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# 5-Azido-4-benzyloxy-2-methoxy-6-methylperhydropyran-3-ol

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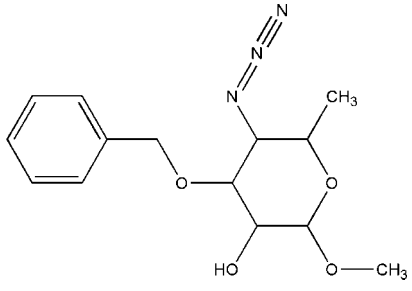
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.049; $wR$ factor = 0.103; data-to-parameter ratio = 8.9.

In the title compound, $C_{14}H_{19}N_3O_4$, the perhydropyran ring adopts a chair conformation. An intramolecular C—H···O hydrogen bond generates an $S$(6) ring motif. In the crystal packing, molecules are linked by O—H···O hydrogen bonds, forming infinite chains along [100].

## Related literature

For background to D-perosamine, see: Jacquinet (2006). For the synthesis of D-perosamine, see: Krishna & Agrawal (2000). For metabolites, see: Grond *et al.* (2000). For ring conformations, see: Cremer & Pople (1975). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).




## Experimental

### Crystal data

$C_{14}H_{19}N_3O_4$ $M_r$ = 293.32
Orthorhombic, $P2_12_12_1$
$a$ = 4.6662 (2) Å
$b$ = 15.3356 (8) Å
$c$ = 20.9273 (12) Å
$V$ = 1497.54 (13) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 100 K
0.27 × 0.11 × 0.08 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.773, $T_{max}$ = 0.980
13029 measured reflections
1742 independent reflections
1334 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.096

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.103
$S$ = 1.09
1742 reflections
196 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H1*O2*···O2$^{i}$ | 0.88 (4) | 1.91 (3) | 2.757 (2) | 161 (3) |
| O2—H1*O2*···O3$^{i}$ | 0.88 (3) | 2.49 (3) | 3.063 (3) | 124 (3) |
| C7—H7*B*···O2 | 0.97 | 2.58 | 3.180 (4) | 120 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2616).

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# supporting information

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## 5-Azido-4-benzyloxy-2-methoxy-6-methylperhydropyran-3-ol

**Hoong-Kun Fun, Wan-Sin Loh, Sankappa Rai, Prakash Shetty and Arun M. Isloor**

### S1. Comment

4-Amino-4,6-dideoxy-D-mannose (*D*-perosamine) was first discovered in the polyene macrolide antibiotic perimycin and was later recognized to be present in the lipopolysaccharide (LPS) of Vivrio cholera (Jacquinet, 2006). Methyl 3-benzyloxy-4-azido-*α*-*D*-rhamnopyranoside is an important intermediate in the synthesis of *D*-perosamine (Krishna & Agrawal, 2000). Rhamnopyranosides were detected as metabolites from five different strains of Streptomycetes (Grond *et al.*, 2000).

The bond lengths (Allen *et al.*, 1987) and angles in the molecule (Fig. 1) are within normal ranges. The perhydropyran ring adopts a chair conformation. The puckering parameters (Cremer & Pople, 1975) are Q = 0.540 (3) Å; Θ = 8.0 (3)° and *φ* = 8.0 (2)°. Intramolecular C7—H7B···O2 hydrogen bonds formed a six-membered ring, producing an *S*(6) ring motif (Bernstein *et al.*, 1995). The dihedral angle formed between the benzene (C1—C6) and perhydropyran (C8—C10/O4/C11/C12) rings is 57.32 (16)°.

In the crystal packing (Fig. 2), the molecules are linked by intermolecular O2—H1O2···O2 and O2—H1O2···O3 hydrogen bonds (Table 1) into an infinite one-dimensional chains along the [100] direction.

