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syn-3-(4-Chlorobenzyl)-1,5-dimethyl-3,7-diazabicyclo[3.3.1]nonan-9-ol

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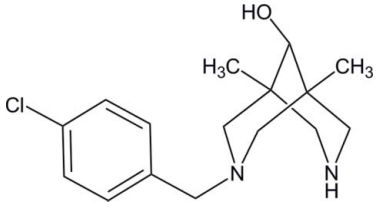
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.107; data-to-parameter ratio = 13.7.

In the title compound, $C_{16}H_{23}ClN_2O$, both six-membered rings adopt chair conformations, thus allowing the formation of an intramolecular N—H···N hydrogen bond. In the crystal, adjacent molecules are combined into chains running along the *ac* diagonal *via* O—H···N hydrogen bonds.

Related literature

For general background to chemistry affording *syn*-3,7-diazabicyclo[3.3.1]nonan-9-ols, see: Vatsadze *et al.* (2006). 3,5,6,7-Tetrasubstituted 3,6-diazabicyclo[3.2.1]octanes, their biological activity as enzyme inhibitors and their X-ray structures have been reported by: Kudryavtsev (2010); Kudryavtsev & Churakov (2012).



Experimental

Crystal data

$C_{16}H_{23}ClN_2O$
M_r = 294.81
Monoclinic, $P2_1/n$
a = 7.9739 (4) Å
b = 16.8120 (9) Å
c = 12.1103 (6) Å
β = 107.520 (1)°
V = 1548.16 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 120 K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.941, T_{max} = 0.953
10450 measured reflections
3747 independent reflections
2976 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
S = 1.02
3747 reflections
273 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N1	0.870 (19)	2.287 (19)	2.8327 (18)	120.8 (16)
O1—H1···N2^{i}	0.87 (2)	1.86 (2)	2.7242 (17)	172 (2)

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2075).

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supporting information

Acta Cryst. (2012). E**68**, o2373 [https://doi.org/10.1107/S1600536812030310]

syn-3-(4-Chlorobenzyl)-1,5-dimethyl-3,7-diazabicyclo[3.3.1]nonan-9-ol

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S1. Comment

In the title compound, both six-membered cycles adopt chair conformation (Fig. 1). The latter allows the formation of intramolecular N—H···N hydrogen bond. The hydroxyl group at the 9th position of the heterocyclic scaffold is situated closer to the tertiary N-atom. In crystal, the adjacent molecules are combined in chains running along *ac*-diagonal *via* O—H···N hydrogen bonds (Fig. 2).

syn-3,7-Diazabicyclo[3.3.1]nonan-9-ols are of interest as a structural motif for enzymes inhibitors. Inhibition of thrombin by substituted 3,6-diazabicyclo[3.2.1]octanes is reported (Kudryavtsev (2010)).

