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1-Amino-*N*,*N*-dibenzyl-1-deoxy-α-D-tagatopyranose methanol solvate

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Key indicators

Single-crystal X-ray study
T = 190 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.095
Data-to-parameter ratio = 10.2

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

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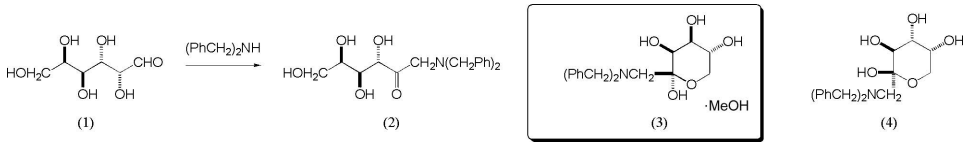
The title tagatosamine, $C_{20}H_{25}NO_5.CH_4O$, formed in the Amadori rearrangement of D-galactose with dibenzylamine, is shown to crystallize as the α-anomer, in contrast to the β-anomer formed in the Amadori reaction of D-glucose with dibenzylamine.

Comment

The Amadori rearrangement, an old and well known reaction (Amadori, 1925; Hodge, 1955), constitutes the first step in the Maillard reaction (Maillard, 1912), the classic browning reaction of food chemistry and one of the most complex reactions known (Martins & Van Boekel, 2005; Kwak & Lim, 2004). Products of the Maillard reaction are responsible for much of the flavour and colour generated during baking and roasting (Mottram *et al.*, 2002). Despite its long standing, however, both the full synthetic potential of the Amadori rearrangement and its role in pathology have yet to be fully understood. The rearrangement is the initial step in the non-enzymatic conjugation of free amines in peptides with reducing carbohydrates to form glycation products *in vivo*; such advanced glycation end-products (AGE) constitute a complex and heterogeneous group of compounds which accumulate in plasma and tissues in diabetes and renal failure (Lapolla *et al.*, 2005; Smit & Lutgers, 2004). Non-enzymatic glycation has also been implicated in processes of ageing, atherosclerosis and in neurodegenerative amyloid pathologies, including Alzheimer's disease (Horvat & Jakas, 2004; Kikuchi *et al.*, 2003).



(1) (2) (3) (4)

D-Galactose (1) on treatment with dibenzylamine in acetic acid, underwent the Amadori rearrangement to give tagatosamine (2) (Grünnagel & Haas, 1969); although the solution NMR of (2) was complex, the formation of crystals allowed the secure identification of the α-anomer (3). Crystallization of the α-anomer of tagatosamine is in direct contrast to the crystallization of the β-anomer of fructosamine (4), the Amadori product formed from D-glucose and dibenzylamine (Hou *et al.*, 2001).

The molecules form independent hydrogen-bonded chains parallel to the *b* axis, incorporating the solvent in the extensive hydrogen-bonding network (Fig. 2).

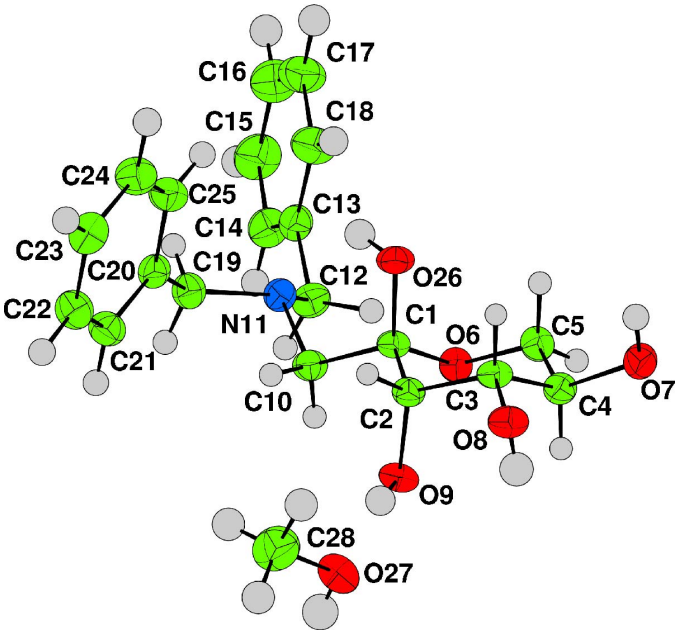


Figure 1
The title compound, with displacement ellipsoids drawn at the 50% probability level.

