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Methyl 2-(4-methoxy-3-nitrobenzamido)-acetate

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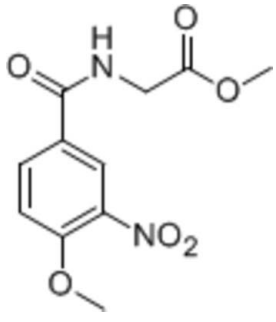
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.155; data-to-parameter ratio = 11.9.

The title compound, $C_{11}H_{12}N_2O_6$, crystallizes with two independent molecules in the asymmetric unit, which differ slightly in conformation. The dihedral angle between the amide O=C—N plane and the attached benzene ring is 19.5 (3)° in one molecule and 23.4 (3)° in the other. In the crystal, the two independent molecules are connected alternately by N—H···O hydrogen bonds, forming a chain along the *a* axis.

Related literature

For the biological activity of compounds with nitro and ester groups, see: Sykes *et al.* (1999). For a related structure, see: Wu *et al.* (2011).



Experimental

Crystal data

$C_{11}H_{12}N_2O_6$
M_r = 268.23
Monoclinic, $P2_1/c$
a = 10.4378 (7) Å
b = 13.9110 (9) Å
c = 17.5420 (15) Å
β = 106.146 (8)°
V = 2446.6 (3) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 291 K
0.28 × 0.26 × 0.24 mm

Data collection

Agilent Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.760, T_{max} = 0.789
10600 measured reflections
4251 independent reflections
3287 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.155
S = 1.04
4251 reflections
356 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O4′^{i}	0.83 (2)	2.26 (2)	3.069 (2)	167 (2)
N2′—H2′···O4	0.83 (2)	2.23 (2)	3.016 (2)	158 (2)

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5151).

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Sykes, B. M., Atwell, G. J., Hogg, A., Wilson, W. R., O'Connor, C. J. & Denny, W. A. (1999). *J. Med. Chem.* **42**, 346–355.
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supporting information

Acta Cryst. (2012). E**68**, o2343 [https://doi.org/10.1107/S1600536812029522]

Methyl 2-(4-methoxy-3-nitrobenzamido)acetate

Xin Zhu and Qiujuan Ma

S1. Comment

The nitro group and ester group are present in many bioactive compounds or be used as prodrug (Sykes *et al.*, 1999). Here we report the crystal structure of $C_{11}H_{12}N_2O_6$, namely, methyl 2-(4-methoxy-3-nitrobenzamido)acetate. In the crystal of the title compound (Fig. 1), the carbonyl group and the adjacent amide group are connected by intermolecular N—H···O hydrogen bonds, forming a chain along the *a* axis (Fig. 2).

S2. Experimental

The title compound (0.25 mmol, 67.0 mg) was dissolved in water-methanol (1 ml / 2 ml *v*/*v*) mixture. Colorless block crystals were separated after several weeks.

S3. Refinement

N-bound H atoms were located in a difference Fourier map and refined freely with a bond-distance restraint of N—H = 0.86 (2) Å. C-bound H-atoms were included in calculated positions and treated as riding atoms, with C—H = 0.93, 0.96 and 0.98 Å for CH(aromatic), CH_3 and CH(methine) H-atoms, respectively, and with U_{iso}(H)= k×U_{eq}(parent C-atom), where k = 1.5 for CH_3 H-atoms and k = 1.2 for other H-atoms.

