Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

N-(2-Acetamido-2-deoxy-β-D-glucopyranosyl)-*N*-(3-azidopropyl)-*O*-methylhydroxylamine

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Received 19 November 2015
Accepted 3 February 2016

Edited by A. J. Lough, University of Toronto, Canada

Keywords: crystal structure; oxyamine glycoside; carbohydrate.

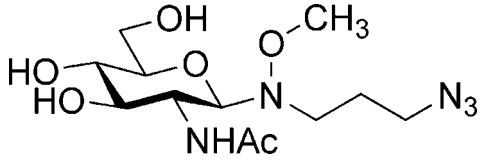
CCDC reference: 1451795

Supporting information: this article has supporting information at journals.iucr.org/e

The structure of the title compound, $C_{12}H_{23}N_5O_6$, solved using adequate data from a thin crystal plate, confirmed that this useful glycoconjugate was obtained in the ring-closed β-pyranose configuration with $^4C_1$ conformation. The molecules are bound by O—H···O(OH) hydrogen bonds, notably in a zigzag $C(2)$ chain along the short b (screw) axis, supplemented with an $R_2^2(12)$ O—H···O(carbonyl) link along the a axis and other $C(2)$ links. The absolute configuration was not unambiguously determined but was known from the synthetic chemistry, which used natural 2-acetamido-2-deoxy-D-glucose as the starting material.

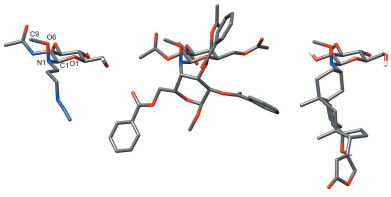
1. Chemical context

Oxyamine glycosides, such as the title compound, can be utilised for the synthesis of a wide variety of complex glycoconjugates (Kwase *et al.*,2014; Munneke *et al.*, 2015; Wang *et al.*, 2013). In particular, the use of an oxyamine bifunctional linker allows for the conjugation of carbohydrates to a substrate of choice, such as proteins, fluorophores and biotin. The crystal structure analysis confirmed that the glycoconjugate was obtained in the ring-closed β-pyranose configuration.



2. Structural commentary

The title compound crystallizes with one independent molecule in the asymmetric unit (Fig. 1) in the C1(R), C2(R), C3(R), C4(S), C5(R) configuration. The absolute configuration was not ambiguously determined but was known from the synthetic chemistry.



3. Supramolecular features

The molecules are bound together with a comprehensive net of O—H···O(alcohol) hydrogen bonds, as well as one N—H···O(carbonyl) and one O—H···O(carbonyl) hydrogen bond (Table 1). The basic interactions are chain $C(2)$ and $C(8)$ types which combine to form a larger chain and rings *e.g.* $R_2^2(12)$, as shown on the right of Fig. 2.

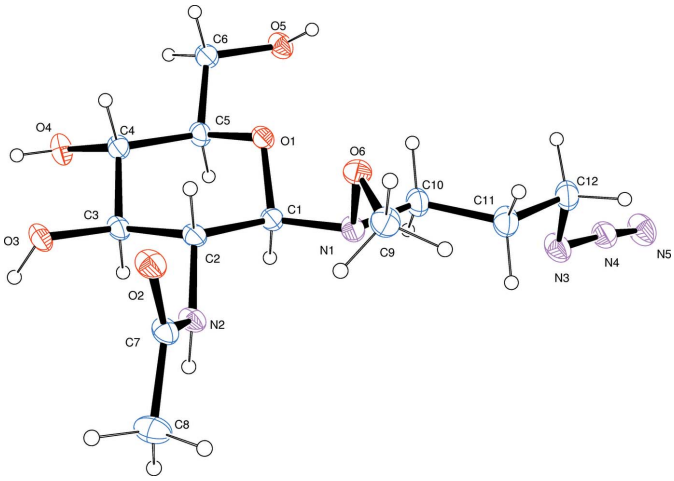


Figure 1
View of the title molecule, drawn with 25% probability displacement ellipsoids.