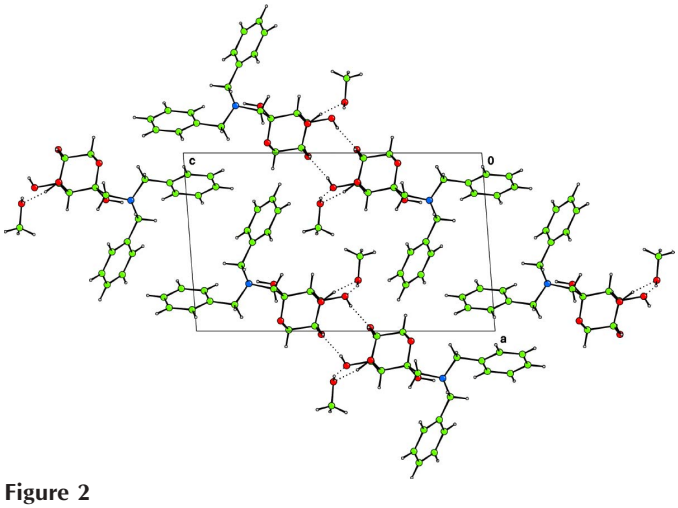


Figure 2
The crystal packing, viewed down the *b* axis.

Experimental

Crystals of the title compound were first obtained by evaporation of a solution in a methanol–water mixture. They were then recrystallized from hot methanol to afford colourless crystals. The full synthetic procedure will be published separately (Hotchkiss *et al.*, 2005).

Crystal data

$C_{20}H_{25}NO_5{\cdot}CH_4O$
M_r = 391.46
Monoclinic, $P2_1$
a = 10.3116 (3) Å
b = 5.9084 (2) Å
c = 17.2641 (6) Å
β = 94.2891 (13)°
V = 1048.87 (6) Å^3
Z = 2
D_x = 1.239 Mg m^{-3}
Mo Kα radiation
Cell parameters from 2207 reflections
θ = 1–27°
μ = 0.09 mm^{-1}
T = 190 K
Block, colourless
0.18 × 0.18 × 0.10 mm

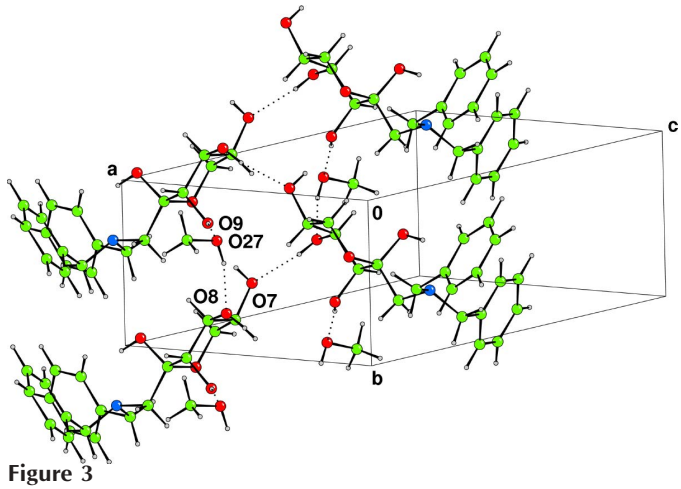


Figure 3
View of a section of one hydrogen-bonded (dashed lines) chain, showing how the solvent and main molecule interact to form the chain.

