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A 1:1 molecular complex of 4-aminocyclohexanol and (4-hydroxycyclohexyl)carbamic acid

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.102
Data-to-parameter ratio = 12.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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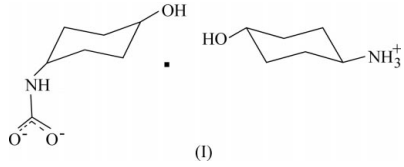
The title molecular complex, 4-ammoniocyclohexanol (4-hydroxycyclohexyl)carbamate, $C_6H_{14}NO^+\cdot C_7H_{12}NO_3^-$, forms an ionic column with N—H···O, O—H···O and C—H···O interactions. There are two different cyclic supramolecular synthons of note. The crystal structures of ionic amino acids also have similar structural patterns.

Comment

The title molecular complex, (I), was obtained during a study of 4-aminocyclohexanol. This type of compound has a tendency to form carbonated adducts by reaction with atmospheric CO_2. In this regard, the crystal structure of 2-aminocyclohexylcarbamate has been reported (Hanessian *et al.*, 1995). In our case, 4-hydroxycyclohexylcarbamic acid initially formed, then crystallized with the original 4-aminocyclohexanol to give a 1:1 ionic molecular complex with proton transfer.



(I)

The molecular structure and atom numbering are given in Fig. 1. The main features are similar to those in the molecular complex of methyl 3-acetoxy-1-ammonio-4-iodocyclohexane-1-carboxylate and trifluoroacetate (Avenoza *et al.*, 1997) and similar to 2-aminocyclohexylcarbamate (Hanessian *et al.*, 1995). The ions form a columnar arrangement with several N—H···O interactions (Table 1); the packing is shown in Fig. 2. Weak C—H···O interactions (Table 1) reinforce the

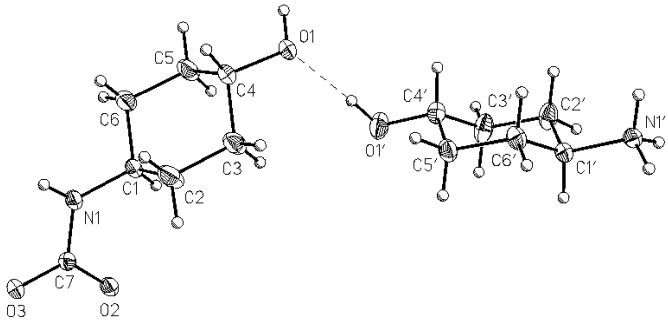


Figure 1
A view of the molecular structure of the title complex, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

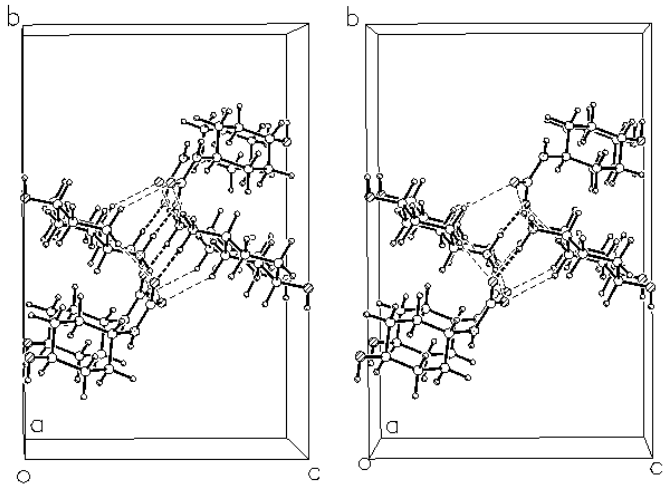


Figure 2
Stereoview of the columnar packing, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

column formation. A closer view of the columnar packing shows that it is composed of two cyclic supramolecular synthons A and B (Fig. 3). Both types of synthon are observed in other ionic amino acids. In the Cambridge Structural Database (Version 5.24, July 2003; Allen, 2002), the crystal structures with refcodes ACXTPY (Bhattacharjee *et al.*, 1975), ACYHXA01 (Valle *et al.*, 1988), DMTYRS (Gaudestad *et al.*, 1976), FOBJUB (Pirrung, 1987), MEMTYR10 (Satyshur & Rao, 1983) RIGSEF (Avenoza *et al.*, 1997) and TOKNUC (Allan *et al.*, 1996) contain synthons A and B.

O—H···O(carboxylate) and O—H···O(hydroxyl) hydrogen bonds act as connectors between the columns.

