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(3-Hydroxypiperidin-1-yl)(4-methylphenyl)-methanone

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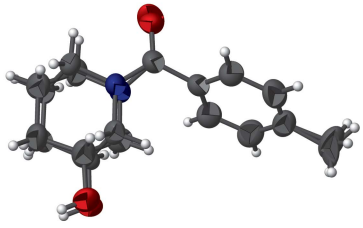
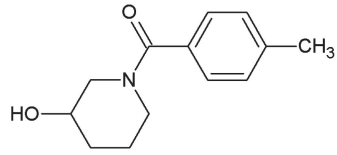
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{13}H_{17}NO_2$, the piperidine ring assumes a chair conformation. The dihedral angle between the mean plane of the piperidine ring and the benzene ring is 45.49 (1)°. In the crystal, molecules are linked by O—H···O intermolecular hydrogen bonds, leading to a molecular chain running along the *c*-axis direction. The atoms of the hydroxy piperidine ring and the methyl group of methylphenyl ring are disordered over two sets of sites with refined occupancies of 0.754 (5) and 0.246 (5).

3D view



Chemical scheme



Structure description

Piperidine and its derivative have played vital roles in the design of pharmaceutical drugs (Das & Brahmachari, 2013). It has been shown that the antioxidant activity of the title molecule can be enhanced by the substitution of hydroxyl, methoxy, nitro and alkyl groups on the piperidine ring system (Ravindernath & Reddy, 2017).

In the compound (Fig. 1), the bond lengths are typical of such derivatives and are in good agreement with literature values (Allen *et al.*, 1987). The C—N distances [1.370 (5)–1.464 (5) Å], C=O distance [1.189 (5) Å] and C—O distance [1.399 (5) Å] are in good agreement with the values of similar reported structures (Revathi *et al.*, 2015; Prathebha *et al.*, 2015). The +*syn*-periplanar(+*sp*) orientation of the keto group with the hydroxy-piperidine ring is revealed by the torsion angle O1—C8—N1—C9 [15.1 (6)]°. The total angle (359.5°) around the N atom indicates sp^2 hybridization of this atom. The piperidine ring (N1/C9–C13) adopts a chair conformation with puckering parameters $q2$ = 0.0097 (4), $q3$ = 0.5605 (4), Q_T= 0.5605 (4) Å, $\varphi 2$ = −22 (21)° and $\theta 2$ = 1.0 (4)°. Atoms

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9B···O1^{i}	0.97	2.66	3.598 (7)	163
O2—H2···O1^{ii}	0.82	2.02	2.802 (7)	159
O2′—H2′···O1′^{ii}	0.82	2.07	2.70 (3)	134

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

C10 and C13 deviate by −0.233 (2) and 0.243 (2) Å, respectively, from the mean plane through all ring atoms.

In the crystal, molecules are linked through O—H···O hydrogen bonds (Table 1, Fig. 2), forming chains running parallel to [001].

Synthesis and crystallization

The title compound was synthesized following a published procedure (Revathi *et al.*, 2015). In a 250 ml round-bottomed flask, 15 ml of ethyl methyl ketone was added to 3-hydroxy piperidine (0.01 mol; 1 g m) and stirred at room temperature. After 5 min, triethylamine (0.02 mol; 1.3 ml) was added and the mixture stirred for 15 min. Then 4-methyl benzoyl chloride (0.02 mol; 1.2 ml) and 15 ml of ethyl methyl ketone were added and the reaction mixture stirred at room temperature for 2 h. A white precipitate was formed which was filtered off. The filtrate was evaporated to give the crude product. It was then recrystallized twice from ethyl methyl ketone to give

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{17}NO_2$
M_r	219.28
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	293
a, b, c (Å)	24.8766 (14), 6.1117 (4), 7.9388 (4)
V (Å^3)	1207.00 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.976, 0.984
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20282, 2385, 1692
R_{int}	0.055
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.099, 1.11
No. of reflections	2385
No. of parameters	230
No. of restraints	99
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.13, −0.11
Absolute structure	Flack x determined using 675 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al*, 2013)
Absolute structure parameter	0.3 (5)

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *ORTEP-3 for Windows* (Farrugia, 2012).