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: none
4394 measured reflections
2601 independent reflections
2044 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 27.5°
$h = -13 \rightarrow 13$
$k = -7 \rightarrow 7$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.095
S = 0.90
2588 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.04P)^2 + 0.24P]$ where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O27—H1···O8^{i}	0.84	1.89	2.700 (3)	161
O7—H4···O9^{ii}	0.78	2.00	2.740 (2)	157
O8—H12···O7^{iii}	0.82	1.95	2.756 (2)	167
O9—H253···O27	0.96	1.77	2.692 (2)	159

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

All of the H atoms were observed in a difference electron-density map. The hydroxyl H atoms were placed as found and the others were positioned geometrically (C—H = 1.0 Å). All were refined with slack restraints and with U_{iso}(H) = 1.2U_{eq}(parent atom), and then refined as riding atoms. In the absence of significant scattering effects, Friedel pairs were merged. The final structure shows voids of 50 Å^3 to be present. These regions were investigated with difference electron-density maps, but no electron density was found within them. Four reflections were removed manually as outliers, whilst some low-angle reflections were omitted from the refinement because they appeared to be obscured by the beam-stop.

Data collection: *COLLECT* (Nonius, 1997); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

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$a = 10.3116$ (3) Å
$b = 5.9084$ (2) Å
$c = 17.2641$ (6) Å
$\beta = 94.2891$ (13)°
$V = 1048.87$ (6) Å^3
$Z = 2$
$F(000) = 420$
$D_x = 1.239$ Mg m^{-3}
Melting point: 125 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2207 reflections
$\theta = 1$–27°
$\mu = 0.09$ mm^{-1}
$T = 190$ K
Block, colourless
0.18 × 0.18 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Graphite monochromator
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4394 measured reflections
2601 independent reflections
2044 reflections with $I > 2\sigma(I)$
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$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -13 \rightarrow 13$
$k = -7 \rightarrow 7$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.095$
$S = 0.90$
2588 reflections
253 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.04P)^2 + 0.24P]$ where $P = [\max(F_o^2,0) + 2F_c^2]/3$
$(\Delta/\sigma)_{max} = 0.000125$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O27	0.28501 (18)	0.6347 (3)	0.55400 (10)	0.0431
C28	0.4200 (3)	0.6523 (6)	0.56632 (18)	0.0602
H16	0.4583	0.7226	0.5201	0.0700*
H26	0.4528	0.4939	0.5730	0.0706*

