IUCrData

ISSN 2414-3146

Received 9 October 2018
Accepted 11 October 2018

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

Keywords: crystal structure; quinoline; hydrogen bond; C—H⋯π.

CCDC reference: 1872739

Structural data: full structural data are available from iucrdata.iucr.org

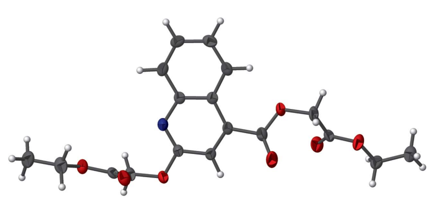
Ethyl 2-{[2-(2-ethoxy-2-oxoethoxy)quinolin-4-yl]-carbonyloxy}acetate

Younos Bouzian,[a]* Fouzia Hlimi,[a] Nada kheira Sebbar,[a] Mohamed El Hafi,[a] Brahim Hni,[a] El Mokhtar Essassi[a] and Joel T. Mague[b]

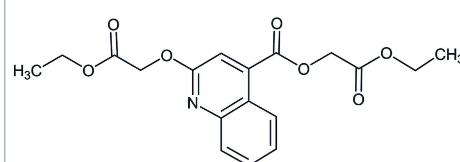
[a]Laboratoire de Chimie Organique Hétérocyclique, Centre de Recherche Des Sciences des Médicaments, Pôle de Compétence Pharmacochimie, Av Ibn Battouta, BP 1014, Faculté des Sciences, Université Mohammed V, Rabat, Morocco, and [b]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: Bouzianyounes@gmail.com

The conformation of the 2-ethoxy-2-oxoethoxy side chain, including a *gauche* $C_e—O—C—C_3$ [72.46 (16)°] (e = ethoxy) unit, in the title compound, $C_{18}H_{19}NO_7$, is partly determined by an intramolecular C—H⋯O hydrogen bond. In the crystal, C—H⋯O hydrogen bonds and C—H⋯π interactions arising from the same methylene group form chains extending along the *a*-axis direction.

3D view



Chemical scheme



Structure description

Quinoline derivatives have various biological properties including antibacterial (Kidwai *et al.*, 2000) antiviral (Wathen *et al.*, 2002), anticancer (Chen *et al.*, 2013) and antimalarial (Kunin & Ellise, 2000) activity. As part of our studies in this area, we now describe the synthesis and structure of the title compound.

As expected, the quinoline core of the molecule is almost planar (r.m.s. deviation = 0.0149) with N1 deviating by the largest amount [0.0272 (9) Å]. The orientation of the inner portion of the side chain emanating from C7 is partially determined by an intramolecular C5—H5⋯O5 hydrogen bond (Fig. 1 and Table 1). In the crystal, the molecules form chains extending along the *a*-axis direction through a combination of C10—H10*A*⋯O2 hydrogen bonds and C10—H10*B*⋯*Cg*2 interactions (Table 1 and Fig. 2). The chains pack with intercalation of the shorter side chains on one side and the longer ones on the other and with the quinoline moieties alternately up and down from one chain to the next (Fig. 3).

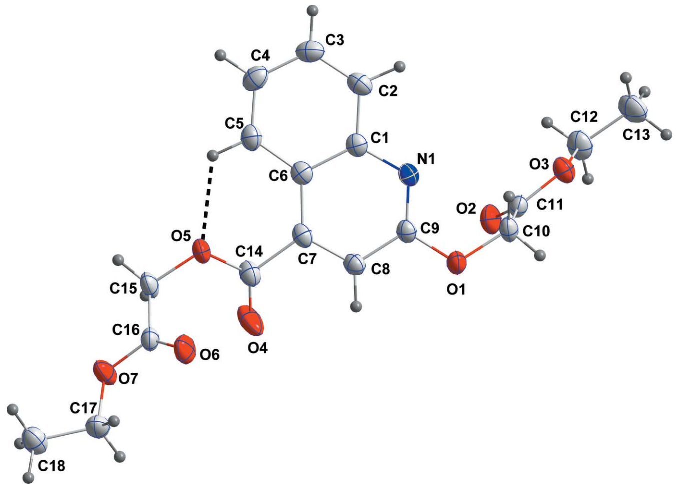


Figure 1
The title molecule showing 50% probability ellipsoids. The intramolecular hydrogen bond is shown by a dashed line.

Synthesis and crystallization

A solution of 0.8 g (4.23 mmol) of 2-oxo-1,2-dihydroquinoline-4-carboxylic acid in 25 ml of DMF was mixed with 0.94 ml (8.46 mmol) ethyl bromoacetate, 1.17 g (8.46 mmol) K_2CO_3 and 0.13 g (0.423 mmol) tetra-*n*-butylammonium bromide (TBAB). The reaction mixture was stirred at room temperature in DMF for 24 h. After removal of salts by filtration, the DMF was evaporated under reduced pressure and the residue obtained was dissolved in dichloromethane. The organic phase was dried over Na_2SO_4 then concentrated *in vacuo*. The resulting mixture was chromatographed on a silica gel column [eluent: ethyl acetate/hexane (1/9)]. Colourless blocks were obtained when the solvent was allowed to evaporate (yield: 20%).