S2. Experimental

The solution of 2.23 g (6.9 mmol) of *anti*-5-(4-chlorobenzyl)-3-formyl- 1,5-dimethyl-3,7-diazabicyclo[3.3.1]nonan-9-ol (Vatsadze *et al.*(2006)) in conc. HCl (molar ratio *ca* 1:120) was refluxed for 21 h. The cooled solution was neutralized with NaOH to the pH 9–10. The precipitate formed was filtered off, washed with water to neutral pH of mother liquor, then once with ether, recrystallized from EtOH. *syn*-3-(4-Chlorobenzyl)-1,5-dimethyl-3,7-diazabicyclo[3.3.1]nonan-9-ol. Yield 1.50 g (74%), colourless crystals, sublimated at 473 K. ^{1}H NMR (dmso-d_6): δ 0.63 (s, 6H, 2CH_3); 2.26–2.41 (m, 6H, H-6a, H-8a, H-4 e, H-4a, H-2 e, H-2a); 2.72 (d, 2H, H-6 e, H-8 e, *J* 13.3); 2.98 (d, 1H, H-9, *J* 4.5); 3.27 (s, 2H, CH_2Ar); 4.74 (d, 1H, OH, *J* 5.0); 7.28, 7.38 (both d, both 2H, CH(3,5)(Ar), CH(2,6)(Ar), *J* 8.3). ^{1}H NMR (dmso-d_6 + CF_3COOH): δ 0.77 (s, 6H, 2CH_3); 2.36 (d, 2H, H-2a, H-4a, *J* 10.6); 2.48 (d, 2H, H-2 e, H-4 e, *J* 12.4); 2.86 (d, 2H, H-6a, H-8a, *J* 11.9); 3.21 (d, 2H, H-6 e, H-8 e, *J* 12.6); 3.24 (s, 1H, H-9); 3.43 (s, 2H, CH_2Ar); 7.34–7.43 (m, 4H, H(Ar)). ^{13}C NMR (dmso-d_6 + CF_3COOH): δ 20.3 (2CH_3); 35.4 (C-1, C-5); 53.7 (C-6, C-8); 56.5 (C-2, C-4); 61.2 (CH_2Ar); 73.4 (C-9); 117.4, 128.7, 131.7, 136.0 (C(Ph)). Anal. Calcd. for $C_{16}H_{23}ClN_2O$: C, 65.20; H, 7.81; N, 9.51. Found: C, 65.52; H, 7.98; N, 9.35.

S3. Refinement

All hydrogen atoms were located in a difference Fourier map and refined isotropically.