### S2. Experimental

To a stirred mixture of methyl 3-benzyloxy-4-methoxysulfonyl-*α*-*D*-rhamnopyranoside (0.50 g, 1.4 mmol) in DMF (5.0 ml) was added sodium azide (0.18 g, 2.8 mmol). The reaction mixture was stirred further at room temperature for 12 h. TLC (30% EtOAc/hexane, Rf-0.5) analysis showed complete conversion. The reaction mixture was concentrated under vacuum and the residue was purified by column chromatography using 25% ethylacetate in petroleum ether to get pure product as colourless crystals (yield: 300.0 mg, 71%, *M.p.* 376–378 K).

### S3. Refinement

Atom H1O2 was located in a difference map and was refined freely. Other H atoms were positioned geometrically [C—H = 0.93 to 0.98 Å] and was refined using a riding model, with $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C). A rotating-group model was applied for the methyl groups. In the absence of significant anomalous dispersion, 1187 Friedel pairs were merged for the final refinement.

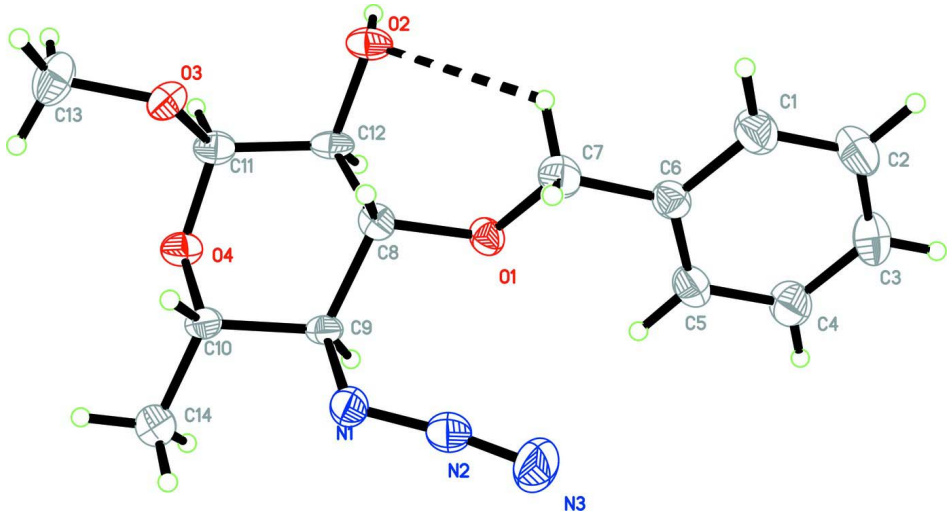


**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom numbering scheme. Intramolecular interaction is shown by dashed line.

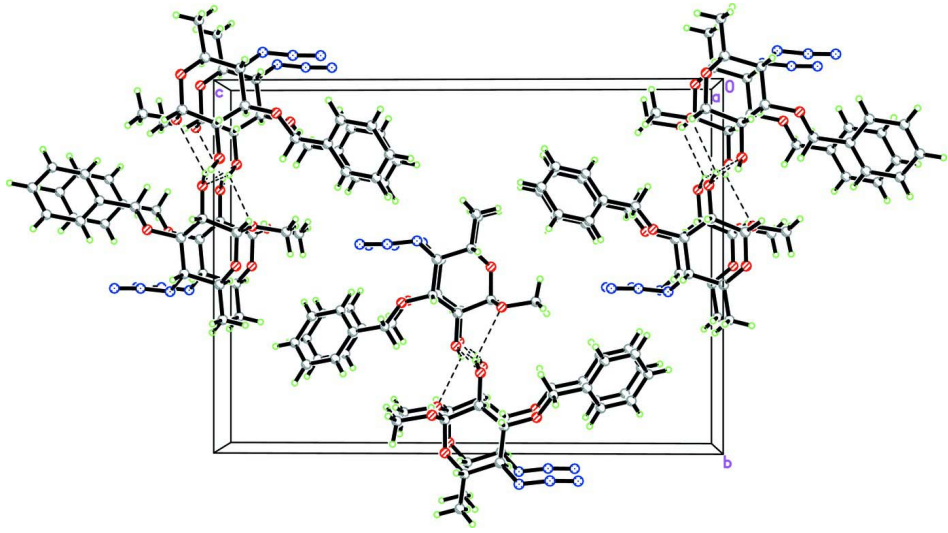


**Figure 2**

The crystal packing of the title compound, viewed along *a* axis. Intermolecular hydrogen bonds are shown by dashed lines.