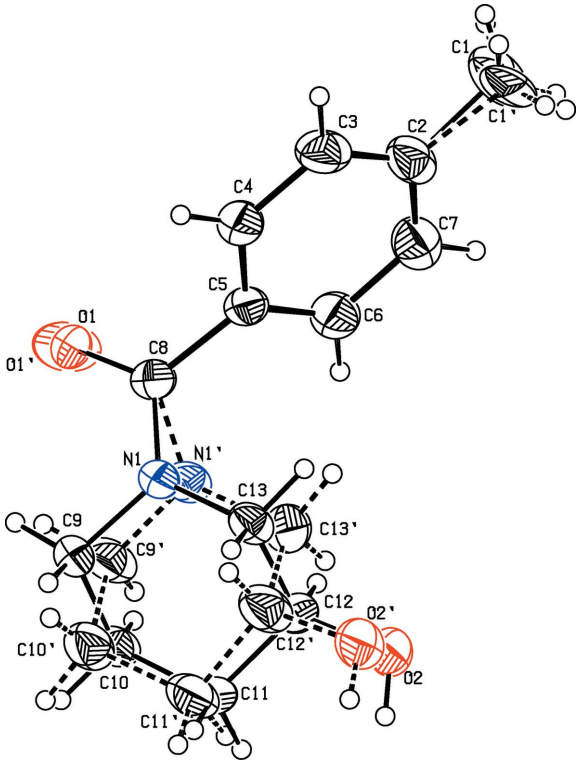


Figure 1
ORTEP-3 for Windows (Farrugia, 2012) plot of the title compound, with displacement ellipsoids drawn at the 30% probability level.

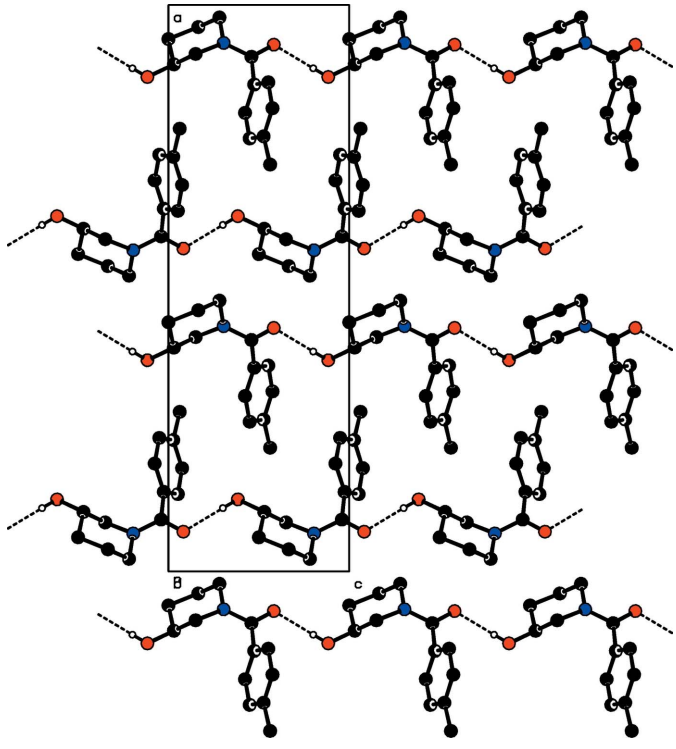


Figure 2
The crystal packing of the title compound, viewed along the *b* axis with hydrogen bonds indicated by dashed lines.

yellow block-like crystals of the title compound (m.p. 70°C, yield 82%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The atoms of the hydroxy piperidine ring and the methyl group of methylphenyl ring are disordered over two sets of sites with refined occupancies of 0.754 (5) and 0.246 (5).