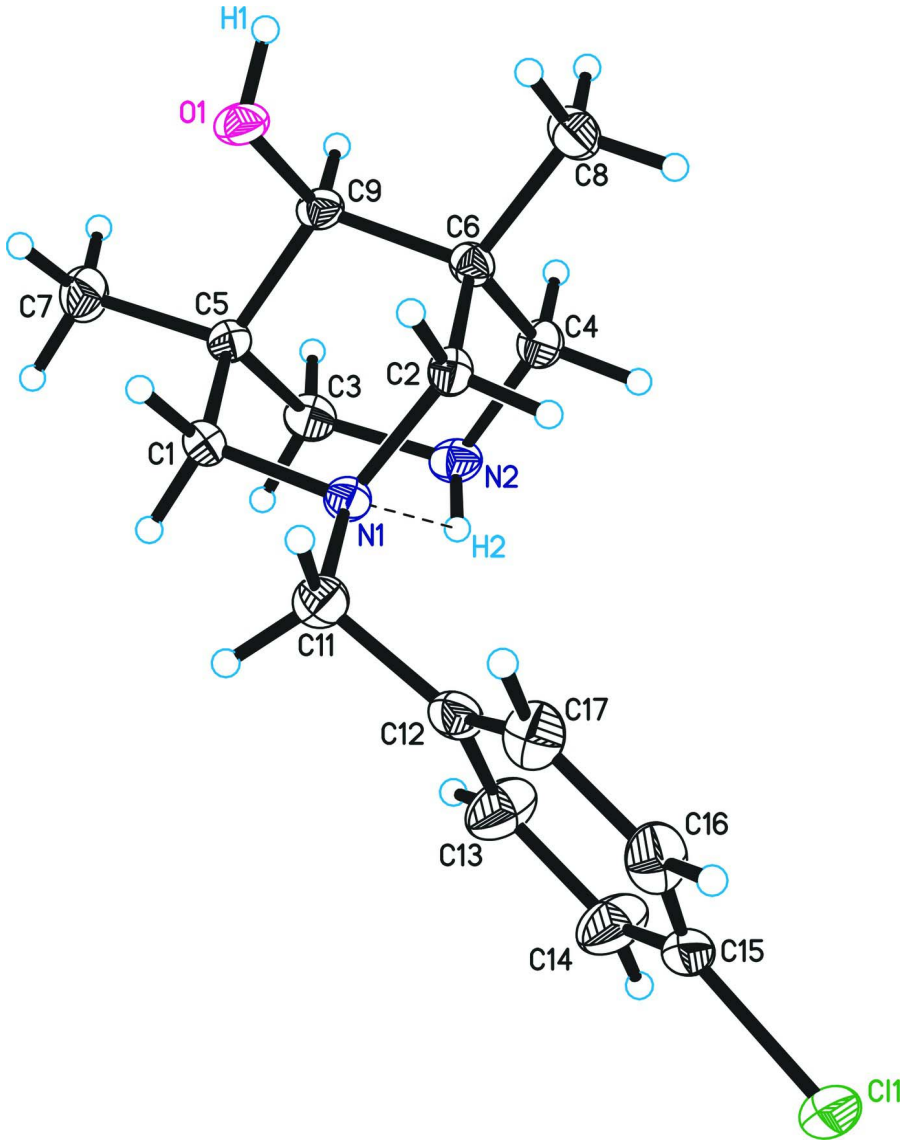

Figure 1

The molecular structure of the title compound, showing the numbering scheme adopted. Displacement ellipsoids are shown at the 50% probability level. Intramolecular hydrogen bond is drawn as dashed line.

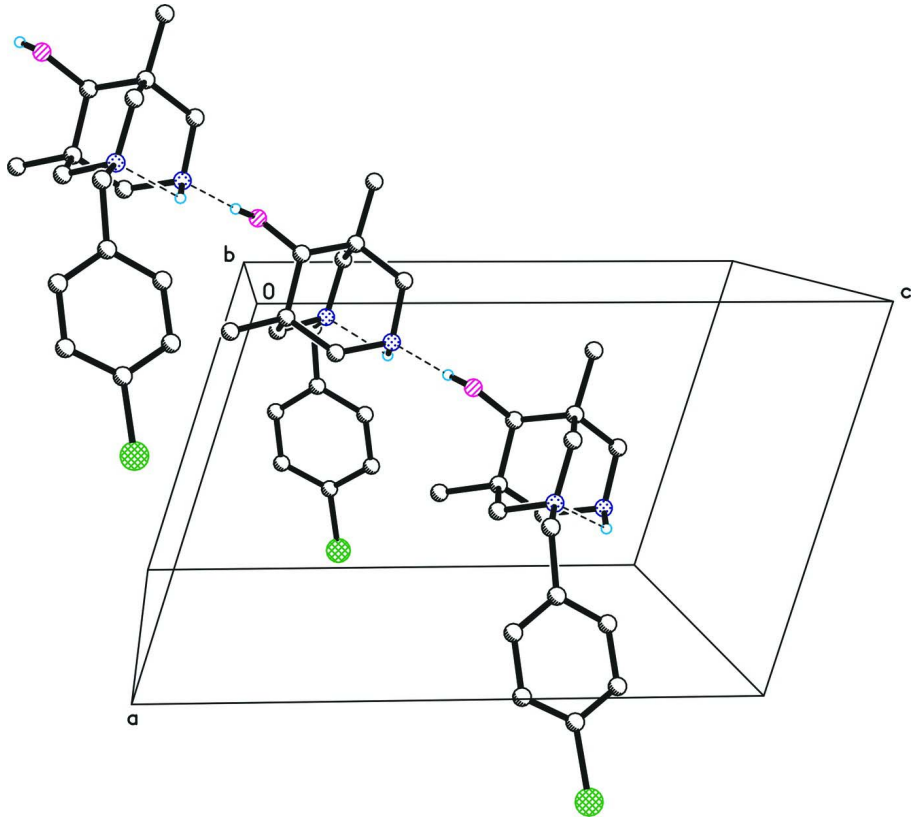

Figure 2

Hydrogen bonded chains spreads along *ac*-diagonal. Hydrogen bonds are drawn as dashed lines.