H28	0.4420	0.7436	0.6152	0.0705*
H1	0.2539	0.7657	0.5502	0.0850*
C1	0.1937 (2)	0.2791 (4)	0.30262 (13)	0.0269
C2	0.2224 (2)	0.2670 (4)	0.39074 (13)	0.0279
C3	0.1704 (2)	0.0479 (4)	0.42317 (13)	0.0286
C4	0.0283 (2)	0.0148 (4)	0.39717 (13)	0.0306
C5	0.0063 (2)	0.0461 (4)	0.30951 (13)	0.0322
O6	0.05706 (15)	0.2580 (3)	0.28426 (9)	0.0306
O7	−0.01900 (16)	−0.2045 (3)	0.41718 (10)	0.0371
O8	0.19461 (17)	0.0441 (3)	0.50611 (9)	0.0353
O9	0.16411 (17)	0.4586 (3)	0.42410 (9)	0.0335
C10	0.2363 (2)	0.5049 (4)	0.26918 (13)	0.0315
N11	0.26608 (19)	0.4749 (4)	0.18718 (11)	0.0304
C12	0.1482 (2)	0.5060 (5)	0.13437 (13)	0.0358
C13	0.1674 (2)	0.4348 (4)	0.05219 (13)	0.0344
C14	0.1193 (3)	0.5681 (5)	−0.00951 (14)	0.0423
C15	0.1306 (3)	0.4988 (6)	−0.08563 (16)	0.0554
C16	0.1902 (3)	0.2987 (7)	−0.10078 (17)	0.0579
C17	0.2386 (3)	0.1632 (6)	−0.04026 (17)	0.0555
C18	0.2263 (3)	0.2303 (5)	0.03591 (16)	0.0481
C19	0.3696 (2)	0.6315 (4)	0.16635 (13)	0.0340
C20	0.4987 (2)	0.5815 (4)	0.20930 (13)	0.0324
C21	0.5556 (3)	0.7338 (5)	0.26329 (14)	0.0370
C22	0.6763 (3)	0.6872 (5)	0.30235 (16)	0.0412
C23	0.7400 (3)	0.4891 (5)	0.28754 (15)	0.0430
C24	0.6836 (3)	0.3355 (5)	0.23441 (16)	0.0443
C25	0.5643 (3)	0.3813 (5)	0.19553 (15)	0.0387
O26	0.26232 (17)	0.1016 (3)	0.27034 (10)	0.0340
H21	0.3177	0.2708	0.4024	0.0323*
H31	0.2202	−0.0785	0.4009	0.0312*
H41	−0.0206	0.1345	0.4227	0.0347*
H51	0.0507	−0.0804	0.2835	0.0355*
H52	−0.0875	0.0447	0.2959	0.0366*
H101	0.3166	0.5510	0.2997	0.0357*
H102	0.1681	0.6217	0.2743	0.0359*
H121	0.0775	0.4143	0.1541	0.0399*
H122	0.1208	0.6670	0.1346	0.0398*
H141	0.0775	0.7145	0.0010	0.0496*
H151	0.0969	0.5954	−0.1284	0.0663*
H161	0.1998	0.2503	−0.1544	0.0681*
H171	0.2807	0.0197	−0.0513	0.0650*
H181	0.2603	0.1343	0.0793	0.0562*
H191	0.3444	0.7889	0.1750	0.0391*
H192	0.3798	0.6099	0.1104	0.0385*
H211	0.5116	0.8764	0.2734	0.0441*
H221	0.7146	0.7960	0.3418	0.0480*
H231	0.8246	0.4558	0.3156	0.0497*
H241	0.7285	0.1924	0.2249	0.0531*