Experimental

Neutralization of the commercially available (Lancaster) hydrochloride salt of 4-aminocyclohexanol by $NaHCO_3$ in water affords the 4-aminocyclohexanol (extracted with EtOAc). The compound crystallized from a 1:1:1 mixture of EtOAc, CH_3CN and EtOH. During the time of crystallization, 4-aminocyclohexanol is carboxylated by atmospheric CO_2 to give the carbamic acid which cocrystallizes with the parent compound to give yellow crystals of the 1:1 molecular complex.

Crystal data

$C_6H_{14}NO^+\cdot C_7H_{12}NO_3^-$
M_r = 274.36
Monoclinic, $P2_1/c$
a = 6.3452 (2) Å
b = 18.6256 (6) Å
c = 12.1664 (4) Å
β = 92.284 (2)°
V = 1436.72 (8) Å^3
Z = 4
D_x = 1.268 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4934 reflections
θ = 2.8–27.5°
μ = 0.09 mm^{-1}
T = 120 (2) K
Plate, yellow
0.22 × 0.12 × 0.04 mm

Data collection

SMART 6K CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.927, T_{max} = 1.000
19783 measured reflections
3308 independent reflections
2537 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 27.5°
$h = -7 \rightarrow 8$
$k = -24 \rightarrow 24$
$l = -15 \rightarrow 15$

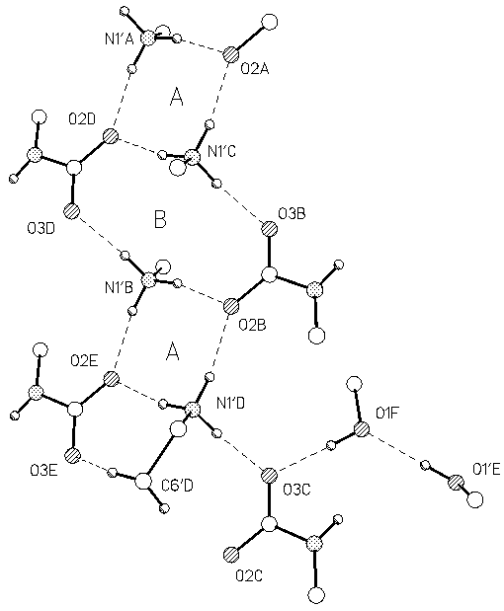


Figure 3
Segment of the crystal structure, showing synthons A and B.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.102
S = 1.01
3308 reflections
276 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.3252P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1′—H1′···O1	0.90 (2)	1.88 (2)	2.784 (2)	176 (1)
O1—H1···O3^{i}	0.90 (2)	1.79 (2)	2.687 (1)	175 (2)
N1′—H111···O2^{ii}	0.94 (2)	1.90 (2)	2.816 (1)	167 (1)
N1′—H112···O3^{iii}	0.95 (2)	1.82 (2)	2.7590 (1)	170 (1)
N1′—H114···O2^{iv}	0.92 (2)	1.87 (2)	2.7870 (1)	169 (1)
C6′—H6D···O3^{ii}	0.96 (2)	2.54 (1)	3.417 (1)	152 (1)

Symmetry codes: (i) $1+x, \frac{3}{2}-y, \frac{1}{2}+z$; (ii) $1+x, y, 1+z$; (iii) $-x, 1-y, 1-z$; (iv) $1-x, 1-y, 1-z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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A 1:1 molecular complex of 4-aminocyclohexanol and (4-hydroxycyclohexyl)-carbamic acid

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4-ammoniocyclohexanol–(4-hydroxycyclohexyl)carbamate (1/1)

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β = 92.284 (2)°
V = 1436.72 (8) Å^3
Z = 4
$F(000)$ = 600
D_x = 1.268 Mg m^{-3}
Melting point: 377 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4934 reflections
θ = 2.8–27.5°
μ = 0.09 mm^{-1}
T = 120 K
Plate, yellow
0.22 × 0.12 × 0.04 mm

