5—H5	0.9800	C20—H20B	0.9600

C6—C7	1.3812 (19)	C20—H20C	0.9600
C6—C11	1.3852 (18)	C21—O4	1.2276 (15)
C7—C8	1.385 (2)	C21—N1	1.3597 (16)
C7—H7	0.9300	C21—C22	1.4976 (17)
C8—C9	1.367 (3)	C22—C23	1.3833 (19)
C8—H8	0.9300	C22—C27	1.3863 (18)
C9—C10	1.372 (3)	C23—C24	1.387 (2)
C9—H9	0.9300	C23—H23	0.9300
C10—C11	1.383 (2)	C24—C25	1.371 (2)
C10—H10	0.9300	C24—H24	0.9300
C11—H11	0.9300	C25—C26	1.372 (2)
C12—C17	1.3782 (19)	C25—H25	0.9300
C12—C13	1.383 (2)	C26—C27	1.382 (2)
C13—C14	1.381 (3)	C26—H26	0.9300
C13—H13	0.9300	C27—H27	0.9300
C14—C15	1.359 (3)	O1—H1A	0.8200

N1—C1—C12	111.53 (9)	C14—C15—C16	119.40 (17)
N1—C1—C2	108.76 (10)	C14—C15—H15	120.3
C12—C1—C2	114.90 (11)	C16—C15—H15	120.3
N1—C1—H1	107.1	C15—C16—C17	120.01 (18)
C12—C1—H1	107.1	C15—C16—H16	120.0
C2—C1—H1	107.1	C17—C16—H16	120.0
C3—C2—C1	113.62 (10)	C12—C17—C16	121.14 (15)
C3—C2—H2A	108.8	C12—C17—H17	119.4
C1—C2—H2A	108.8	C16—C17—H17	119.4
C3—C2—H2B	108.8	O2—C18—O3	122.55 (12)
C1—C2—H2B	108.8	O2—C18—C4	124.16 (13)
H2A—C2—H2B	107.7	O3—C18—C4	113.28 (11)
O1—C3—C4	123.70 (12)	O3—C19—C20	109.75 (14)
O1—C3—C2	112.47 (11)	O3—C19—H19A	109.7
C4—C3—C2	123.74 (11)	C20—C19—H19A	109.7
C3—C4—C18	118.69 (11)	O3—C19—H19B	109.7
C3—C4—C5	122.01 (11)	C20—C19—H19B	109.7
C18—C4—C5	118.95 (11)	H19A—C19—H19B	108.2
N1—C5—C4	109.42 (9)	C19—C20—H20A	109.5
N1—C5—C6	113.34 (9)	C19—C20—H20B	109.5
C4—C5—C6	115.47 (10)	H20A—C20—H20B	109.5
N1—C5—H5	105.9	C19—C20—H20C	109.5
C4—C5—H5	105.9	H20A—C20—H20C	109.5
C6—C5—H5	105.9	H20B—C20—H20C	109.5
C7—C6—C11	118.09 (12)	O4—C21—N1	122.22 (11)
C7—C6—C5	122.82 (11)	O4—C21—C22	118.89 (11)
C11—C6—C5	118.96 (11)	N1—C21—C22	118.87 (11)
C6—C7—C8	121.02 (14)	C23—C22—C27	119.20 (13)
C6—C7—H7	119.5	C23—C22—C21	118.91 (12)
C8—C7—H7	119.5	C27—C22—C21	121.59 (12)
C9—C8—C7	120.12 (16)	C22—C23—C24	120.09 (14)