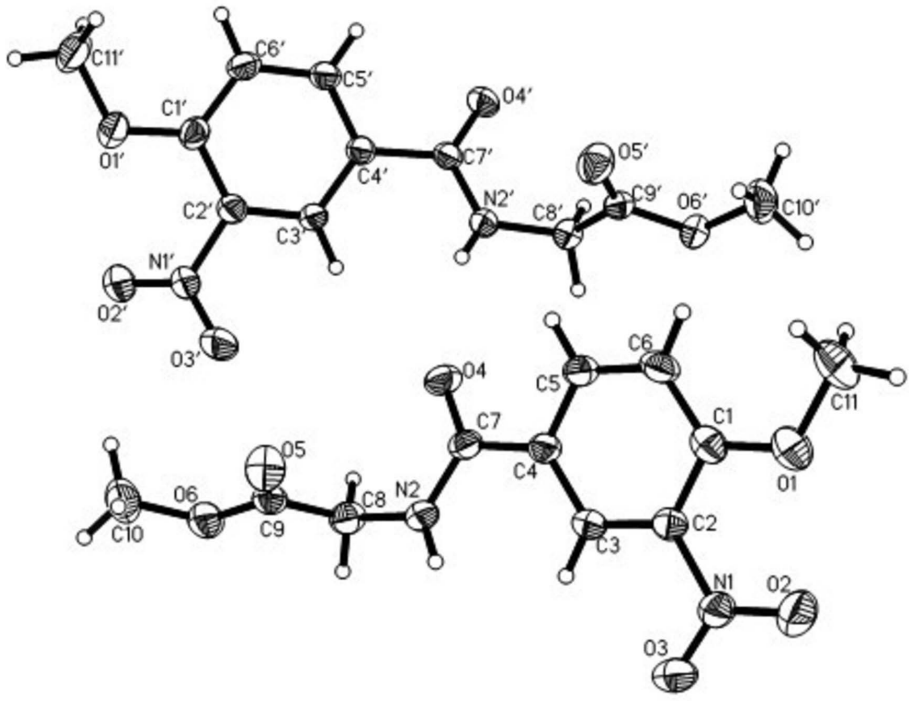

Figure 1

A view of the molecular structure of the title compound The displacement ellipsoids are drawn at the 30% probability level.

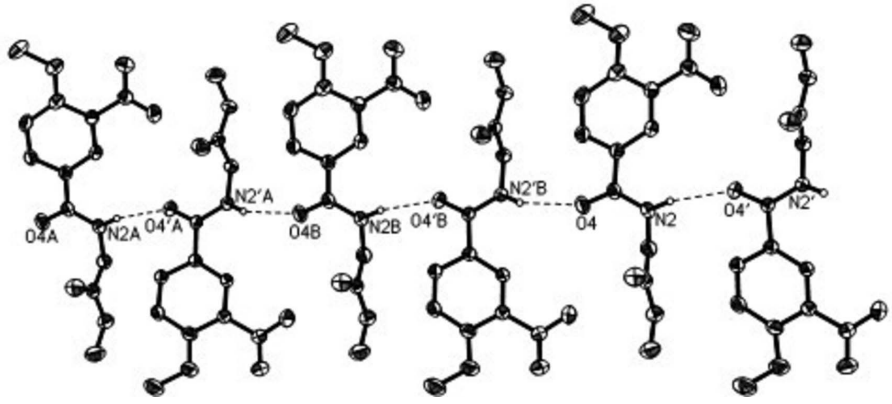

Figure 2

A view of the hydrogen bonded polymeric chain. The hydrogen bonds are shown as dashed lines.

Methyl 2-(4-methoxy-3-nitrobenzamido)acetate

Crystal data

$C_{11}H_{12}N_2O_6$
M_r = 268.23
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.4378 (7) Å
b = 13.9110 (9) Å
c = 17.5420 (15) Å
β = 106.146 (8)°
V = 2446.6 (3) Å^3
Z = 8
$F(000)$ = 1120
D_x = 1.456 Mg m^{-3}

Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3206 reflections
θ = 3.2–67.0°
μ = 1.03 mm^{-1}
T = 291 K
Block, colorless
0.28 × 0.26 × 0.24 mm