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171493 [https://doi.org/10.1107/S2414314617014936]

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Crystal data

$C_{13}H_{17}NO_2$
M_r = 219.28
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
a = 24.8766 (14) Å
b = 6.1117 (4) Å
c = 7.9388 (4) Å
V = 1207.00 (12) Å^3
Z = 4
$F(000)$ = 472
D_x = 1.207 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2385 reflections
θ = 0.8–0.7°
μ = 0.08 mm^{-1}
T = 293 K
Block, yellow
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and \ f scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.976, T_{max} = 0.984
20282 measured reflections
2385 independent reflections
1692 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 26.0°, θ_{min} = 3.3°
h = −30→30
k = −7→7
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.099
S = 1.11
2385 reflections
230 parameters
99 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
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.0531P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.141 (11)
Absolute structure: Flack x determined using 675 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons et al. (2013)
Absolute structure parameter: 0.3 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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.
H atoms were positioned geometrically and treated as riding on their parent atoms and refined with, C—H distance of 0.93–0.98 Å, O—H of 0.82 Å with U_{iso}(H)= 1.5 U_{eq}(c-methyl),and U_{iso}(H)= 1.2Ueq(C) for other H atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C3	0.18222 (11)	−0.4020 (4)	1.0752 (3)	0.0762 (7)	
H3	0.1791	−0.5388	1.1256	0.091*	
C4	0.13647 (8)	−0.2764 (3)	1.0519 (3)	0.0670 (6)	
H4	0.1032	−0.3274	1.0885	0.080*	
C5	0.14041 (8)	−0.0763 (3)	0.9743 (2)	0.0576 (5)	
C6	0.19040 (9)	−0.0040 (4)	0.9234 (3)	0.0701 (6)	
H6	0.1935	0.1314	0.8708	0.084*	
C7	0.23570 (8)	−0.1285 (4)	0.9492 (3)	0.0748 (6)	
H7	0.2690	−0.0765	0.9145	0.090*	
C8	0.09139 (9)	0.0653 (3)	0.9589 (3)	0.0666 (6)	
C2	0.23190 (9)	−0.3301 (4)	1.0261 (3)	0.0733 (7)	
C1	0.2817 (3)	−0.4667 (13)	1.0622 (13)	0.116 (3)	0.754 (5)
H1A	0.3073	−0.4472	0.9729	0.174*	0.754 (5)
H1B	0.2719	−0.6183	1.0694	0.174*	0.754 (5)
H1C	0.2974	−0.4208	1.1669	0.174*	0.754 (5)
C9	0.02203 (13)	0.2386 (6)	0.7818 (4)	0.0590 (8)	0.754 (5)
H9A	0.0114	0.2993	0.8897	0.071*	0.754 (5)
H9B	−0.0085	0.1612	0.7347	0.071*	0.754 (5)
C10	0.03892 (17)	0.4199 (6)	0.6648 (5)	0.0643 (10)	0.754 (5)
H10A	0.0666	0.5071	0.7187	0.077*	0.754 (5)
H10B	0.0084	0.5144	0.6428	0.077*	0.754 (5)
C11	0.06016 (18)	0.3312 (8)	0.4998 (5)	0.0669 (12)	0.754 (5)
H11A	0.0312	0.2601	0.4389	0.080*	0.754 (5)
H11B	0.0734	0.4511	0.4313	0.080*	0.754 (5)
C12	0.10493 (16)	0.1694 (7)	0.5298 (4)	0.0621 (9)	0.754 (5)
H12	0.1339	0.2492	0.5867	0.075*	0.754 (5)
C13	0.08638 (13)	−0.0078 (5)	0.6499 (3)	0.0529 (8)	0.754 (5)
H13A	0.0579	−0.0923	0.5978	0.063*	0.754 (5)
H13B	0.1160	−0.1060	0.6740	0.063*	0.754 (5)
N1	0.06702 (11)	0.0872 (5)	0.8051 (3)	0.0498 (7)	0.754 (5)
O1	0.0701 (2)	0.1339 (12)	1.0822 (7)	0.0802 (15)	0.754 (5)
O2	0.12710 (16)	0.0789 (9)	0.3835 (4)	0.1091 (16)	0.754 (5)
H2	0.1118	0.1294	0.3007	0.164*	0.754 (5)
C1′	0.2820 (6)	−0.480 (4)	1.037 (3)	0.095 (7)	0.246 (5)