syn-3-(4-Chlorobenzyl)-1,5-dimethyl-3,7-diazabicyclo[3.3.1]nonan-9-ol

Crystal data

$C_{16}H_{23}ClN_2O$
$M_r = 294.81$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.9739\ (4)$ Å
$b = 16.8120\ (9)$ Å
$c = 12.1103\ (6)$ Å
$\beta = 107.520\ (1)°$
$V = 1548.16\ (14)$ Å^3
$Z = 4$
$F(000) = 632$
$D_x = 1.265$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4857 reflections
$\theta = 2.7–30.0°$
$\mu = 0.25$ mm^{-1}
$T = 120$ K
Prism, colourless
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K **[or APEXII?]** diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.941$, $T_{max} = 0.953$
10450 measured reflections
3747 independent reflections
2976 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.1°$
$h = -10\rightarrow9$
$k = -22\rightarrow14$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.107$
$S = 1.02$
3747 reflections
273 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 0.4862P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ 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}
Cl1	0.97589 (5)	1.10266 (3)	0.39054 (4)	0.03592 (14)
O1	−0.15380 (14)	0.82506 (6)	−0.00656 (9)	0.0220 (2)
N1	0.16827 (16)	0.92965 (7)	0.19544 (10)	0.0176 (3)
N2	0.22587 (17)	0.78671 (8)	0.32531 (11)	0.0211 (3)
C1	−0.01659 (19)	0.92287 (8)	0.19298 (13)	0.0180 (3)
C2	0.20407 (19)	0.88120 (9)	0.10373 (13)	0.0176 (3)
C3	0.0379 (2)	0.79594 (9)	0.31288 (13)	0.0216 (3)
C4	0.2528 (2)	0.75254 (9)	0.22011 (13)	0.0204 (3)
C5	−0.07319 (18)	0.83646 (8)	0.20054 (12)	0.0173 (3)
C6	0.14948 (19)	0.79358 (8)	0.10650 (12)	0.0168 (3)
C7	−0.2661 (2)	0.83514 (11)	0.19815 (17)	0.0265 (3)
C8	0.1851 (2)	0.74991 (10)	0.00522 (14)	0.0244 (3)
C9	−0.04692 (19)	0.79066 (8)	0.09780 (12)	0.0173 (3)
C11	0.2140 (2)	1.01297 (9)	0.18344 (15)	0.0224 (3)
C12	0.4088 (2)	1.02924 (8)	0.23069 (14)	0.0212 (3)
C13	0.4991 (2)	1.01062 (12)	0.34495 (15)	0.0332 (4)
C14	0.6739 (2)	1.03189 (12)	0.39435 (16)	0.0350 (4)
C15	0.7590 (2)	1.07151 (9)	0.32730 (15)	0.0249 (3)
C16	0.6764 (2)	1.08801 (10)	0.21243 (16)	0.0284 (4)
C17	0.5000 (2)	1.06683 (10)	0.16459 (15)	0.0267 (4)
H1	−0.185 (3)	0.7863 (13)	−0.056 (2)	0.047 (6)*
H2	0.275 (2)	0.8334 (12)	0.3320 (17)	0.029 (5)*
H9	−0.082 (2)	0.7325 (11)	0.1019 (15)	0.024 (5)*
H11	−0.029 (2)	0.9525 (9)	0.2591 (14)	0.014 (4)*
H12	−0.097 (2)	0.9484 (10)	0.1210 (15)	0.022 (4)*