Data collection

Agilent Xcalibur Eos Gemini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.760, T_{max} = 0.789
10600 measured reflections
4251 independent reflections
3287 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 67.0°, θ_{min} = 4.1°
h = −12→12
k = −16→16
l = −20→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.155
S = 1.04
4251 reflections
356 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 0.8379P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00093 (17)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.7104 (2)	0.31701 (14)	0.29328 (12)	0.0732 (6)
O1′	0.18346 (19)	1.11580 (13)	0.30677 (12)	0.0671 (5)
O2	0.9503 (2)	0.31213 (17)	0.3839 (2)	0.1162 (11)
O2′	0.4242 (2)	1.12599 (15)	0.40786 (18)	0.0981 (9)
O3	1.0472 (2)	0.44345 (17)	0.41534 (18)	0.1013 (9)
O3′	0.5286 (2)	0.99534 (16)	0.41347 (19)	0.1039 (9)
O4	0.58759 (15)	0.72298 (13)	0.42220 (11)	0.0593 (5)
O4′	0.09322 (15)	0.69905 (12)	0.43303 (11)	0.0576 (5)
O5	0.7439 (2)	0.90062 (15)	0.34121 (12)	0.0724 (6)
O5′	0.2464 (2)	0.54205 (14)	0.32784 (11)	0.0677 (5)
O6	0.82081 (18)	0.99909 (13)	0.44488 (13)	0.0688 (5)

O6′	0.33449 (16)	0.43396 (11)	0.42284 (11)	0.0563 (4)
N1	0.9474 (2)	0.39794 (16)	0.38787 (13)	0.0579 (5)
N1′	0.4254 (2)	1.04059 (14)	0.39950 (14)	0.0569 (5)
N2	0.80857 (19)	0.74112 (15)	0.44094 (13)	0.0523 (5)
N2′	0.31167 (18)	0.68992 (14)	0.43984 (12)	0.0473 (5)
C1	0.7024 (2)	0.40601 (18)	0.32103 (14)	0.0530 (6)
C1′	0.1806 (2)	1.02642 (16)	0.33482 (14)	0.0483 (5)
C2	0.8203 (2)	0.44932 (17)	0.36718 (13)	0.0457 (5)
C2′	0.3009 (2)	0.98568 (16)	0.38040 (14)	0.0454 (5)
C3	0.8207 (2)	0.54128 (17)	0.39638 (13)	0.0443 (5)
H3	0.9007	0.5688	0.4253	0.053*
C3′	0.3080 (2)	0.89318 (15)	0.40887 (13)	0.0432 (5)
H3′	0.3896	0.8679	0.4377	0.052*
C4	0.7030 (2)	0.59338 (17)	0.38321 (13)	0.0458 (5)
C4′	0.1937 (2)	0.83750 (16)	0.39470 (13)	0.0433 (5)
C5	0.5861 (2)	0.55008 (19)	0.33762 (15)	0.0545 (6)
H5	0.5061	0.5836	0.3283	0.065*
C5′	0.0740 (2)	0.87772 (17)	0.35111 (14)	0.0486 (5)
H5′	−0.0038	0.8417	0.3423	0.058*
C6	0.5852 (2)	0.45980 (19)	0.30610 (16)	0.0588 (7)
H6	0.5058	0.4342	0.2745	0.071*
C6′	0.0668 (2)	0.96912 (17)	0.32055 (15)	0.0530 (6)
H6′	−0.0146	0.9930	0.2901	0.064*
C7	0.6947 (2)	0.69072 (17)	0.41681 (13)	0.0464 (5)
C7′	0.1950 (2)	0.73673 (16)	0.42440 (13)	0.0426 (5)
C8	0.8122 (3)	0.83675 (19)	0.47275 (15)	0.0569 (6)
H8A	0.8988	0.8474	0.5103	0.068*
H8B	0.7455	0.8418	0.5015	0.068*
C8′	0.3254 (2)	0.59067 (16)	0.46412 (14)	0.0495 (6)
H8′A	0.2655	0.5777	0.4964	0.059*
H8′B	0.4158	0.5799	0.4969	0.059*
C9	0.7875 (2)	0.91368 (18)	0.41080 (17)	0.0528 (6)
C9′	0.2959 (2)	0.52156 (16)	0.39587 (14)	0.0458 (5)
C10	0.7937 (3)	1.0825 (2)	0.3943 (2)	0.0863 (10)
H10D	0.8540	1.1333	0.4180	0.130*
H10E	0.7036	1.1033	0.3878	0.130*
H10F	0.8055	1.0667	0.3434	0.130*
C10′	0.3005 (3)	0.3553 (2)	0.3677 (2)	0.0757 (9)
H10A	0.3653	0.3050	0.3839	0.114*
H10B	0.2997	0.3773	0.3156	0.114*
H10C	0.2138	0.3312	0.3666	0.114*
C11	0.5910 (4)	0.2707 (2)	0.2494 (2)	0.0936 (11)
H11D	0.5337	0.2608	0.2831	0.140*
H11E	0.6125	0.2098	0.2304	0.140*
H11F	0.5463	0.3103	0.2052	0.140*
C11′	0.0631 (3)	1.1560 (2)	0.25777 (19)	0.0801 (9)
H11A	−0.0002	1.1630	0.2880	0.120*
H11B	0.0270	1.1143	0.2134	0.120*