### 5-Azido-4-benzyloxy-2-methoxy-6-methylperhydropyran-3-ol

*Crystal data*

$C_{14}H_{19}N_3O_4$
$M_r = 293.32$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 4.6662\ (2)$ Å
$b = 15.3356\ (8)$ Å
$c = 20.9273\ (12)$ Å
$V = 1497.54\ (13)$ Å$^3$
$Z = 4$
$F(000) = 624$
$D_x = 1.301$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1880 reflections
$\theta = 2.4$–$29.9°$

$\mu$ = 0.10 mm$^{-1}$
$T$ = 100 K

Block, colourless
0.27 × 0.11 × 0.08 mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.773, $T_{max}$ = 0.980

13029 measured reflections
1742 independent reflections
1334 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.096
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 2.0°
$h$ = −5→5
$k$ = −18→17
$l$ = −25→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.103
$S$ = 1.09
1742 reflections
196 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
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.0881 (4) | 0.40074 (13) | 0.13521 (10) | 0.0229 (5) |
| O2 | 0.0911 (5) | 0.28256 (14) | 0.02574 (11) | 0.0251 (5) |
| O3 | 0.3176 (5) | 0.39026 (14) | −0.06657 (9) | 0.0236 (5) |
| O4 | −0.0200 (5) | 0.49881 (14) | −0.04434 (10) | 0.0250 (5) |
| N1 | 0.3572 (6) | 0.56890 (17) | 0.10102 (12) | 0.0260 (7) |
| N2 | 0.3482 (6) | 0.56020 (18) | 0.16023 (14) | 0.0306 (7) |
| N3 | 0.3680 (9) | 0.5600 (2) | 0.21422 (15) | 0.0537 (11) |
| C1 | 0.2228 (8) | 0.2487 (2) | 0.26646 (17) | 0.0341 (9) |
| H1A | 0.3517 | 0.2100 | 0.2479 | 0.041* |
| C2 | 0.1203 (8) | 0.2318 (2) | 0.32682 (17) | 0.0389 (9) |
| H2A | 0.1795 | 0.1820 | 0.3485 | 0.047* |