H21	0.328 (2)	0.8846 (10)	0.1130 (14)	0.017 (4)*
H22	0.144 (2)	0.9043 (10)	0.0278 (15)	0.018 (4)*
H31	−0.013 (2)	0.7404 (11)	0.3163 (16)	0.027 (5)*
H32	0.032 (2)	0.8250 (10)	0.3794 (16)	0.021 (4)*
H41	0.219 (2)	0.6942 (10)	0.2163 (14)	0.017 (4)*
H42	0.382 (2)	0.7540 (10)	0.2280 (14)	0.018 (4)*
H13	0.438 (3)	0.9822 (12)	0.3919 (18)	0.041 (6)*
H14	0.737 (3)	1.0203 (13)	0.4736 (19)	0.043 (6)*
H16	0.736 (3)	1.1168 (14)	0.168 (2)	0.054 (7)*
H17	0.438 (3)	1.0795 (12)	0.0842 (19)	0.043 (6)*
H71	−0.343 (3)	0.8633 (12)	0.1288 (18)	0.040 (6)*
H72	−0.309 (3)	0.7796 (13)	0.1971 (19)	0.046 (6)*
H73	−0.279 (3)	0.8637 (13)	0.2655 (19)	0.046 (6)*
H81	0.309 (3)	0.7521 (12)	0.0095 (17)	0.036 (5)*
H82	0.116 (2)	0.7740 (11)	−0.0672 (17)	0.029 (5)*
H83	0.151 (2)	0.6936 (12)	0.0048 (15)	0.027 (5)*
H111	0.153 (2)	1.0450 (11)	0.2285 (16)	0.029 (5)*
H112	0.172 (2)	1.0293 (11)	0.1034 (17)	0.032 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0236 (2)	0.0411 (3)	0.0449 (3)	−0.01249 (17)	0.01322 (18)	−0.0198 (2)
O1	0.0232 (6)	0.0192 (5)	0.0174 (5)	0.0022 (4)	−0.0034 (4)	−0.0017 (4)
N1	0.0177 (6)	0.0145 (6)	0.0201 (6)	−0.0009 (4)	0.0047 (5)	−0.0012 (5)
N2	0.0240 (7)	0.0205 (6)	0.0159 (6)	−0.0001 (5)	0.0017 (5)	0.0010 (5)
C1	0.0180 (7)	0.0165 (7)	0.0196 (7)	0.0016 (5)	0.0059 (6)	−0.0023 (6)
C2	0.0162 (7)	0.0189 (7)	0.0177 (7)	0.0014 (5)	0.0051 (6)	0.0010 (5)
C3	0.0262 (8)	0.0226 (8)	0.0167 (7)	−0.0007 (6)	0.0074 (6)	0.0013 (6)
C4	0.0203 (7)	0.0194 (7)	0.0191 (7)	0.0041 (6)	0.0026 (6)	0.0026 (6)
C5	0.0162 (7)	0.0168 (7)	0.0184 (7)	−0.0009 (5)	0.0046 (6)	−0.0012 (5)
C6	0.0192 (7)	0.0157 (7)	0.0152 (7)	0.0023 (5)	0.0045 (6)	0.0001 (5)
C7	0.0201 (8)	0.0281 (9)	0.0335 (9)	−0.0020 (6)	0.0115 (7)	−0.0024 (7)
C8	0.0279 (9)	0.0247 (8)	0.0215 (8)	0.0045 (6)	0.0086 (7)	−0.0019 (6)
C9	0.0185 (7)	0.0146 (7)	0.0159 (7)	0.0008 (5)	0.0007 (5)	0.0003 (5)
C11	0.0230 (8)	0.0158 (7)	0.0267 (8)	−0.0008 (6)	0.0048 (6)	0.0015 (6)
C12	0.0239 (8)	0.0152 (7)	0.0253 (8)	−0.0020 (6)	0.0084 (6)	−0.0038 (6)
C13	0.0274 (9)	0.0496 (11)	0.0237 (9)	−0.0135 (8)	0.0093 (7)	−0.0002 (8)
C14	0.0277 (9)	0.0543 (12)	0.0217 (9)	−0.0116 (8)	0.0053 (7)	−0.0041 (8)
C15	0.0203 (7)	0.0236 (8)	0.0329 (9)	−0.0061 (6)	0.0108 (7)	−0.0114 (7)
C16	0.0287 (9)	0.0229 (8)	0.0379 (9)	−0.0015 (6)	0.0166 (8)	0.0046 (7)
C17	0.0271 (8)	0.0238 (8)	0.0294 (9)	0.0018 (6)	0.0087 (7)	0.0064 (7)

Geometric parameters (Å, º)