4. Database survey

The Cambridge Structural Database (CSD, Version 5.36, update 3; Groom & Allen, 2014) was searched for *N*-alkyl-*N*-(tetrahydro-2*H*-pyran-2-yl)oxyamines, and two structures were found, both of which are *N*-β-glycosyloxyamines, *viz*. an *N*-β-glucopyranosyloxyamine (Langenhan *et al.*, 2005) and an *N*-β-galactopyranosyloxyamine (Renaudet & Dumy, 2002). Interestingly, all three structures have a similar conformation around the anomeric linkage, with O6—N1—C1—O1 and C9—O6—N1—C1 torsion angles of 62.9 (8) and 115.6 (2) for the glucosyloxyamine derivative, 50.8 (1) and 126.3 (8) for the galactosyloxyamine and 64.2 (4) and 127.1 (3) for the title compound (Fig. 3). A configuration that allows both the methoxy group to adopt a pseudoaxial orientation, and positions the nitrogen for optimal overlap between the nitrogen lone pair and the C1—O1 σ* (n → σ* interaction).

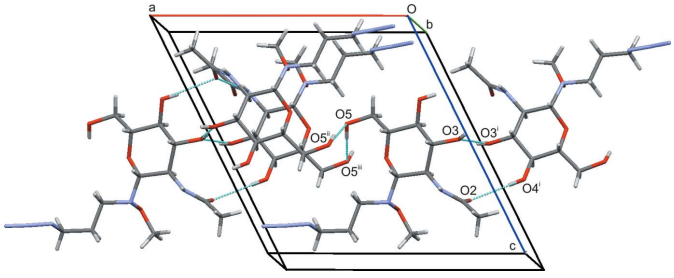


Figure 2
The unit-cell contents viewed along approximately the *b* axis. Some intermolecular binding contacts are shown as blue dotted lines. [Symmetry codes: (i) $-x, y+\frac{1}{2}, 1-z$; (ii) $1-x, y-\frac{1}{2}, 1-z$; (iii) $1-x, y+\frac{1}{2}, 1-z$.]

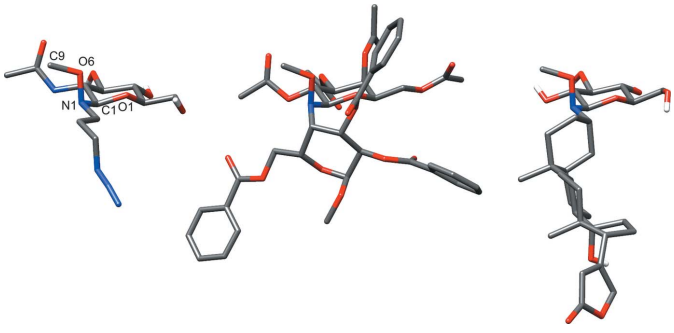


Figure 3
The O6—N1—C1—O1 and C9—O6—N1—C1 torsion angles of *N*-glycosyloxyamines: left – title compound; middle – *N*-β-glucopyranosyloxyamine (Langenhan *et al.*, 2005); right – *N*-β-galactopyranosyloxyamine (Renaudet & Dumy, 2002).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*O*···O3^{i}	0.84	1.79	2.616 (5)	167
O4—H4*O*···O2^{i}	0.80 (7)	2.23 (7)	3.027 (4)	170 (8)
O5—H5*O*···O5^{ii}	0.90 (8)	1.98 (8)	2.855 (4)	167 (7)
N2—H2*N*···O2^{iii}	0.93 (7)	2.08 (6)	2.961 (5)	158 (5)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{23}N_5O_6$
M_r	333.35
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	120
a, *b*, *c* (Å)	13.5605 (18), 4.7386 (3), 14.140 (2)
β (°)	118.181 (19)
V (Å^3)	800.9 (2)
Z	2
Radiation type	Cu *Kα*
μ (mm^{-1})	0.95
Crystal size (mm)	0.57 × 0.14 × 0.02
Data collection	
Diffractometer	Agilent SuperNova Dual Source diffractometer with an Atlas detector
Absorption correction	Gaussian (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.792, 0.985
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6061, 2355, 2073
R_{int}	0.053
(sin θ/λ)$_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.059, 0.165, 1.03
No. of reflections	2355
No. of parameters	221
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.32
Absolute structure	Flack *x* determined using 619 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons & Flack, 2004)
Absolute structure parameter	0.2 (4)