Data collection

SMART 6k CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
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Detector resolution: 8 pixels mm^{-1}
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19783 measured reflections
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R_{int} = 0.038
θ_{max} = 27.5°, θ_{min} = 2.0°
h = −7→8
k = −24→24
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.102
S = 1.01
3308 reflections
276 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.3252P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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}
O3	−0.46270 (13)	0.63687 (5)	0.01886 (7)	0.0216 (2)
O2	−0.15113 (14)	0.58448 (5)	0.05544 (7)	0.0223 (2)
O1	0.35337 (16)	0.73442 (5)	0.48724 (8)	0.0300 (2)
N1′	0.74068 (18)	0.46768 (6)	0.91750 (8)	0.0182 (2)
O1′	0.56745 (17)	0.60426 (6)	0.50683 (8)	0.0303 (2)
N1	−0.21577 (18)	0.69590 (6)	0.12248 (9)	0.0227 (2)
C7	−0.27812 (19)	0.63633 (6)	0.06402 (9)	0.0172 (2)
C1	−0.0410 (2)	0.69605 (7)	0.20400 (10)	0.0197 (3)
C1′	0.68231 (19)	0.48446 (7)	0.79946 (10)	0.0182 (3)
C4	0.1752 (2)	0.74117 (7)	0.41197 (10)	0.0220 (3)
C5	0.2403 (2)	0.76883 (8)	0.30124 (11)	0.0290 (3)
C5′	0.4282 (2)	0.54960 (7)	0.67150 (10)	0.0217 (3)
C4′	0.6106 (2)	0.58854 (7)	0.61997 (10)	0.0229 (3)
C6′	0.4831 (2)	0.52980 (7)	0.79140 (10)	0.0206 (3)
C3′	0.8078 (2)	0.54205 (8)	0.62791 (12)	0.0291 (3)
C6	0.0536 (3)	0.77048 (8)	0.21763 (12)	0.0298 (3)
C2′	0.8658 (2)	0.52213 (8)	0.74691 (12)	0.0266 (3)
C3	0.0736 (3)	0.66789 (8)	0.39996 (12)	0.0321 (3)
C2	−0.1096 (2)	0.66843 (9)	0.31494 (12)	0.0310 (3)
H1A	0.066 (2)	0.6656 (8)	0.1757 (12)	0.020 (3)*
H1B	0.658 (2)	0.4379 (7)	0.7637 (11)	0.015 (3)*
H2D	0.893 (2)	0.5668 (9)	0.7913 (13)	0.028 (4)*
H6D	0.506 (2)	0.5722 (8)	0.8348 (12)	0.021 (4)*
H4′	0.636 (2)	0.6353 (8)	0.6590 (12)	0.021 (4)*
H5D	0.400 (2)	0.5061 (8)	0.6273 (12)	0.020 (4)*
H4	0.073 (3)	0.7753 (9)	0.4436 (13)	0.030 (4)*
H3D	0.925 (3)	0.5664 (9)	0.5937 (14)	0.033 (4)*
H5C	0.307 (3)	0.5814 (9)	0.6675 (13)	0.030 (4)*
H115	−0.315 (3)	0.7273 (10)	0.1311 (14)	0.038 (5)*
H114	0.870 (3)	0.4447 (9)	0.9227 (13)	0.031 (4)*
H2A	−0.221 (3)	0.7018 (11)	0.3403 (15)	0.047 (5)*
H112	0.641 (3)	0.4352 (9)	0.9465 (14)	0.038 (5)*
H111	0.756 (2)	0.5090 (9)	0.9608 (13)	0.027 (4)*
H6C	0.370 (2)	0.5034 (8)	0.8226 (12)	0.021 (4)*
H5A	0.352 (3)	0.7351 (10)	0.2737 (15)	0.042 (5)*