| | | | | |
|---|---|---|---|---|
| C3 | −0.0706 (8) | 0.2888 (3) | 0.35523 (17) | 0.0379 (9) |
| H3A | −0.1405 | 0.2776 | 0.3960 | 0.045* |
| C4 | −0.1561 (9) | 0.3619 (2) | 0.32269 (16) | 0.0362 (9) |
| H4A | −0.2856 | 0.4003 | 0.3413 | 0.043* |
| C5 | −0.0489 (8) | 0.3786 (2) | 0.26165 (16) | 0.0314 (9) |
| H5A | −0.1051 | 0.4289 | 0.2402 | 0.038* |
| C6 | 0.1390 (7) | 0.3216 (2) | 0.23289 (15) | 0.0245 (7) |
| C7 | 0.2586 (8) | 0.3380 (2) | 0.16733 (16) | 0.0309 (9) |
| H7A | 0.4541 | 0.3590 | 0.1708 | 0.037* |
| H7B | 0.2607 | 0.2840 | 0.1431 | 0.037* |
| C8 | 0.1803 (7) | 0.4219 (2) | 0.07207 (14) | 0.0209 (7) |
| H8A | 0.3837 | 0.4073 | 0.0675 | 0.025* |
| C9 | 0.1415 (7) | 0.51995 (19) | 0.06387 (14) | 0.0193 (7) |
| H9A | −0.0498 | 0.5361 | 0.0791 | 0.023* |
| C10 | 0.1727 (7) | 0.5493 (2) | −0.00515 (14) | 0.0215 (7) |
| H10A | 0.3703 | 0.5397 | −0.0193 | 0.026* |
| C11 | 0.0416 (7) | 0.4086 (2) | −0.04432 (15) | 0.0241 (8) |
| H11A | −0.0965 | 0.3794 | −0.0723 | 0.029* |
| C12 | 0.0088 (7) | 0.37161 (19) | 0.02287 (15) | 0.0214 (7) |
| H12A | −0.1941 | 0.3754 | 0.0347 | 0.026* |
| C13 | 0.3436 (8) | 0.4054 (3) | −0.13393 (15) | 0.0361 (9) |
| H13A | 0.5309 | 0.3880 | −0.1480 | 0.054* |
| H13B | 0.3159 | 0.4662 | −0.1427 | 0.054* |
| H13C | 0.2012 | 0.3720 | −0.1562 | 0.054* |
| C14 | 0.0949 (9) | 0.6437 (2) | −0.01442 (16) | 0.0364 (9) |
| H14A | 0.1146 | 0.6588 | −0.0587 | 0.055* |
| H14B | 0.2203 | 0.6795 | 0.0107 | 0.055* |
| H14C | −0.0997 | 0.6530 | −0.0012 | 0.055* |
| H1O2 | −0.060 (8) | 0.251 (2) | 0.0151 (15) | 0.028 (10)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0225 (12) | 0.0219 (12) | 0.0243 (11) | 0.0014 (10) | 0.0055 (10) | 0.0037 (10) |
| O2 | 0.0200 (12) | 0.0185 (12) | 0.0368 (13) | −0.0030 (11) | 0.0015 (11) | −0.0055 (10) |
| O3 | 0.0222 (11) | 0.0283 (13) | 0.0205 (11) | 0.0038 (11) | −0.0013 (10) | −0.0046 (10) |
| O4 | 0.0249 (12) | 0.0218 (12) | 0.0282 (12) | 0.0030 (11) | −0.0041 (10) | −0.0033 (10) |
| N1 | 0.0301 (16) | 0.0255 (17) | 0.0224 (16) | −0.0079 (14) | 0.0009 (14) | −0.0004 (12) |
| N2 | 0.0360 (17) | 0.0250 (17) | 0.0307 (19) | −0.0096 (14) | −0.0032 (15) | −0.0024 (13) |
| N3 | 0.084 (3) | 0.049 (2) | 0.0274 (18) | −0.028 (2) | −0.0075 (19) | −0.0015 (15) |
| C1 | 0.036 (2) | 0.032 (2) | 0.035 (2) | 0.0072 (17) | 0.0014 (17) | 0.0053 (17) |
| C2 | 0.044 (2) | 0.032 (2) | 0.040 (2) | 0.003 (2) | 0.000 (2) | 0.0127 (18) |
| C3 | 0.040 (2) | 0.045 (2) | 0.0295 (19) | −0.002 (2) | 0.0026 (18) | 0.0106 (18) |
| C4 | 0.040 (2) | 0.036 (2) | 0.0329 (19) | 0.0034 (19) | 0.0131 (19) | 0.0041 (17) |
| C5 | 0.038 (2) | 0.0257 (19) | 0.0300 (19) | 0.0002 (18) | 0.0039 (18) | 0.0061 (16) |
| C6 | 0.0246 (18) | 0.0220 (18) | 0.0267 (17) | −0.0019 (16) | −0.0029 (16) | 0.0018 (15) |
| C7 | 0.0305 (19) | 0.031 (2) | 0.0315 (19) | 0.0135 (17) | 0.0029 (16) | 0.0033 (16) |
| C8 | 0.0170 (16) | 0.0213 (18) | 0.0244 (17) | −0.0001 (15) | 0.0013 (15) | 0.0015 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0197 (16) | 0.0150 (16) | 0.0233 (16) | 0.0001 (14) | 0.0031 (15) | −0.0037 (13) |
| C10 | 0.0238 (17) | 0.0185 (17) | 0.0224 (16) | −0.0001 (15) | 0.0005 (15) | −0.0037 (14) |
| C11 | 0.0224 (16) | 0.0213 (18) | 0.0286 (18) | −0.0019 (15) | −0.0045 (15) | −0.0047 (15) |
| C12 | 0.0153 (15) | 0.0157 (16) | 0.0333 (18) | 0.0017 (14) | 0.0013 (15) | −0.0062 (14) |
| C13 | 0.035 (2) | 0.052 (2) | 0.0214 (17) | 0.004 (2) | −0.0043 (18) | −0.0014 (17) |
| C14 | 0.052 (2) | 0.028 (2) | 0.0291 (19) | 0.0020 (19) | 0.0024 (19) | 0.0017 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C7 | 1.418 (4) | C5—H5A | 0.9300 |
| O1—C8 | 1.427 (4) | C6—C7 | 1.502 (4) |
| O2—C12 | 1.420 (3) | C7—H7A | 0.9700 |
| O2—H1O2 | 0.88 (4) | C7—H7B | 0.9700 |
| O3—C11 | 1.398 (4) | C8—C12 | 1.515 (4) |
| O3—C13 | 1.434 (4) | C8—C9 | 1.524 (4) |
| O4—C11 | 1.412 (4) | C8—H8A | 0.9800 |
| O4—C10 | 1.443 (4) | C9—C10 | 1.520 (4) |
| N1—N2 | 1.247 (4) | C9—H9A | 0.9800 |
| N1—C9 | 1.477 (4) | C10—C14 | 1.505 (4) |
| N2—N3 | 1.134 (4) | C10—H10A | 0.9800 |
| C1—C2 | 1.375 (5) | C11—C12 | 1.524 (4) |
| C1—C6 | 1.376 (5) | C11—H11A | 0.9800 |
| C1—H1A | 0.9300 | C12—H12A | 0.9800 |
| C2—C3 | 1.382 (5) | C13—H13A | 0.9600 |
| C2—H2A | 0.9300 | C13—H13B | 0.9600 |
| C3—C4 | 1.371 (5) | C13—H13C | 0.9600 |
| C3—H3A | 0.9300 | C14—H14A | 0.9600 |
| C4—C5 | 1.396 (5) | C14—H14B | 0.9600 |
| C4—H4A | 0.9300 | C14—H14C | 0.9600 |
| C5—C6 | 1.378 (5) | | |