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2012* and *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

5. Synthesis and crystallization

N-(2-Acetamido-2-deoxy-β-D-glucopyranosyl)-*N*-(3-azidopropyl)-*O*-methylhydroxylamine was prepared as described in Munneke *et al.* (2015) from 3-azido-1-methoxyaminopropane and commercially available *N*-acetylglucosamine. The title compound was recrystallized from freshly distilled MeOH–Et_2O (1:8 *v*/*v*).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All methyl H atoms were constrained to an ideal geometry (C—H = 0.98 Å) with U_{iso}(H) = 1.5U_{eq}(C), but were allowed to rotate freely about the adjacent C—C bond. All other O,C-bound H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.99 (methylene) and 1.0 (tertiary) Å, O—H = 0.84 Å and with U_{iso}(H) = 1.2U_{eq}(C,O). The nitrogen H atom was located in a difference Fourier map and refined with U_{iso}(H) = 1.2U_{eq}(N).

Acknowledgements

We thank Dr M. Polson of the University of Canterbury, New Zealand, for the data collection.

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supporting information

Acta Cryst. (2016). E**72**, 340-342 [doi:10.1107/S2056989016002164]

N-(2-Acetamido-2-deoxy-*β*-D-glucopyranosyl)-*N*-(3-azidopropyl)-*O*-methylhydroxylamine

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2012* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

N-(2-Acetamido-2-deoxy-*β*-*D*-glucopyranosyl)-*N*-(3-azidopropyl)-*O*-methylhydroxylamine

Crystal data

$C_{12}H_{23}N_5O_6$
$M_r = 333.35$
Monoclinic, $P2_1$
$a = 13.5605\ (18)$ Å
$b = 4.7386\ (3)$ Å
$c = 14.140\ (2)$ Å
$\beta = 118.181\ (19)°$
$V = 800.9\ (2)$ Å^3
$Z = 2$
$F(000) = 356$
$D_x = 1.382$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2327 reflections
$\theta = 3.7–75.3°$
$\mu = 0.95$ mm^{-1}
$T = 120$ K
Needle, colourless
0.57 × 0.14 × 0.02 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: sealed X-ray tube, SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.6501 pixels mm^{-1}
ω scans
Absorption correction: gaussian (*CrysAlis PRO*; Agilent, 2014)
$T_{min} = 0.792$, $T_{max} = 0.985$
6061 measured reflections
2355 independent reflections
2073 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 66.6°$, $\theta_{min} = 3.6°$
$h = -16\rightarrow16$
$k = -5\rightarrow5$
$l = -17\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.165$
$S = 1.03$
2355 reflections
221 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1194P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Absolute structure: Flack *x* determined using 619 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons & Flack, 2004)
Absolute structure parameter: 0.2 (4)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.3682 (2)	0.2828 (6)	0.5792 (2)	0.0314 (7)
O2	0.1361 (3)	0.5357 (7)	0.7397 (3)	0.0378 (8)
O3	0.0442 (2)	0.1637 (7)	0.5080 (3)	0.0368 (8)
H3O	0.007 (4)	0.017 (14)	0.498 (6)	0.055*
O4	0.1155 (3)	0.0380 (8)	0.3491 (3)	0.0426 (8)
H4O	0.050 (6)	0.058 (17)	0.328 (5)	0.064*
O5	0.4546 (3)	0.2456 (8)	0.4382 (3)	0.0401 (8)
H5O	0.486 (6)	0.385 (16)	0.486 (6)	0.060*
O6	0.4312 (3)	0.5384 (7)	0.7784 (3)	0.0369 (7)
N1	0.4434 (3)	0.2390 (8)	0.7677 (3)	0.0329 (8)
N2	0.2088 (3)	0.1158 (8)	0.7250 (3)	0.0326 (8)
H2N	0.205 (4)	−0.077 (14)	0.732 (4)	0.039*
N3	0.7789 (3)	−0.1042 (10)	0.8833 (4)	0.0480 (11)
N4	0.8722 (3)	−0.1684 (10)	0.8948 (4)	0.0451 (10)
N5	0.9545 (4)	−0.2571 (12)	0.9039 (4)	0.0566 (12)
C1	0.3557 (3)	0.1498 (10)	0.6645 (4)	0.0308 (9)
H1	0.3616	−0.0591	0.6585	0.037*
C2	0.2369 (3)	0.2191 (9)	0.6435 (3)	0.0304 (9)
H2	0.2276	0.4289	0.6387	0.036*
C3	0.1552 (3)	0.0914 (9)	0.5340 (4)	0.0318 (9)
H3	0.1626	−0.1187	0.5392	0.038*
C4	0.1797 (3)	0.1921 (9)	0.4452 (4)	0.0320 (9)
H4	0.1613	0.3974	0.4317	0.038*
C5	0.3030 (3)	0.1481 (10)	0.4789 (4)	0.0338 (10)
H5	0.3197	−0.0587	0.4869	0.041*
C6	0.3382 (4)	0.2715 (11)	0.4006 (4)	0.0349 (9)
H6A	0.2977	0.1734	0.3308	0.042*
H6B	0.3172	0.4735	0.3890	0.042*
C7	0.1536 (3)	0.2815 (10)	0.7623 (4)	0.0324 (9)
C8	0.1154 (4)	0.1435 (11)	0.8351 (4)	0.0436 (11)
H8A	0.1627	0.2070	0.9090	0.065*
H8B	0.1212	−0.0619	0.8313	0.065*
H8C	0.0375	0.1955	0.8123	0.065*
C9	0.4282 (4)	0.5914 (10)	0.8765 (4)	0.0395 (11)
H9A	0.4977	0.5240	0.9370	0.059*