H1′1	0.3139	−0.3949	1.0188	0.142*	0.246 (5)
H1′2	0.2796	−0.5919	0.9519	0.142*	0.246 (5)
H1′3	0.2835	−0.5473	1.1460	0.142*	0.246 (5)
C9′	0.0545 (5)	0.363 (2)	0.7878 (13)	0.081 (4)	0.246 (5)
H9′1	0.0743	0.4953	0.7602	0.097*	0.246 (5)
H9′2	0.0362	0.3883	0.8940	0.097*	0.246 (5)
C10′	0.0136 (5)	0.325 (3)	0.6554 (15)	0.081 (4)	0.246 (5)
H10C	−0.0066	0.4583	0.6364	0.097*	0.246 (5)
H10D	−0.0114	0.2131	0.6933	0.097*	0.246 (5)
C11′	0.0396 (6)	0.251 (3)	0.4900 (19)	0.087 (5)	0.246 (5)
H11C	0.0121	0.2065	0.4106	0.104*	0.246 (5)
H11D	0.0596	0.3717	0.4407	0.104*	0.246 (5)
C12′	0.0770 (6)	0.062 (2)	0.5267 (15)	0.083 (4)	0.246 (5)
H12′	0.0547	−0.0547	0.5744	0.100*	0.246 (5)
C13′	0.1182 (4)	0.1118 (19)	0.6524 (12)	0.071 (3)	0.246 (5)
H13C	0.1417	0.2262	0.6103	0.085*	0.246 (5)
H13D	0.1398	−0.0174	0.6734	0.085*	0.246 (5)
N1′	0.0927 (4)	0.1837 (17)	0.8095 (9)	0.064 (3)	0.246 (5)
O1′	0.0737 (10)	0.179 (4)	1.098 (3)	0.110 (8)	0.246 (5)
O2′	0.1012 (5)	−0.0230 (18)	0.3875 (13)	0.084 (3)	0.246 (5)
H2′	0.0802	−0.0193	0.3079	0.126*	0.246 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C3	0.1035 (19)	0.0606 (13)	0.0644 (13)	0.0231 (12)	−0.0065 (13)	0.0065 (11)
C4	0.0729 (13)	0.0679 (14)	0.0601 (12)	0.0152 (10)	0.0062 (10)	0.0074 (10)
C5	0.0705 (13)	0.0611 (12)	0.0413 (9)	0.0178 (10)	0.0010 (9)	0.0032 (9)
C6	0.0805 (14)	0.0612 (11)	0.0686 (14)	0.0120 (11)	0.0052 (11)	0.0074 (10)
C7	0.0665 (13)	0.0795 (16)	0.0784 (14)	0.0045 (12)	−0.0032 (12)	−0.0057 (12)
C8	0.0769 (13)	0.0750 (14)	0.0477 (11)	0.0262 (11)	0.0040 (11)	0.0086 (10)
C2	0.0765 (16)	0.0815 (16)	0.0618 (14)	0.0287 (13)	−0.0157 (11)	−0.0186 (12)
C1	0.126 (6)	0.120 (6)	0.100 (5)	0.078 (5)	−0.028 (3)	−0.044 (4)
C9	0.0543 (17)	0.071 (2)	0.0519 (17)	0.0210 (15)	0.0023 (13)	0.0046 (14)
C10	0.075 (2)	0.059 (2)	0.059 (2)	0.0239 (16)	−0.0076 (18)	0.0038 (17)
C11	0.075 (3)	0.080 (2)	0.0464 (19)	0.0186 (19)	−0.0010 (17)	0.0135 (17)
C12	0.062 (2)	0.086 (2)	0.0380 (16)	0.0183 (17)	0.0000 (13)	0.0011 (16)
C13	0.0557 (16)	0.0535 (17)	0.0494 (16)	0.0130 (14)	−0.0132 (12)	−0.0121 (13)
N1	0.0508 (15)	0.0529 (15)	0.0457 (12)	0.0118 (12)	−0.0007 (11)	0.0038 (11)
O1	0.082 (2)	0.119 (4)	0.040 (2)	0.046 (2)	0.0107 (16)	0.002 (2)
O2	0.096 (3)	0.186 (5)	0.0448 (12)	0.071 (3)	0.0066 (16)	−0.003 (2)
C1′	0.041 (8)	0.153 (18)	0.090 (12)	0.015 (7)	−0.032 (7)	0.037 (11)
C9′	0.097 (8)	0.083 (7)	0.062 (6)	0.046 (6)	−0.020 (5)	−0.015 (5)
C10′	0.077 (8)	0.108 (9)	0.058 (6)	0.033 (6)	−0.016 (6)	−0.015 (7)
C11′	0.092 (9)	0.108 (10)	0.060 (6)	0.050 (8)	−0.019 (6)	−0.009 (7)
C12′	0.096 (8)	0.093 (8)	0.062 (6)	0.043 (7)	−0.019 (6)	−0.019 (6)
C13′	0.079 (7)	0.069 (6)	0.064 (6)	0.016 (6)	0.007 (5)	0.000 (5)
N1′	0.075 (6)	0.076 (6)	0.040 (4)	0.028 (5)	−0.014 (4)	−0.015 (4)