H11C	0.0814	1.2179	0.2389	0.120*
H2′	0.3781 (19)	0.7135 (17)	0.4293 (14)	0.049 (7)*
H2	0.8799 (19)	0.7210 (17)	0.4351 (15)	0.049 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0720 (12)	0.0635 (12)	0.0763 (13)	−0.0131 (10)	0.0076 (10)	−0.0211 (10)
O1′	0.0693 (11)	0.0466 (10)	0.0737 (12)	0.0043 (9)	0.0004 (9)	0.0127 (9)
O2	0.0815 (16)	0.0625 (14)	0.180 (3)	0.0145 (12)	−0.0038 (17)	−0.0290 (16)
O2′	0.0691 (13)	0.0446 (12)	0.163 (2)	−0.0081 (10)	0.0032 (14)	0.0035 (13)
O3	0.0439 (11)	0.0780 (15)	0.173 (3)	0.0028 (10)	0.0148 (13)	−0.0273 (16)
O3′	0.0447 (11)	0.0661 (14)	0.199 (3)	−0.0027 (10)	0.0301 (14)	0.0091 (15)
O4	0.0399 (8)	0.0660 (11)	0.0736 (11)	0.0104 (8)	0.0183 (8)	0.0060 (9)
O4′	0.0395 (8)	0.0518 (10)	0.0837 (12)	−0.0066 (7)	0.0210 (8)	0.0000 (9)
O5	0.0894 (14)	0.0647 (12)	0.0632 (12)	−0.0003 (11)	0.0215 (11)	−0.0005 (9)
O5′	0.0811 (13)	0.0605 (11)	0.0553 (11)	0.0090 (10)	0.0086 (10)	0.0041 (9)
O6	0.0583 (10)	0.0522 (11)	0.0941 (14)	−0.0040 (8)	0.0180 (10)	−0.0118 (10)
O6′	0.0528 (9)	0.0393 (9)	0.0741 (11)	0.0058 (7)	0.0132 (8)	0.0056 (8)
N1	0.0502 (12)	0.0539 (13)	0.0684 (13)	0.0031 (10)	0.0143 (10)	−0.0125 (10)
N1′	0.0493 (11)	0.0408 (11)	0.0788 (15)	−0.0036 (9)	0.0149 (10)	0.0020 (10)
N2	0.0395 (10)	0.0490 (12)	0.0679 (13)	0.0062 (9)	0.0140 (9)	−0.0024 (10)
N2′	0.0375 (9)	0.0394 (10)	0.0666 (13)	−0.0009 (8)	0.0168 (9)	0.0045 (9)
C1	0.0555 (14)	0.0541 (14)	0.0476 (13)	−0.0105 (11)	0.0112 (11)	−0.0020 (11)
C1′	0.0517 (13)	0.0397 (12)	0.0506 (13)	0.0065 (10)	0.0095 (10)	−0.0031 (10)
C2	0.0425 (11)	0.0498 (13)	0.0456 (12)	−0.0012 (10)	0.0137 (10)	0.0001 (10)
C2′	0.0402 (11)	0.0408 (12)	0.0546 (13)	−0.0012 (9)	0.0120 (10)	−0.0048 (10)
C3	0.0367 (10)	0.0510 (13)	0.0449 (12)	−0.0048 (9)	0.0110 (9)	0.0004 (10)
C3′	0.0352 (10)	0.0391 (11)	0.0519 (12)	0.0022 (9)	0.0066 (9)	−0.0029 (9)
C4	0.0374 (11)	0.0491 (13)	0.0504 (12)	−0.0006 (9)	0.0113 (9)	0.0100 (10)
C4′	0.0379 (11)	0.0395 (11)	0.0515 (12)	0.0002 (9)	0.0109 (9)	−0.0070 (10)
C5	0.0384 (12)	0.0568 (15)	0.0643 (15)	0.0003 (10)	0.0077 (11)	0.0135 (12)
C5′	0.0364 (11)	0.0449 (12)	0.0614 (14)	0.0004 (9)	0.0087 (10)	−0.0089 (10)
C6	0.0425 (12)	0.0654 (16)	0.0598 (15)	−0.0136 (11)	−0.0003 (11)	0.0053 (13)
C6′	0.0397 (11)	0.0505 (14)	0.0610 (14)	0.0076 (10)	0.0011 (10)	−0.0072 (11)
C7	0.0382 (11)	0.0536 (13)	0.0471 (12)	0.0056 (10)	0.0116 (9)	0.0109 (10)
C7′	0.0351 (10)	0.0414 (12)	0.0504 (12)	−0.0035 (9)	0.0107 (9)	−0.0060 (9)
C8	0.0499 (13)	0.0579 (15)	0.0592 (15)	0.0042 (11)	0.0090 (11)	−0.0081 (12)
C8′	0.0456 (12)	0.0432 (12)	0.0568 (14)	0.0009 (10)	0.0096 (10)	0.0064 (10)
C9	0.0385 (11)	0.0514 (14)	0.0693 (17)	0.0001 (10)	0.0162 (11)	−0.0076 (12)
C9′	0.0349 (10)	0.0453 (12)	0.0553 (14)	0.0019 (9)	0.0096 (10)	0.0067 (10)
C10	0.088 (2)	0.0523 (17)	0.130 (3)	−0.0070 (16)	0.050 (2)	0.0034 (18)
C10′	0.082 (2)	0.0484 (15)	0.103 (2)	−0.0009 (14)	0.0353 (18)	−0.0128 (15)
C11	0.092 (2)	0.074 (2)	0.101 (3)	−0.0303 (18)	0.005 (2)	−0.0312 (19)
C11′	0.091 (2)	0.0580 (17)	0.0742 (19)	0.0170 (16)	−0.0049 (17)	0.0139 (14)