| | | | |
|---|---|---|---|
| C7—O1—C8 | 115.1 (2) | N1—C9—C10 | 106.5 (2) |
| C12—O2—H1O2 | 107 (2) | N1—C9—C8 | 111.2 (3) |
| C11—O3—C13 | 111.9 (2) | C10—C9—C8 | 112.8 (2) |
| C11—O4—C10 | 113.5 (2) | N1—C9—H9A | 108.7 |
| N2—N1—C9 | 116.5 (3) | C10—C9—H9A | 108.7 |
| N3—N2—N1 | 171.1 (4) | C8—C9—H9A | 108.7 |
| C2—C1—C6 | 121.5 (3) | O4—C10—C14 | 107.0 (3) |
| C2—C1—H1A | 119.2 | O4—C10—C9 | 108.8 (2) |
| C6—C1—H1A | 119.2 | C14—C10—C9 | 112.6 (3) |
| C1—C2—C3 | 120.0 (3) | O4—C10—H10A | 109.5 |
| C1—C2—H2A | 120.0 | C14—C10—H10A | 109.5 |
| C3—C2—H2A | 120.0 | C9—C10—H10A | 109.5 |
| C4—C3—C2 | 119.4 (3) | O3—C11—O4 | 112.6 (3) |
| C4—C3—H3A | 120.3 | O3—C11—C12 | 109.0 (3) |
| C2—C3—H3A | 120.3 | O4—C11—C12 | 110.2 (3) |
| C3—C4—C5 | 120.1 (3) | O3—C11—H11A | 108.3 |
| C3—C4—H4A | 120.0 | O4—C11—H11A | 108.3 |