H9B	0.3644	0.4919	0.8757	0.059*
H9C	0.4203	0.7945	0.8842	0.059*
C10	0.5538 (3)	0.1952 (11)	0.7742 (4)	0.0389 (11)
H10A	0.5617	0.3227	0.7227	0.047*
H10B	0.5589	−0.0014	0.7532	0.047*
C11	0.6489 (4)	0.2502 (12)	0.8862 (4)	0.0443 (11)
H11A	0.6441	0.4474	0.9068	0.053*
H11B	0.6405	0.1240	0.9378	0.053*
C12	0.7623 (4)	0.2026 (12)	0.8934 (4)	0.0451 (12)
H12A	0.7675	0.3074	0.8353	0.054*
H12B	0.8216	0.2735	0.9630	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0257 (13)	0.0269 (16)	0.0409 (16)	−0.0022 (12)	0.0150 (12)	0.0014 (13)
O2	0.0370 (16)	0.0236 (16)	0.056 (2)	0.0021 (13)	0.0245 (15)	0.0010 (15)
O3	0.0235 (13)	0.0265 (16)	0.060 (2)	−0.0025 (12)	0.0190 (14)	−0.0003 (15)
O4	0.0270 (15)	0.047 (2)	0.0476 (19)	−0.0046 (16)	0.0129 (14)	−0.0117 (17)
O5	0.0322 (15)	0.0397 (19)	0.0533 (19)	−0.0004 (14)	0.0243 (14)	−0.0017 (17)
O6	0.0412 (17)	0.0222 (15)	0.0421 (17)	−0.0018 (14)	0.0152 (14)	0.0019 (14)
N1	0.0277 (17)	0.0250 (19)	0.042 (2)	0.0011 (14)	0.0130 (15)	0.0004 (15)
N2	0.0313 (17)	0.0212 (18)	0.049 (2)	0.0013 (14)	0.0223 (16)	0.0030 (15)
N3	0.033 (2)	0.042 (2)	0.066 (3)	−0.0007 (19)	0.021 (2)	0.001 (2)
N4	0.038 (2)	0.042 (2)	0.051 (2)	−0.0025 (18)	0.0174 (19)	0.0016 (19)
N5	0.036 (2)	0.055 (3)	0.079 (3)	0.003 (2)	0.027 (2)	−0.002 (3)
C1	0.0266 (19)	0.027 (2)	0.037 (2)	0.0008 (17)	0.0136 (17)	0.0035 (17)
C2	0.0266 (19)	0.022 (2)	0.045 (2)	0.0031 (16)	0.0187 (18)	0.0052 (18)
C3	0.0256 (19)	0.021 (2)	0.047 (2)	0.0000 (16)	0.0160 (18)	0.0006 (18)
C4	0.027 (2)	0.026 (2)	0.041 (2)	0.0014 (17)	0.0143 (18)	0.0008 (19)
C5	0.0249 (19)	0.033 (2)	0.042 (2)	0.0018 (18)	0.0146 (17)	0.0022 (19)
C6	0.033 (2)	0.034 (2)	0.039 (2)	−0.002 (2)	0.0172 (18)	0.000 (2)
C7	0.0297 (19)	0.022 (2)	0.045 (2)	−0.0016 (17)	0.0173 (18)	−0.0012 (18)
C8	0.056 (3)	0.028 (2)	0.061 (3)	0.000 (2)	0.039 (2)	0.003 (2)
C9	0.042 (2)	0.030 (2)	0.041 (2)	−0.0021 (19)	0.016 (2)	−0.004 (2)
C10	0.027 (2)	0.040 (3)	0.044 (3)	0.0000 (19)	0.0112 (19)	0.001 (2)
C11	0.034 (2)	0.044 (3)	0.046 (3)	0.001 (2)	0.012 (2)	−0.001 (2)
C12	0.033 (2)	0.040 (3)	0.048 (3)	−0.002 (2)	0.007 (2)	0.000 (2)