Geometric parameters (Å, º)

O1—C1	1.341 (3)	C3—H3	0.9300
O1—C11	1.424 (3)	C3′—C4′	1.385 (3)
O1′—C1′	1.340 (3)	C3′—H3′	0.9300
O1′—C11′	1.424 (3)	C4—C5	1.396 (3)
O2—N1	1.197 (3)	C4—C7	1.489 (3)
O2′—N1′	1.197 (3)	C4′—C5′	1.389 (3)
O3—N1	1.200 (3)	C4′—C7′	1.494 (3)
O3′—N1′	1.213 (3)	C5—C6	1.371 (4)
O4—C7	1.233 (3)	C5—H5	0.9300
O4′—C7′	1.231 (2)	C5′—C6′	1.374 (3)
O5—C9	1.192 (3)	C5′—H5′	0.9300
O5′—C9′	1.195 (3)	C6—H6	0.9300
O6—C9	1.332 (3)	C6′—H6′	0.9300
O6—C10	1.440 (4)	C8—C9	1.496 (4)
O6′—C9′	1.328 (3)	C8—H8A	0.9700
O6′—C10′	1.438 (3)	C8—H8B	0.9700
N1—C2	1.461 (3)	C8′—C9′	1.499 (3)
N1′—C2′	1.463 (3)	C8′—H8′A	0.9700
N2—C7	1.343 (3)	C8′—H8′B	0.9700
N2—C8	1.439 (3)	C10—H10D	0.9600
N2—H2	0.828 (16)	C10—H10E	0.9600
N2′—C7′	1.341 (3)	C10—H10F	0.9600
N2′—C8′	1.440 (3)	C10′—H10A	0.9600
N2′—H2′	0.833 (16)	C10′—H10B	0.9600
C1—C6	1.395 (4)	C10′—H10C	0.9600
C1—C2	1.407 (3)	C11—H11D	0.9600
C1′—C6′	1.394 (3)	C11—H11E	0.9600
C1′—C2′	1.407 (3)	C11—H11F	0.9600
C2—C3	1.378 (3)	C11′—H11A	0.9600
C2′—C3′	1.375 (3)	C11′—H11B	0.9600
C3—C4	1.389 (3)	C11′—H11C	0.9600
C1—O1—C11	118.7 (2)	C5′—C6′—H6′	119.7
C1′—O1′—C11′	118.7 (2)	C1′—C6′—H6′	119.7
C9—O6—C10	117.4 (2)	O4—C7—N2	121.9 (2)
C9′—O6′—C10′	117.7 (2)	O4—C7—C4	121.0 (2)
O2—N1—O3	121.1 (2)	N2—C7—C4	117.11 (19)
O2—N1—C2	120.6 (2)	O4′—C7′—N2′	122.3 (2)
O3—N1—C2	118.0 (2)	O4′—C7′—C4′	121.19 (19)
O2′—N1′—O3′	121.9 (2)	N2′—C7′—C4′	116.47 (18)
O2′—N1′—C2′	120.5 (2)	N2—C8—C9	113.5 (2)
O3′—N1′—C2′	117.2 (2)	N2—C8—H8A	108.9
C7—N2—C8	122.0 (2)	C9—C8—H8A	108.9
C7—N2—H2	122.2 (18)	N2—C8—H8B	108.9
C8—N2—H2	115.6 (18)	C9—C8—H8B	108.9
C7′—N2′—C8′	122.38 (19)	H8A—C8—H8B	107.7