O1′	0.188 (15)	0.085 (8)	0.057 (8)	0.075 (8)	−0.027 (7)	−0.036 (6)
O2′	0.100 (8)	0.097 (7)	0.054 (4)	0.045 (5)	−0.003 (5)	−0.024 (4)

Geometric parameters (Å, º)

C3—C2	1.368 (3)	C11—H11B	0.9700
C3—C4	1.385 (3)	C12—O2	1.399 (5)
C3—H3	0.9300	C12—C13	1.515 (5)
C4—C5	1.373 (3)	C12—H12	0.9800
C4—H4	0.9300	C13—N1	1.444 (3)
C5—C6	1.380 (3)	C13—H13A	0.9700
C5—C8	1.500 (3)	C13—H13B	0.9700
C6—C7	1.375 (3)	O2—H2	0.8200
C6—H6	0.9300	C1′—H1′1	0.9600
C7—C2	1.379 (3)	C1′—H1′2	0.9600
C7—H7	0.9300	C1′—H1′3	0.9600
C8—O1	1.189 (5)	C9′—N1′	1.463 (11)
C8—N1	1.370 (3)	C9′—C10′	1.481 (14)
C8—O1′	1.37 (2)	C9′—H9′1	0.9700
C8—N1′	1.390 (9)	C9′—H9′2	0.9700
C2—C1	1.522 (5)	C10′—C11′	1.531 (15)
C2—C1′	1.551 (13)	C10′—H10C	0.9700
C1—H1A	0.9600	C10′—H10D	0.9700
C1—H1B	0.9600	C11′—C12′	1.512 (14)
C1—H1C	0.9600	C11′—H11C	0.9700
C9—N1	1.464 (3)	C11′—H11D	0.9700
C9—C10	1.506 (5)	C12′—O2′	1.362 (15)
C9—H9A	0.9700	C12′—C13′	1.463 (14)
C9—H9B	0.9700	C12′—H12′	0.9800
C10—C11	1.513 (5)	C13′—N1′	1.467 (11)
C10—H10A	0.9700	C13′—H13C	0.9700
C10—H10B	0.9700	C13′—H13D	0.9700
C11—C12	1.508 (5)	O2′—H2′	0.8200
C11—H11A	0.9700		