C9—C8—H8	119.9	C22—C23—H23	120.0
C7—C8—H8	119.9	C24—C23—H23	120.0
C8—C9—C10	119.73 (14)	C25—C24—C23	120.07 (15)
C8—C9—H9	120.1	C25—C24—H24	120.0
C10—C9—H9	120.1	C23—C24—H24	120.0
C9—C10—C11	120.26 (15)	C24—C25—C26	120.31 (14)
C9—C10—H10	119.9	C24—C25—H25	119.8
C11—C10—H10	119.9	C26—C25—H25	119.8
C10—C11—C6	120.77 (14)	C25—C26—C27	120.03 (14)
C10—C11—H11	119.6	C25—C26—H26	120.0
C6—C11—H11	119.6	C27—C26—H26	120.0
C17—C12—C13	118.23 (14)	C26—C27—C22	120.27 (14)
C17—C12—C1	118.10 (12)	C26—C27—H27	119.9
C13—C12—C1	123.64 (13)	C22—C27—H27	119.9
C14—C13—C12	120.02 (17)	C21—N1—C5	118.15 (10)
C14—C13—H13	120.0	C21—N1—C1	124.93 (10)
C12—C13—H13	120.0	C5—N1—C1	116.82 (9)
C15—C14—C13	121.17 (18)	C3—O1—H1A	109.5
C15—C14—H14	119.4	C18—O3—C19	118.01 (12)
C13—C14—H14	119.4		

N1—C1—C2—C3	−39.33 (16)	C1—C12—C17—C16	−179.77 (14)
C12—C1—C2—C3	86.47 (15)	C15—C16—C17—C12	0.1 (3)
C1—C2—C3—O1	−170.79 (12)	C3—C4—C18—O2	8.2 (2)
C1—C2—C3—C4	12.3 (2)	C5—C4—C18—O2	−178.52 (12)
O1—C3—C4—C18	−3.4 (2)	C3—C4—C18—O3	−170.63 (12)
C2—C3—C4—C18	173.15 (13)	C5—C4—C18—O3	2.68 (17)
O1—C3—C4—C5	−176.51 (12)	O4—C21—C22—C23	57.04 (17)
C2—C3—C4—C5	0.1 (2)	N1—C21—C22—C23	−124.55 (13)
C3—C4—C5—N1	15.95 (16)	O4—C21—C22—C27	−116.66 (15)
C18—C4—C5—N1	−157.13 (11)	N1—C21—C22—C27	61.75 (17)
C3—C4—C5—C6	−113.35 (13)	C27—C22—C23—C24	−1.6 (2)
C18—C4—C5—C6	73.57 (14)	C21—C22—C23—C24	−175.44 (13)
N1—C5—C6—C7	−130.38 (13)	C22—C23—C24—C25	1.5 (2)
C4—C5—C6—C7	−3.03 (17)	C23—C24—C25—C26	−0.3 (2)
N1—C5—C6—C11	53.88 (14)	C24—C25—C26—C27	−0.8 (2)
C4—C5—C6—C11	−178.77 (11)	C25—C26—C27—C22	0.6 (2)
C11—C6—C7—C8	0.4 (2)	C23—C22—C27—C26	0.5 (2)
C5—C6—C7—C8	−175.42 (14)	C21—C22—C27—C26	174.22 (13)
C6—C7—C8—C9	−1.0 (3)	O4—C21—N1—C5	11.51 (17)
C7—C8—C9—C10	1.0 (3)	C22—C21—N1—C5	−166.85 (10)
C8—C9—C10—C11	−0.3 (3)	O4—C21—N1—C1	−172.21 (11)
C9—C10—C11—C6	−0.4 (2)	C22—C21—N1—C1	9.43 (17)
C7—C6—C11—C10	0.3 (2)	C4—C5—N1—C21	129.05 (11)
C5—C6—C11—C10	176.29 (13)	C6—C5—N1—C21	−100.50 (12)
N1—C1—C12—C17	−68.07 (15)	C4—C5—N1—C1	−47.53 (13)
C2—C1—C12—C17	167.57 (11)	C6—C5—N1—C1	82.92 (12)
N1—C1—C12—C13	113.98 (14)	C12—C1—N1—C21	116.28 (12)

C2—C1—C12—C13	−10.38 (18)	C2—C1—N1—C21	−115.98 (13)
C17—C12—C13—C14	1.8 (2)	C12—C1—N1—C5	−67.39 (13)
C1—C12—C13—C14	179.77 (16)	C2—C1—N1—C5	60.35 (13)
C12—C13—C14—C15	−0.4 (3)	O2—C18—O3—C19	4.6 (2)
C13—C14—C15—C16	−1.3 (3)	C4—C18—O3—C19	−176.56 (12)
C14—C15—C16—C17	1.4 (3)	C20—C19—O3—C18	90.67 (17)
C13—C12—C17—C16	−1.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O2	0.82	1.85	2.570 (2)	146