H251	0.5240	0.2730	0.1585	0.0450*
H252	0.2777	0.1573	0.2176	0.0601*
H4	0.0315	−0.2956	0.4058	0.0456*
H12	0.1412	0.1313	0.5224	0.0747*
H253	0.2184	0.4880	0.4706	0.0579*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O27	0.0463 (11)	0.0351 (10)	0.0464 (10)	0.0013 (9)	−0.0067 (8)	−0.0026 (9)
C28	0.055 (2)	0.064 (2)	0.0628 (19)	0.0040 (19)	0.0081 (15)	−0.0019 (18)
C1	0.0289 (12)	0.0242 (11)	0.0280 (11)	0.0047 (10)	0.0035 (9)	−0.0019 (10)
C2	0.0266 (12)	0.0256 (12)	0.0316 (12)	0.0034 (10)	0.0021 (9)	−0.0021 (10)
C3	0.0340 (13)	0.0281 (12)	0.0238 (11)	0.0063 (11)	0.0036 (10)	−0.0007 (10)
C4	0.0316 (13)	0.0259 (12)	0.0348 (12)	0.0042 (11)	0.0060 (10)	0.0031 (10)
C5	0.0311 (13)	0.0302 (13)	0.0349 (13)	0.0007 (11)	−0.0002 (10)	0.0017 (11)
O6	0.0292 (9)	0.0296 (9)	0.0327 (8)	0.0024 (8)	−0.0009 (7)	0.0044 (8)
O7	0.0349 (9)	0.0303 (9)	0.0471 (10)	0.0021 (8)	0.0097 (8)	0.0050 (8)
O8	0.0430 (10)	0.0353 (9)	0.0273 (8)	0.0085 (8)	0.0018 (7)	0.0005 (7)
O9	0.0432 (10)	0.0280 (9)	0.0290 (8)	0.0064 (8)	0.0004 (7)	−0.0053 (8)
C10	0.0371 (14)	0.0291 (13)	0.0289 (12)	0.0027 (11)	0.0060 (10)	−0.0003 (10)
N11	0.0334 (11)	0.0310 (10)	0.0270 (9)	−0.0008 (9)	0.0034 (8)	0.0018 (9)
C12	0.0314 (13)	0.0415 (14)	0.0342 (13)	0.0049 (12)	0.0014 (10)	−0.0002 (12)
C13	0.0338 (13)	0.0372 (14)	0.0322 (13)	−0.0030 (12)	0.0032 (10)	0.0011 (12)
C14	0.0449 (16)	0.0445 (16)	0.0373 (14)	0.0019 (13)	0.0029 (12)	0.0041 (13)
C15	0.068 (2)	0.063 (2)	0.0352 (15)	0.0013 (19)	0.0042 (13)	0.0077 (16)
C16	0.071 (2)	0.068 (2)	0.0349 (15)	−0.007 (2)	0.0066 (14)	−0.0077 (16)
C17	0.072 (2)	0.0473 (18)	0.0485 (17)	0.0027 (17)	0.0113 (15)	−0.0105 (15)
C18	0.0624 (19)	0.0406 (16)	0.0414 (14)	0.0063 (15)	0.0048 (13)	−0.0004 (14)
C19	0.0369 (14)	0.0317 (13)	0.0336 (13)	−0.0006 (12)	0.0037 (10)	0.0044 (11)
C20	0.0357 (14)	0.0307 (13)	0.0318 (12)	0.0001 (11)	0.0080 (10)	0.0048 (11)
C21	0.0431 (15)	0.0312 (13)	0.0371 (13)	0.0011 (12)	0.0052 (11)	−0.0002 (12)
C22	0.0415 (16)	0.0416 (15)	0.0400 (14)	−0.0024 (13)	−0.0011 (12)	−0.0017 (12)
C23	0.0382 (15)	0.0501 (17)	0.0404 (14)	0.0024 (14)	0.0012 (11)	0.0069 (14)
C24	0.0409 (16)	0.0404 (15)	0.0516 (16)	0.0087 (13)	0.0030 (13)	0.0009 (13)
C25	0.0444 (16)	0.0363 (14)	0.0355 (14)	0.0021 (13)	0.0038 (12)	−0.0034 (12)
O26	0.0405 (10)	0.0283 (9)	0.0343 (9)	0.0079 (8)	0.0098 (7)	−0.0026 (7)

Geometric parameters (Å, º)

O27—C28	1.397 (3)	C12—C13	1.507 (3)
O27—H1	0.839	C12—H121	0.989
C28—H16	1.006	C12—H122	0.992
C28—H26	0.999	C13—C14	1.386 (4)
C28—H28	1.012	C13—C18	1.390 (4)
C1—C2	1.529 (3)	C14—C15	1.390 (4)
C1—O6	1.427 (3)	C14—H141	0.990
C1—C10	1.531 (3)	C15—C16	1.367 (5)

C1—O26	1.403 (3)	C15—H151	0.975
C2—C3	1.524 (3)	C16—C17	1.380 (5)
C2—O9	1.423 (3)	C16—H161	0.980
C2—H21	0.989	C17—C18	1.388 (4)
C3—C4	1.513 (3)	C17—H171	0.978
C3—O8	1.435 (3)	C18—H181	0.984
C3—H31	0.999	C19—C20	1.503 (3)
C4—C5	1.525 (3)	C19—H191	0.980
C4—O7	1.435 (3)	C19—H192	0.987
C4—H41	0.991	C20—C21	1.393 (4)
C5—O6	1.437 (3)	C20—C25	1.392 (4)
C5—H51	1.000	C21—C22	1.398 (4)
C5—H52	0.979	C21—H211	0.978
O7—H4	0.784	C22—C23	1.375 (4)
O8—H12	0.820	C22—H221	0.997
O9—H253	0.960	C23—C24	1.387 (4)
C10—N11	1.481 (3)	C23—H231	0.985
C10—H101	0.985	C24—C25	1.383 (4)
C10—H102	0.994	C24—H241	0.983
N11—C12	1.475 (3)	C25—H251	0.976
N11—C19	1.477 (3)	O26—H252	0.992