Cl1—C15	1.7476 (16)	C6—C8	1.528 (2)
O1—C9	1.4175 (17)	C6—C9	1.538 (2)
O1—H1	0.87 (2)	C7—H71	1.00 (2)

N1—C11	1.4656 (19)	C7—H72	0.99 (2)
N1—C1	1.4698 (19)	C7—H73	0.98 (2)
N1—C2	1.4729 (19)	C8—H81	0.97 (2)
N2—C3	1.469 (2)	C8—H82	0.971 (19)
N2—C4	1.471 (2)	C8—H83	0.984 (19)
N2—H2	0.870 (19)	C9—H9	1.021 (18)
C1—C5	1.532 (2)	C11—C12	1.510 (2)
C1—H11	0.972 (16)	C11—H111	0.993 (19)
C1—H12	1.010 (18)	C11—H112	0.97 (2)
C2—C6	1.539 (2)	C12—C17	1.386 (2)
C2—H21	0.962 (17)	C12—C13	1.390 (2)
C2—H22	0.980 (17)	C13—C14	1.388 (2)
C3—C5	1.541 (2)	C13—H13	0.98 (2)
C3—H31	1.026 (19)	C14—C15	1.377 (2)
C3—H32	0.955 (18)	C14—H14	0.96 (2)
C4—C6	1.5381 (19)	C15—C16	1.376 (3)
C4—H41	1.014 (17)	C16—C17	1.397 (2)
C4—H42	1.005 (17)	C16—H16	0.95 (2)
C5—C7	1.530 (2)	C17—H17	0.97 (2)
C5—C9	1.530 (2)		

C9—O1—H1	106.2 (15)	C5—C7—H71	111.5 (12)
C11—N1—C1	110.47 (11)	C5—C7—H72	110.7 (12)
C11—N1—C2	110.08 (12)	H71—C7—H72	108.4 (17)
C1—N1—C2	111.27 (11)	C5—C7—H73	109.4 (12)
C3—N2—C4	111.30 (12)	H71—C7—H73	106.2 (17)
C3—N2—H2	109.3 (13)	H72—C7—H73	110.6 (18)
C4—N2—H2	104.8 (13)	C6—C8—H81	111.8 (12)
N1—C1—C5	112.58 (11)	C6—C8—H82	109.5 (11)
N1—C1—H11	106.9 (9)	H81—C8—H82	108.6 (16)
C5—C1—H11	109.4 (9)	C6—C8—H83	110.5 (11)
N1—C1—H12	111.0 (10)	H81—C8—H83	108.0 (16)
C5—C1—H12	109.4 (10)	H82—C8—H83	108.5 (15)
H11—C1—H12	107.3 (13)	O1—C9—C5	109.08 (11)
N1—C2—C6	113.11 (12)	O1—C9—C6	111.99 (12)
N1—C2—H21	107.7 (10)	C5—C9—C6	108.29 (11)
C6—C2—H21	110.0 (10)	O1—C9—H9	109.6 (10)
N1—C2—H22	109.7 (10)	C5—C9—H9	109.6 (10)
C6—C2—H22	109.8 (10)	C6—C9—H9	108.2 (10)
H21—C2—H22	106.2 (14)	N1—C11—C12	113.18 (12)
N2—C3—C5	115.77 (12)	N1—C11—H111	106.7 (11)
N2—C3—H31	107.9 (10)	C12—C11—H111	108.2 (11)
C5—C3—H31	107.9 (10)	N1—C11—H112	110.5 (11)
N2—C3—H32	106.1 (11)	C12—C11—H112	109.6 (11)
C5—C3—H32	110.9 (10)	H111—C11—H112	108.5 (15)
H31—C3—H32	108.0 (15)	C17—C12—C13	118.22 (15)
N2—C4—C6	114.89 (12)	C17—C12—C11	121.53 (15)
N2—C4—H41	108.1 (9)	C13—C12—C11	120.16 (14)