Geometric parameters (Å, º)

O1—C5	1.420 (6)	C3—C4	1.520 (6)
O1—C1	1.441 (5)	C3—H3	1.0000
O2—C7	1.240 (6)	C4—C5	1.521 (5)
O3—C3	1.413 (5)	C4—H4	1.0000
O3—H3O	0.84 (8)	C5—C6	1.515 (6)
O4—C4	1.421 (6)	C5—H5	1.0000
O4—H4O	0.80 (7)	C6—H6A	0.9900

O5—C6	1.413 (5)	C6—H6B	0.9900
O5—H5O	0.90 (8)	C7—C8	1.502 (6)
O6—C9	1.430 (6)	C8—H8A	0.9800
O6—N1	1.445 (5)	C8—H8B	0.9800
N1—C1	1.443 (6)	C8—H8C	0.9800
N1—C10	1.470 (5)	C9—H9A	0.9800
N2—C7	1.352 (6)	C9—H9B	0.9800
N2—C2	1.459 (5)	C9—H9C	0.9800
N2—H2N	0.93 (7)	C10—C11	1.520 (6)
N3—N4	1.235 (6)	C10—H10A	0.9900
N3—C12	1.488 (7)	C10—H10B	0.9900
N4—N5	1.141 (6)	C11—C12	1.510 (7)
C1—C2	1.529 (5)	C11—H11A	0.9900
C1—H1	1.0000	C11—H11B	0.9900
C2—C3	1.539 (6)	C12—H12A	0.9900
C2—H2	1.0000	C12—H12B	0.9900

C5—O1—C1	112.0 (3)	C6—C5—H5	109.1
C3—O3—H3O	109.5	C4—C5—H5	109.1
C4—O4—H4O	112 (5)	O5—C6—C5	111.9 (3)
C6—O5—H5O	106 (5)	O5—C6—H6A	109.2
C9—O6—N1	109.4 (3)	C5—C6—H6A	109.2
C1—N1—O6	108.2 (3)	O5—C6—H6B	109.2
C1—N1—C10	110.6 (3)	C5—C6—H6B	109.2
O6—N1—C10	107.2 (3)	H6A—C6—H6B	107.9
C7—N2—C2	120.9 (4)	O2—C7—N2	122.5 (4)
C7—N2—H2N	118 (3)	O2—C7—C8	120.9 (4)
C2—N2—H2N	118 (3)	N2—C7—C8	116.6 (4)
N4—N3—C12	114.8 (4)	C7—C8—H8A	109.5
N5—N4—N3	172.6 (6)	C7—C8—H8B	109.5
O1—C1—N1	110.6 (3)	H8A—C8—H8B	109.5
O1—C1—C2	105.9 (3)	C7—C8—H8C	109.5
N1—C1—C2	115.1 (4)	H8A—C8—H8C	109.5
O1—C1—H1	108.4	H8B—C8—H8C	109.5
N1—C1—H1	108.4	O6—C9—H9A	109.5
C2—C1—H1	108.4	O6—C9—H9B	109.5
N2—C2—C1	114.7 (3)	H9A—C9—H9B	109.5
N2—C2—C3	109.3 (3)	O6—C9—H9C	109.5
C1—C2—C3	107.6 (3)	H9A—C9—H9C	109.5
N2—C2—H2	108.4	H9B—C9—H9C	109.5
C1—C2—H2	108.4	N1—C10—C11	112.2 (4)
C3—C2—H2	108.4	N1—C10—H10A	109.2
O3—C3—C4	109.3 (4)	C11—C10—H10A	109.2
O3—C3—C2	109.8 (3)	N1—C10—H10B	109.2
C4—C3—C2	111.9 (3)	C11—C10—H10B	109.2
O3—C3—H3	108.6	H10A—C10—H10B	107.9
C4—C3—H3	108.6	C12—C11—C10	112.3 (4)
C2—C3—H3	108.6	C12—C11—H11A	109.1