C2—C3—C4	121.7 (2)	C11—C12—C13	110.1 (3)
C2—C3—H3	119.1	O2—C12—H12	106.8
C4—C3—H3	119.1	C11—C12—H12	106.8
C5—C4—C3	119.7 (2)	C13—C12—H12	106.8
C5—C4—H4	120.2	N1—C13—C12	110.6 (3)
C3—C4—H4	120.2	N1—C13—H13A	109.5
C4—C5—C6	118.73 (18)	C12—C13—H13A	109.5
C4—C5—C8	119.50 (18)	N1—C13—H13B	109.5
C6—C5—C8	121.60 (18)	C12—C13—H13B	109.5
C7—C6—C5	121.2 (2)	H13A—C13—H13B	108.1
C7—C6—H6	119.4	C8—N1—C13	125.0 (2)
C5—C6—H6	119.4	C8—N1—C9	120.8 (2)
C6—C7—C2	120.3 (2)	C13—N1—C9	113.7 (2)

C6—C7—H7	119.9	C12—O2—H2	109.5
C2—C7—H7	119.9	C2—C1′—H1′1	109.5
O1—C8—N1	120.1 (3)	C2—C1′—H1′2	109.5
O1—C8—O1′	11.4 (14)	H1′1—C1′—H1′2	109.5
N1—C8—O1′	121.5 (11)	C2—C1′—H1′3	109.5
O1—C8—N1′	121.9 (5)	H1′1—C1′—H1′3	109.5
N1—C8—N1′	36.8 (4)	H1′2—C1′—H1′3	109.5
O1′—C8—N1′	115.3 (11)	N1′—C9′—C10′	114.2 (9)
O1—C8—C5	119.9 (3)	N1′—C9′—H9′1	108.7
N1—C8—C5	119.25 (19)	C10′—C9′—H9′1	108.7
O1′—C8—C5	119.2 (11)	N1′—C9′—H9′2	108.7
N1′—C8—C5	110.5 (4)	C10′—C9′—H9′2	108.7
C3—C2—C7	118.40 (19)	H9′1—C9′—H9′2	107.6
C3—C2—C1	120.4 (5)	C9′—C10′—C11′	111.4 (10)
C7—C2—C1	121.2 (5)	C9′—C10′—H10C	109.3
C3—C2—C1′	121.3 (9)	C11′—C10′—H10C	109.3
C7—C2—C1′	119.9 (9)	C9′—C10′—H10D	109.3
C1—C2—C1′	8.1 (13)	C11′—C10′—H10D	109.3
C2—C1—H1A	109.5	H10C—C10′—H10D	108.0
C2—C1—H1B	109.5	C12′—C11′—C10′	108.5 (11)
C2—C1—H1C	109.5	C12′—C11′—H11C	110.0
N1—C9—C10	109.2 (2)	C10′—C11′—H11C	110.0
N1—C9—H9A	109.8	C12′—C11′—H11D	110.0
C10—C9—H9A	109.8	C10′—C11′—H11D	110.0
N1—C9—H9B	109.8	H11C—C11′—H11D	108.4
C10—C9—H9B	109.8	O2′—C12′—C13′	108.8 (10)
H9A—C9—H9B	108.3	O2′—C12′—C11′	114.1 (11)
C9—C10—C11	111.6 (3)	C13′—C12′—C11′	113.8 (11)
C9—C10—H10A	109.3	O2′—C12′—H12′	106.5
C11—C10—H10A	109.3	C13′—C12′—H12′	106.5
C9—C10—H10B	109.3	C11′—C12′—H12′	106.5
C11—C10—H10B	109.3	C12′—C13′—N1′	109.8 (8)
H10A—C10—H10B	108.0	C12′—C13′—H13C	109.7
C12—C11—C10	110.9 (3)	N1′—C13′—H13C	109.7
C12—C11—H11A	109.5	C12′—C13′—H13D	109.7
C10—C11—H11A	109.5	N1′—C13′—H13D	109.7
C12—C11—H11B	109.5	H13C—C13′—H13D	108.2
C10—C11—H11B	109.5	C8—N1′—C9′	118.4 (8)
H11A—C11—H11B	108.1	C8—N1′—C13′	125.4 (7)
O2—C12—C11	114.8 (3)	C9′—N1′—C13′	114.0 (8)
O2—C12—C13	111.1 (3)	C12′—O2′—H2′	109.5