C6—C4—H41	109.2 (9)	C14—C13—C12	121.57 (16)
N2—C4—H42	108.7 (10)	C14—C13—H13	119.2 (12)
C6—C4—H42	109.4 (10)	C12—C13—H13	119.2 (12)
H41—C4—H42	106.2 (13)	C15—C14—C13	118.67 (17)
C7—C5—C9	111.12 (12)	C15—C14—H14	118.9 (13)
C7—C5—C1	108.97 (12)	C13—C14—H14	122.4 (13)
C9—C5—C1	108.28 (12)	C16—C15—C14	121.53 (16)
C7—C5—C3	108.52 (13)	C16—C15—Cl1	119.45 (13)
C9—C5—C3	108.21 (12)	C14—C15—Cl1	119.01 (14)
C1—C5—C3	111.76 (12)	C15—C16—C17	118.92 (16)
C8—C6—C4	108.87 (12)	C15—C16—H16	120.4 (15)
C8—C6—C9	111.18 (12)	C17—C16—H16	120.5 (14)
C4—C6—C9	107.90 (12)	C12—C17—C16	121.00 (16)
C8—C6—C2	108.67 (12)	C12—C17—H17	118.8 (13)
C4—C6—C2	111.71 (12)	C16—C17—H17	120.2 (13)
C9—C6—C2	108.54 (11)		

C11—N1—C1—C5	177.79 (12)	C3—C5—C9—C6	−60.28 (14)
C2—N1—C1—C5	55.20 (16)	C8—C6—C9—O1	−58.82 (15)
C11—N1—C2—C6	−176.75 (12)	C4—C6—C9—O1	−178.14 (11)
C1—N1—C2—C6	−53.93 (15)	C2—C6—C9—O1	60.65 (15)
C4—N2—C3—C5	−48.59 (17)	C8—C6—C9—C5	−179.14 (12)
C3—N2—C4—C6	49.63 (17)	C4—C6—C9—C5	61.55 (14)
N1—C1—C5—C7	179.66 (13)	C2—C6—C9—C5	−59.66 (14)
N1—C1—C5—C9	−59.36 (15)	C1—N1—C11—C12	157.40 (13)
N1—C1—C5—C3	59.73 (16)	C2—N1—C11—C12	−79.32 (16)
N2—C3—C5—C7	175.66 (13)	N1—C11—C12—C17	127.48 (16)
N2—C3—C5—C9	54.98 (16)	N1—C11—C12—C13	−56.2 (2)
N2—C3—C5—C1	−64.15 (16)	C17—C12—C13—C14	2.9 (3)
N2—C4—C6—C8	−177.88 (13)	C11—C12—C13—C14	−173.55 (17)
N2—C4—C6—C9	−57.11 (16)	C12—C13—C14—C15	−0.8 (3)
N2—C4—C6—C2	62.10 (17)	C13—C14—C15—C16	−2.1 (3)
N1—C2—C6—C8	177.65 (12)	C13—C14—C15—Cl1	177.03 (15)
N1—C2—C6—C4	−62.22 (16)	C14—C15—C16—C17	2.7 (3)
N1—C2—C6—C9	56.62 (15)	Cl1—C15—C16—C17	−176.40 (13)
C7—C5—C9—O1	58.55 (16)	C13—C12—C17—C16	−2.2 (2)
C1—C5—C9—O1	−61.09 (15)	C11—C12—C17—C16	174.16 (15)
C3—C5—C9—O1	177.60 (12)	C15—C16—C17—C12	−0.5 (3)
C7—C5—C9—C6	−179.33 (12)	C5—C9—O1—H1	−147.5 (15)
C1—C5—C9—C6	61.02 (14)	C6—C9—O1—H1	92.6 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1	0.870 (19)	2.287 (19)	2.8327 (18)	120.8 (16)
O1—H1···N2^{i}	0.87 (2)	1.86 (2)	2.7242 (17)	172 (2)

Symmetry code: (i) $x-1/2, -y+3/2, z-1/2$.