C7′—N2′—H2′	122.0 (17)	N2′—C8′—C9′	113.4 (2)
C8′—N2′—H2′	115.0 (17)	N2′—C8′—H8′A	108.9
O1—C1—C6	124.5 (2)	C9′—C8′—H8′A	108.9
O1—C1—C2	118.1 (2)	N2′—C8′—H8′B	108.9
C6—C1—C2	117.4 (2)	C9′—C8′—H8′B	108.9
O1′—C1′—C6′	124.7 (2)	H8′A—C8′—H8′B	107.7
O1′—C1′—C2′	118.3 (2)	O5—C9—O6	125.0 (3)
C6′—C1′—C2′	116.9 (2)	O5—C9—C8	125.1 (2)
C3—C2—C1	121.5 (2)	O6—C9—C8	110.0 (2)
C3—C2—N1	117.0 (2)	O5′—C9′—O6′	125.3 (2)
C1—C2—N1	121.5 (2)	O5′—C9′—C8′	125.5 (2)
C3′—C2′—C1′	122.2 (2)	O6′—C9′—C8′	109.2 (2)
C3′—C2′—N1′	116.83 (19)	O6—C10—H10D	109.5
C1′—C2′—N1′	121.0 (2)	O6—C10—H10E	109.5
C2—C3—C4	120.8 (2)	H10D—C10—H10E	109.5
C2—C3—H3	119.6	O6—C10—H10F	109.5
C4—C3—H3	119.6	H10D—C10—H10F	109.5
C2′—C3′—C4′	120.1 (2)	H10E—C10—H10F	109.5
C2′—C3′—H3′	119.9	O6′—C10′—H10A	109.5
C4′—C3′—H3′	119.9	O6′—C10′—H10B	109.5
C3—C4—C5	117.5 (2)	H10A—C10′—H10B	109.5
C3—C4—C7	123.7 (2)	O6′—C10′—H10C	109.5
C5—C4—C7	118.8 (2)	H10A—C10′—H10C	109.5
C3′—C4′—C5′	118.1 (2)	H10B—C10′—H10C	109.5
C3′—C4′—C7′	122.56 (19)	O1—C11—H11D	109.5
C5′—C4′—C7′	119.31 (19)	O1—C11—H11E	109.5
C6—C5—C4	122.2 (2)	H11D—C11—H11E	109.5
C6—C5—H5	118.9	O1—C11—H11F	109.5
C4—C5—H5	118.9	H11D—C11—H11F	109.5
C6′—C5′—C4′	122.0 (2)	H11E—C11—H11F	109.5
C6′—C5′—H5′	119.0	O1′—C11′—H11A	109.5
C4′—C5′—H5′	119.0	O1′—C11′—H11B	109.5
C5—C6—C1	120.5 (2)	H11A—C11′—H11B	109.5
C5—C6—H6	119.7	O1′—C11′—H11C	109.5
C1—C6—H6	119.7	H11A—C11′—H11C	109.5
C5′—C6′—C1′	120.5 (2)	H11B—C11′—H11C	109.5