O4—C4—C3	110.8 (4)	C10—C11—H11A	109.1
O4—C4—C5	108.4 (3)	C12—C11—H11B	109.1
C3—C4—C5	109.5 (3)	C10—C11—H11B	109.1
O4—C4—H4	109.4	H11A—C11—H11B	107.9
C3—C4—H4	109.4	N3—C12—C11	109.5 (4)
C5—C4—H4	109.4	N3—C12—H12A	109.8
O1—C5—C6	107.1 (3)	C11—C12—H12A	109.8
O1—C5—C4	109.0 (3)	N3—C12—H12B	109.8
C6—C5—C4	113.4 (4)	C11—C12—H12B	109.8
O1—C5—H5	109.1	H12A—C12—H12B	108.2

C9—O6—N1—C1	127.1 (3)	C2—C3—C4—O4	170.7 (3)
C9—O6—N1—C10	−113.6 (4)	O3—C3—C4—C5	173.0 (4)
C5—O1—C1—N1	164.6 (3)	C2—C3—C4—C5	51.1 (5)
C5—O1—C1—C2	−70.2 (4)	C1—O1—C5—C6	−170.3 (3)
O6—N1—C1—O1	64.2 (4)	C1—O1—C5—C4	66.7 (4)
C10—N1—C1—O1	−52.9 (5)	O4—C4—C5—O1	−175.5 (3)
O6—N1—C1—C2	−55.6 (4)	C3—C4—C5—O1	−54.5 (5)
C10—N1—C1—C2	−172.8 (4)	O4—C4—C5—C6	65.3 (5)
C7—N2—C2—C1	136.0 (4)	C3—C4—C5—C6	−173.7 (4)
C7—N2—C2—C3	−103.1 (4)	O1—C5—C6—O5	55.3 (5)
O1—C1—C2—N2	−176.8 (3)	C4—C5—C6—O5	175.6 (4)
N1—C1—C2—N2	−54.4 (5)	C2—N2—C7—O2	−8.8 (7)
O1—C1—C2—C3	61.4 (4)	C2—N2—C7—C8	172.2 (4)
N1—C1—C2—C3	−176.2 (3)	C1—N1—C10—C11	−172.5 (4)
N2—C2—C3—O3	58.2 (4)	O6—N1—C10—C11	69.7 (5)
C1—C2—C3—O3	−176.7 (3)	N1—C10—C11—C12	179.5 (4)
N2—C2—C3—C4	179.7 (3)	N4—N3—C12—C11	−175.7 (4)
C1—C2—C3—C4	−55.1 (4)	C10—C11—C12—N3	−69.7 (6)
O3—C3—C4—O4	−67.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*O*···O3^{i}	0.84	1.79	2.616 (5)	167
O4—H4*O*···O2^{i}	0.80 (7)	2.23 (7)	3.027 (4)	170 (8)
O5—H5*O*···O5^{ii}	0.90 (8)	1.98 (8)	2.855 (4)	167 (7)
N2—H2*N*···O2^{iii}	0.93 (7)	2.08 (6)	2.961 (5)	158 (5)

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