H1′	0.498 (3)	0.6467 (10)	0.5041 (15)	0.042 (5)*
H3C	0.776 (3)	0.4966 (11)	0.5837 (15)	0.045 (5)*
H2C	0.988 (3)	0.4894 (9)	0.7499 (13)	0.036 (4)*
H3A	0.188 (3)	0.6337 (10)	0.3776 (14)	0.042 (5)*
H6B	−0.058 (3)	0.8024 (10)	0.2441 (14)	0.035 (4)*
H2B	−0.171 (3)	0.6200 (10)	0.3086 (14)	0.039 (5)*
H6A	0.095 (3)	0.7889 (10)	0.1460 (16)	0.047 (5)*
H3B	0.026 (3)	0.6536 (11)	0.4732 (17)	0.053 (5)*
H1	0.419 (3)	0.7770 (11)	0.4939 (16)	0.049 (5)*
H5B	0.305 (3)	0.8174 (10)	0.3088 (14)	0.042 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0175 (5)	0.0204 (4)	0.0262 (5)	−0.0009 (3)	−0.0078 (3)	0.0008 (3)
O2	0.0191 (5)	0.0202 (4)	0.0270 (5)	0.0026 (3)	−0.0060 (4)	−0.0046 (3)
O1	0.0349 (6)	0.0212 (5)	0.0322 (5)	−0.0039 (4)	−0.0202 (4)	0.0027 (4)
N1′	0.0167 (5)	0.0184 (5)	0.0191 (5)	0.0002 (4)	−0.0026 (4)	−0.0002 (4)
O1′	0.0362 (6)	0.0308 (5)	0.0235 (5)	0.0065 (4)	−0.0022 (4)	0.0075 (4)
N1	0.0207 (6)	0.0201 (5)	0.0264 (6)	0.0044 (4)	−0.0096 (4)	−0.0048 (4)
C7	0.0183 (6)	0.0169 (6)	0.0161 (5)	−0.0012 (4)	−0.0022 (4)	0.0021 (4)
C1	0.0179 (6)	0.0203 (6)	0.0202 (6)	0.0010 (5)	−0.0064 (5)	−0.0024 (5)
C1′	0.0176 (6)	0.0193 (6)	0.0176 (6)	0.0000 (5)	−0.0024 (4)	0.0007 (4)
C4	0.0230 (7)	0.0213 (6)	0.0211 (6)	0.0002 (5)	−0.0085 (5)	−0.0019 (5)
C5	0.0296 (8)	0.0294 (7)	0.0272 (7)	−0.0137 (6)	−0.0101 (6)	0.0048 (5)
C5′	0.0187 (6)	0.0248 (6)	0.0211 (6)	0.0023 (5)	−0.0047 (5)	0.0005 (5)
C4′	0.0239 (7)	0.0218 (6)	0.0227 (6)	0.0006 (5)	−0.0041 (5)	0.0039 (5)
C6′	0.0163 (6)	0.0257 (6)	0.0196 (6)	0.0022 (5)	−0.0026 (5)	−0.0002 (5)
C3′	0.0218 (7)	0.0360 (8)	0.0297 (7)	0.0044 (6)	0.0044 (6)	0.0145 (6)
C6	0.0380 (8)	0.0245 (7)	0.0258 (7)	−0.0089 (6)	−0.0134 (6)	0.0050 (5)
C2′	0.0159 (6)	0.0324 (7)	0.0311 (7)	0.0008 (5)	−0.0021 (5)	0.0113 (6)
C3	0.0432 (9)	0.0297 (7)	0.0223 (7)	−0.0158 (7)	−0.0113 (6)	0.0072 (6)
C2	0.0318 (8)	0.0352 (8)	0.0253 (7)	−0.0162 (6)	−0.0065 (6)	0.0024 (6)

Geometric parameters (Å, º)

O3—C7	1.2737 (14)	C5—H5A	1.016 (19)
O2—C7	1.2647 (15)	C5—H5B	0.996 (19)
O1—C4	1.4316 (15)	C5′—C4′	1.5224 (19)
O1—H1	0.90 (2)	C5′—C6′	1.5314 (17)
N1′—C1′	1.5016 (15)	C5′—H5D	0.984 (15)
N1′—H114	0.924 (18)	C5′—H5C	0.971 (17)
N1′—H112	0.953 (18)	C4′—C3′	1.5215 (19)
N1′—H111	0.937 (17)	C4′—H4′	1.002 (15)
O1′—C4′	1.4231 (15)	C6′—H6D	0.959 (15)
O1′—H1′	0.905 (19)	C6′—H6C	0.961 (16)
N1—C7	1.3679 (15)	C3′—C2′	1.5253 (19)
N1—C1	1.4578 (15)	C3′—H3D	0.980 (18)

N1—H115	0.869 (19)	C3′—H3C	1.019 (19)
C1—C6	1.5170 (18)	C6—H6B	0.990 (18)
C1—C2	1.5240 (19)	C6—H6A	0.982 (19)
C1—H1A	0.958 (15)	C2′—H2D	1.003 (16)
C1′—C6′	1.5198 (17)	C2′—H2C	0.984 (18)
C1′—C2′	1.5216 (18)	C3—C2	1.5249 (19)
C1′—H1B	0.979 (14)	C3—H3A	1.011 (19)
C4—C3	1.5141 (18)	C3—H3B	0.99 (2)
C4—C5	1.5151 (19)	C2—H2A	1.00 (2)
C4—H4	0.996 (16)	C2—H2B	0.983 (18)
C5—C6	1.5310 (19)		