C11—O1—C1—C6	−3.9 (4)	C3′—C4′—C5′—C6′	1.6 (3)
C11—O1—C1—C2	177.3 (3)	C7′—C4′—C5′—C6′	−178.4 (2)
C11′—O1′—C1′—C6′	−1.0 (4)	C4—C5—C6—C1	2.2 (4)
C11′—O1′—C1′—C2′	177.4 (2)	O1—C1—C6—C5	179.4 (2)
O1—C1—C2—C3	178.6 (2)	C2—C1—C6—C5	−1.9 (4)
C6—C1—C2—C3	−0.2 (3)	C4′—C5′—C6′—C1′	−2.2 (4)
O1—C1—C2—N1	−2.8 (3)	O1′—C1′—C6′—C5′	179.2 (2)
C6—C1—C2—N1	178.3 (2)	C2′—C1′—C6′—C5′	0.9 (4)
O2—N1—C2—C3	159.7 (3)	C8—N2—C7—O4	−1.6 (4)
O3—N1—C2—C3	−13.9 (4)	C8—N2—C7—C4	178.6 (2)
O2—N1—C2—C1	−18.9 (4)	C3—C4—C7—O4	−160.1 (2)

O3—N1—C2—C1	167.5 (3)	C5—C4—C7—O4	18.0 (3)
O1′—C1′—C2′—C3′	−177.4 (2)	C3—C4—C7—N2	19.8 (3)
C6′—C1′—C2′—C3′	1.0 (3)	C5—C4—C7—N2	−162.1 (2)
O1′—C1′—C2′—N1′	2.4 (3)	C8′—N2′—C7′—O4′	3.0 (4)
C6′—C1′—C2′—N1′	−179.1 (2)	C8′—N2′—C7′—C4′	−176.1 (2)
O2′—N1′—C2′—C3′	−148.6 (3)	C3′—C4′—C7′—O4′	157.6 (2)
O3′—N1′—C2′—C3′	24.8 (4)	C5′—C4′—C7′—O4′	−22.4 (3)
O2′—N1′—C2′—C1′	31.6 (4)	C3′—C4′—C7′—N2′	−23.3 (3)
O3′—N1′—C2′—C1′	−155.0 (3)	C5′—C4′—C7′—N2′	156.7 (2)
C1—C2—C3—C4	2.1 (3)	C7—N2—C8—C9	−88.1 (3)
N1—C2—C3—C4	−176.5 (2)	C7′—N2′—C8′—C9′	87.3 (3)
C1′—C2′—C3′—C4′	−1.6 (4)	C10—O6—C9—O5	4.3 (4)
N1′—C2′—C3′—C4′	178.5 (2)	C10—O6—C9—C8	−175.3 (2)
C2—C3—C4—C5	−1.8 (3)	N2—C8—C9—O5	13.9 (4)
C2—C3—C4—C7	176.4 (2)	N2—C8—C9—O6	−166.5 (2)
C2′—C3′—C4′—C5′	0.3 (3)	C10′—O6′—C9′—O5′	−7.6 (4)
C2′—C3′—C4′—C7′	−179.7 (2)	C10′—O6′—C9′—C8′	172.9 (2)
C3—C4—C5—C6	−0.3 (4)	N2′—C8′—C9′—O5′	−10.9 (3)
C7—C4—C5—C6	−178.6 (2)	N2′—C8′—C9′—O6′	168.53 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4′^{i}	0.83 (2)	2.26 (2)	3.069 (2)	167 (2)
N2′—H2′···O4	0.83 (2)	2.23 (2)	3.016 (2)	158 (2)

Symmetry code: (i) *x*+1, *y*, *z*.