| | | | |
|---|---|---|---|
| C5—C4—H4A | 120.0 | C12—C11—H11A | 108.3 |
| C6—C5—C4 | 120.7 (3) | O2—C12—C8 | 108.5 (2) |
| C6—C5—H5A | 119.6 | O2—C12—C11 | 111.7 (2) |
| C4—C5—H5A | 119.6 | C8—C12—C11 | 112.6 (3) |
| C1—C6—C5 | 118.3 (3) | O2—C12—H12A | 107.9 |
| C1—C6—C7 | 119.8 (3) | C8—C12—H12A | 107.9 |
| C5—C6—C7 | 121.9 (3) | C11—C12—H12A | 107.9 |
| O1—C7—C6 | 109.8 (3) | O3—C13—H13A | 109.5 |
| O1—C7—H7A | 109.7 | O3—C13—H13B | 109.5 |
| C6—C7—H7A | 109.7 | H13A—C13—H13B | 109.5 |
| O1—C7—H7B | 109.7 | O3—C13—H13C | 109.5 |
| C6—C7—H7B | 109.7 | H13A—C13—H13C | 109.5 |
| H7A—C7—H7B | 108.2 | H13B—C13—H13C | 109.5 |
| O1—C8—C12 | 110.8 (2) | C10—C14—H14A | 109.5 |
| O1—C8—C9 | 107.0 (2) | C10—C14—H14B | 109.5 |
| C12—C8—C9 | 111.3 (3) | H14A—C14—H14B | 109.5 |
| O1—C8—H8A | 109.2 | C10—C14—H14C | 109.5 |
| C12—C8—H8A | 109.2 | H14A—C14—H14C | 109.5 |
| C9—C8—H8A | 109.2 | H14B—C14—H14C | 109.5 |

| | | | |
|---|---|---|---|
| C9—N1—N2—N3 | −177 (2) | C12—C8—C9—C10 | −47.1 (4) |
| C6—C1—C2—C3 | −0.2 (6) | C11—O4—C10—C14 | 175.5 (3) |
| C1—C2—C3—C4 | 0.0 (6) | C11—O4—C10—C9 | −62.7 (3) |
| C2—C3—C4—C5 | −0.5 (6) | N1—C9—C10—O4 | 176.0 (2) |
| C3—C4—C5—C6 | 1.2 (6) | C8—C9—C10—O4 | 53.7 (3) |
| C2—C1—C6—C5 | 0.9 (5) | N1—C9—C10—C14 | −65.6 (3) |
| C2—C1—C6—C7 | 179.4 (3) | C8—C9—C10—C14 | 172.2 (3) |
| C4—C5—C6—C1 | −1.4 (5) | C13—O3—C11—O4 | −70.6 (3) |
| C4—C5—C6—C7 | −179.8 (3) | C13—O3—C11—C12 | 166.9 (2) |
| C8—O1—C7—C6 | −179.9 (3) | C10—O4—C11—O3 | −59.5 (3) |
| C1—C6—C7—O1 | 163.7 (3) | C10—O4—C11—C12 | 62.4 (3) |
| C5—C6—C7—O1 | −17.8 (5) | O1—C8—C12—O2 | −71.0 (3) |
| C7—O1—C8—C12 | 98.3 (3) | C9—C8—C12—O2 | 170.1 (3) |
| C7—O1—C8—C9 | −140.2 (3) | O1—C8—C12—C11 | 164.8 (2) |
| N2—N1—C9—C10 | 173.4 (3) | C9—C8—C12—C11 | 45.9 (3) |
| N2—N1—C9—C8 | −63.3 (4) | O3—C11—C12—O2 | −51.3 (3) |
| O1—C8—C9—N1 | 72.2 (3) | O4—C11—C12—O2 | −175.3 (2) |
| C12—C8—C9—N1 | −166.7 (2) | O3—C11—C12—C8 | 71.1 (3) |
| O1—C8—C9—C10 | −168.2 (2) | O4—C11—C12—C8 | −52.9 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H1*O2*···O2$^{i}$ | 0.88 (4) | 1.91 (3) | 2.757 (2) | 161 (3) |
| O2—H1*O2*···O3$^{i}$ | 0.88 (3) | 2.49 (3) | 3.063 (3) | 124 (3) |
| C7—H7*B*···O2 | 0.97 | 2.58 | 3.180 (4) | 120 |

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