C4—O1—H1	109.3 (12)	H5D—C5′—H5C	110.4 (13)
C1′—N1′—H114	110.2 (10)	O1′—C4′—C3′	107.74 (11)
C1′—N1′—H112	110.1 (10)	O1′—C4′—C5′	112.09 (11)
H114—N1′—H112	106.3 (14)	C3′—C4′—C5′	109.85 (11)
C1′—N1′—H111	112.6 (9)	O1′—C4′—H4′	107.5 (8)
H114—N1′—H111	105.6 (14)	C3′—C4′—H4′	110.5 (8)
H112—N1′—H111	111.7 (14)	C5′—C4′—H4′	109.1 (8)
C4′—O1′—H1′	106.9 (12)	C1′—C6′—C5′	110.64 (10)
C7—N1—C1	123.48 (11)	C1′—C6′—H6D	108.3 (9)
C7—N1—H115	114.4 (12)	C5′—C6′—H6D	110.5 (9)
C1—N1—H115	116.9 (12)	C1′—C6′—H6C	108.8 (9)
O2—C7—O3	123.25 (11)	C5′—C6′—H6C	110.8 (9)
O2—C7—N1	119.36 (11)	H6D—C6′—H6C	107.7 (12)
O3—C7—N1	117.38 (11)	C4′—C3′—C2′	111.42 (12)
N1—C1—C6	111.28 (10)	C4′—C3′—H3D	110.3 (10)
N1—C1—C2	111.45 (11)	C2′—C3′—H3D	110.9 (10)
C6—C1—C2	109.71 (11)	C4′—C3′—H3C	107.1 (11)
N1—C1—H1A	106.5 (8)	C2′—C3′—H3C	109.5 (10)
C6—C1—H1A	107.3 (9)	H3D—C3′—H3C	107.4 (14)
C2—C1—H1A	110.5 (9)	C1—C6—C5	110.28 (11)
N1′—C1′—C6′	110.50 (10)	C1—C6—H6B	107.4 (10)
N1′—C1′—C2′	109.52 (10)	C5—C6—H6B	110.0 (10)
C6′—C1′—C2′	111.39 (10)	C1—C6—H6A	110.0 (11)
N1′—C1′—H1B	105.6 (8)	C5—C6—H6A	111.6 (11)
C6′—C1′—H1B	110.2 (8)	H6B—C6—H6A	107.4 (15)
C2′—C1′—H1B	109.4 (8)	C1′—C2′—C3′	110.58 (11)
O1—C4—C3	107.75 (10)	C1′—C2′—H2D	106.0 (9)
O1—C4—C5	111.25 (11)	C3′—C2′—H2D	109.9 (9)
C3—C4—C5	110.54 (11)	C1′—C2′—H2C	108.2 (10)
O1—C4—H4	108.5 (9)	C3′—C2′—H2C	110.2 (10)
C3—C4—H4	109.3 (9)	H2D—C2′—H2C	111.9 (13)
C5—C4—H4	109.4 (9)	C4—C3—C2	111.69 (12)
C4—C5—C6	111.49 (12)	C4—C3—H3A	106.7 (10)
C4—C5—H5A	107.6 (10)	C2—C3—H3A	111.0 (10)
C6—C5—H5A	109.1 (10)	C4—C3—H3B	107.4 (12)
C4—C5—H5B	110.7 (10)	C2—C3—H3B	111.2 (12)

C6—C5—H5B	110.5 (10)	H3A—C3—H3B	108.7 (15)
H5A—C5—H5B	107.4 (14)	C1—C2—C3	111.49 (12)
C4′—C5′—C6′	111.03 (10)	C1—C2—H2A	107.1 (11)
C4′—C5′—H5D	107.0 (8)	C3—C2—H2A	109.0 (11)
C6′—C5′—H5D	110.6 (8)	C1—C2—H2B	111.4 (10)
C4′—C5′—H5C	107.6 (9)	C3—C2—H2B	109.5 (10)
C6′—C5′—H5C	110.2 (9)	H2A—C2—H2B	108.2 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1′—H1′···O1	0.90 (2)	1.88 (2)	2.784 (2)	176 (1)
O1—H1···O3^{i}	0.90 (2)	1.79 (2)	2.687 (1)	175 (2)
N1′—H111···O2^{ii}	0.94 (2)	1.90 (2)	2.816 (1)	167 (1)
N1′—H112···O3^{iii}	0.95 (2)	1.82 (2)	2.7590 (1)	170 (1)
N1′—H114···O2^{iv}	0.92 (2)	1.87 (2)	2.7870 (1)	169 (1)
C6′—H6*D*···O3^{ii}	0.96 (2)	2.54 (1)	3.417 (1)	152 (1)

Symmetry codes: (i) *x*+1, −*y*+3/2, *z*+1/2; (ii) *x*+1, *y*, *z*+1; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1.