C28—O27—H1	108.4	N11—C12—C13	112.8 (2)
O27—C28—H16	110.8	N11—C12—H121	108.2
O27—C28—H26	105.8	C13—C12—H121	108.9
H16—C28—H26	109.2	N11—C12—H122	109.8
O27—C28—H28	108.9	C13—C12—H122	109.2
H16—C28—H28	111.3	H121—C12—H122	107.8
H26—C28—H28	110.5	C12—C13—C14	120.0 (2)
C2—C1—O6	109.4 (1)	C12—C13—C18	121.5 (2)
C2—C1—C10	112.1 (2)	C14—C13—C18	118.4 (2)
O6—C1—C10	107.4 (2)	C13—C14—C15	120.6 (3)
C2—C1—O26	107.1 (2)	C13—C14—H141	119.4
O6—C1—O26	111.4 (2)	C15—C14—H141	120.0
C10—C1—O26	109.5 (2)	C14—C15—C16	120.4 (3)
C1—C2—C3	111.0 (2)	C14—C15—H151	119.5
C1—C2—O9	108.0 (2)	C16—C15—H151	120.1
C3—C2—O9	110.8 (2)	C15—C16—C17	120.0 (3)
C1—C2—H21	108.4	C15—C16—H161	120.8
C3—C2—H21	108.5	C17—C16—H161	119.3
O9—C2—H21	110.1	C16—C17—C18	119.9 (3)
C2—C3—C4	111.1 (2)	C16—C17—H171	119.7
C2—C3—O8	109.9 (2)	C18—C17—H171	120.4
C4—C3—O8	112.7 (2)	C13—C18—C17	120.8 (3)
C2—C3—H31	106.8	C13—C18—H181	118.9
C4—C3—H31	107.7	C17—C18—H181	120.3
O8—C3—H31	108.4	N11—C19—C20	112.7 (2)
C3—C4—C5	110.3 (2)	N11—C19—H191	110.7

C3—C4—O7	112.5 (2)	C20—C19—H191	110.3
C5—C4—O7	108.7 (2)	N11—C19—H192	106.8
C3—C4—H41	106.9	C20—C19—H192	107.6
C5—C4—H41	108.2	H191—C19—H192	108.7
O7—C4—H41	110.1	C19—C20—C21	121.1 (2)
C4—C5—O6	112.1 (2)	C19—C20—C25	120.4 (2)
C4—C5—H51	108.4	C21—C20—C25	118.5 (2)
O6—C5—H51	109.0	C20—C21—C22	120.7 (2)
C4—C5—H52	107.9	C20—C21—H211	119.8
O6—C5—H52	108.1	C22—C21—H211	119.5
H51—C5—H52	111.3	C21—C22—C23	119.9 (3)
C5—O6—C1	112.6 (2)	C21—C22—H221	119.7
C4—O7—H4	108.4	C23—C22—H221	120.4
C3—O8—H12	105.2	C22—C23—C24	119.8 (3)
C2—O9—H253	104.2	C22—C23—H231	119.8
C1—C10—N11	110.0 (2)	C24—C23—H231	120.4
C1—C10—H101	107.0	C23—C24—C25	120.4 (3)
N11—C10—H101	108.6	C23—C24—H241	119.6
C1—C10—H102	110.3	C25—C24—H241	120.0
N11—C10—H102	111.5	C20—C25—C24	120.7 (3)
H101—C10—H102	109.4	C20—C25—H251	118.70
C10—N11—C12	110.8 (2)	C24—C25—H251	120.60
C10—N11—C19	111.2 (2)	C1—O26—H252	103.7
C12—N11—C19	110.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O27—H1···O8^{i}	0.84	1.89	2.700 (3)	161
O7—H4···O9^{ii}	0.78	2.00	2.740 (2)	157
O8—H12···O7^{iii}	0.82	1.95	2.756 (2)	167
O9—H253···O27	0.96	1.77	2.692 (2)	159

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