C2—C3—C4—C5	1.4 (3)	N1′—C8—N1—C13	82.2 (6)
C3—C4—C5—C6	−0.9 (3)	C5—C8—N1—C13	−3.4 (4)
C3—C4—C5—C8	−176.20 (19)	O1—C8—N1—C9	15.1 (6)
C4—C5—C6—C7	0.0 (3)	O1′—C8—N1—C9	1.9 (13)
C8—C5—C6—C7	175.2 (2)	N1′—C8—N1—C9	−89.1 (6)
C5—C6—C7—C2	0.3 (3)	C5—C8—N1—C9	−174.6 (2)

C4—C5—C8—O1	63.9 (5)	C12—C13—N1—C8	−112.6 (4)
C6—C5—C8—O1	−111.3 (5)	C12—C13—N1—C9	59.2 (4)
C4—C5—C8—N1	−106.4 (3)	C10—C9—N1—C8	114.0 (4)
C6—C5—C8—N1	78.4 (3)	C10—C9—N1—C13	−58.2 (4)
C4—C5—C8—O1′	77.0 (13)	N1′—C9′—C10′—C11′	−50.2 (19)
C6—C5—C8—O1′	−98.2 (12)	C9′—C10′—C11′—C12′	51.2 (19)
C4—C5—C8—N1′	−146.0 (5)	C10′—C11′—C12′—O2′	177.8 (13)
C6—C5—C8—N1′	38.8 (6)	C10′—C11′—C12′—C13′	−56.6 (19)
C4—C3—C2—C7	−1.1 (3)	O2′—C12′—C13′—N1′	−174.5 (10)
C4—C3—C2—C1	176.7 (4)	C11′—C12′—C13′—N1′	57.1 (17)
C4—C3—C2—C1′	−174.0 (12)	O1—C8—N1′—C9′	−18.1 (12)
C6—C7—C2—C3	0.2 (3)	N1—C8—N1′—C9′	80.7 (10)
C6—C7—C2—C1	−177.6 (4)	O1′—C8—N1′—C9′	−28.7 (16)
C6—C7—C2—C1′	173.2 (12)	C5—C8—N1′—C9′	−167.5 (8)
N1—C9—C10—C11	54.8 (5)	O1—C8—N1′—C13′	179.8 (9)
C9—C10—C11—C12	−54.5 (5)	N1—C8—N1′—C13′	−81.4 (10)
C10—C11—C12—O2	−179.9 (4)	O1′—C8—N1′—C13′	169.2 (14)
C10—C11—C12—C13	53.9 (5)	C5—C8—N1′—C13′	30.3 (12)
O2—C12—C13—N1	176.0 (3)	C10′—C9′—N1′—C8	−112.8 (14)
C11—C12—C13—N1	−55.7 (4)	C10′—C9′—N1′—C13′	51.3 (17)
O1—C8—N1—C13	−173.6 (5)	C12′—C13′—N1′—C8	109.9 (14)
O1′—C8—N1—C13	173.2 (13)	C12′—C13′—N1′—C9′	−52.9 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*B*···O1^{i}	0.97	2.66	3.598 (7)	163
O2—H2···O1^{ii}	0.82	2.02	2.802 (7)	159
O2′—H2′···O1′^{ii}	0.82	2.07	2.70 (3)	134

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