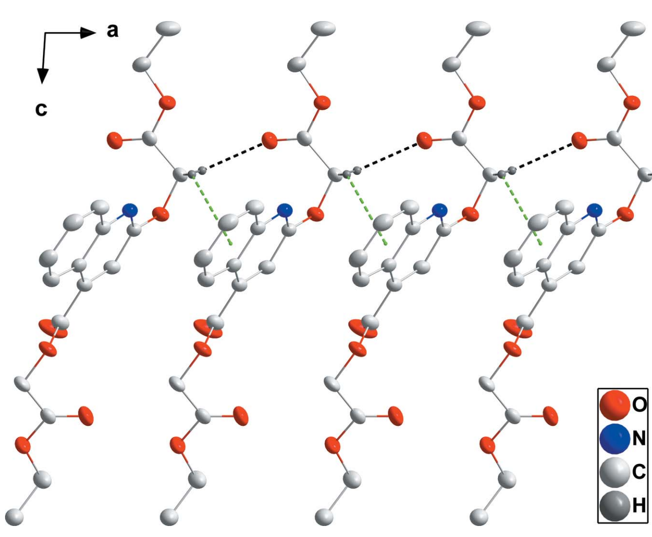


Figure 2
A portion of the hydrogen-bonded chain viewed along the *b*-axis direction. C—H⋯O hydrogen bonds and C—H⋯π(ring) interactions are shown, respectively, by black and green dashed lines.

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

*Cg*2 is the centroid of the C1–C6 ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C5—H5⋯O5	0.977 (19)	2.244 (17)	2.8681 (17)	120.7 (14)
C10—H10*A*⋯O2^{i}	0.954 (19)	2.435 (19)	3.3079 (16)	152.1 (15)
C10—H10*B*⋯*Cg*2^{i}	0.983 (17)	3.249 (16)	4.0173 (14)	136.3 (15)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{19}NO_7$
M_r	361.34
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, *b*, *c* (Å)	4.9417 (2), 7.6157 (3), 23.4472 (9)
α, β, γ (°)	94.490 (2), 92.997 (2), 98.136 (2)
V (Å^3)	869.06 (6)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	0.91
Crystal size (mm)	0.19 × 0.14 × 0.08
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.85, 0.93
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6827, 3301, 2894
R_{int}	0.023
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.037, 0.099, 1.03
No. of reflections	3301
No. of parameters	312
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.20

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

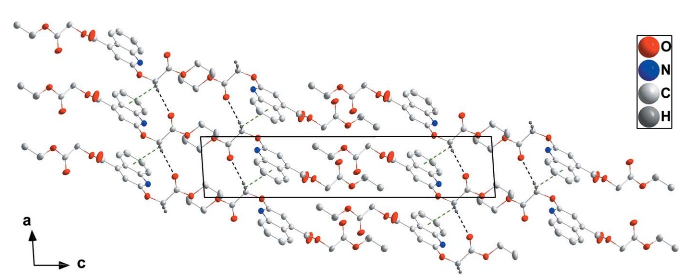


Figure 3
Packing viewed along the *b*-axis direction with intermolecular interactions depicted as in Fig. 2.

Funding information

The support of NSF–MRI Grant No. 1228232 for the purchase of the diffractometer and Tulane University for support of the Tulane Crystallography Laboratory are gratefully acknowledged.

References

Brandenburg, K. & Putz, H. (2012). *DIAMOND*, Crystal Impact GbR, Bonn, Germany.
Bruker (2016). *APEX3*, *SAINT* and *SADABS*. Bruker AXS, Inc., Madison, Wisconsin, USA.
Chen, H., Yang, Z., Ding, C., Chu, L., Zhang, Y., Terry, K., Liu, H., Shen, Q. & Zhou, J. (2013). *Eur. J. Med. Chem.* **62**, 498–507.
Kidwai, M., Bhushan, K., Sapra, P., Saxena, R. & Gupta, R. (2000). *Bioorg. Med. Chem.* **8**, 69–72.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Kunin, C. M. & Ellis, W. Y. (2000). *Antimicrob. Agents Chemother.* **44**, 848–852.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Wathen, M. W. (2002). *Rev. Med. Virol.* **12**, 167–178.

full crystallographic data

IUCrData (2018). **3**, x181438 [https://doi.org/10.1107/S2414314618014384]

Ethyl 2-{[2-(2-ethoxy-2-oxoethoxy)quinolin-4-yl]carbonyloxy}acetate

Younos Bouzian, Fouzia Hlimi, Nada kheira Sebbar, Mohamed El Hafi, Brahim Hni, El Mokhtar Essassi and Joel T. Mague

Ethyl 2-{[2-(2-ethoxy-2-oxoethoxy)quinolin-4-yl]carbonyloxy}acetate

Crystal data

$C_{18}H_{19}NO_7$
M_r = 361.34
Triclinic, $P\overline{1}$
a = 4.9417 (2) Å
b = 7.6157 (3) Å
c = 23.4472 (9) Å
α = 94.490 (2)°
β = 92.997 (2)°
γ = 98.136 (2)°
V = 869.06 (6) Å^3
Z = 2
F(000) = 380
D_x = 1.381 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 5397 reflections
θ = 3.8–74.5°
μ = 0.91 mm^{-1}
T = 150 K
Block, colourless
0.19 × 0.14 × 0.08 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.85, T_{max} = 0.93
6827 measured reflections
3301 independent reflections
2894 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 74.5°, θ_{min} = 3.8°
h = −5→6
k = −9→9
l = −27→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
S = 1.03
3301 reflections
312 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.2771P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL-2018/1* (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0144 (10)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.9795 (2)	0.19616 (13)	0.19654 (4)	0.0298 (2)
O2	0.6525 (2)	0.10059 (14)	0.09687 (4)	0.0347 (3)
O3	0.9762 (2)	0.24142 (13)	0.04573 (4)	0.0314 (2)
O4	0.3329 (3)	0.15037 (15)	0.35154 (5)	0.0549 (4)
O5	0.3071 (2)	0.43440 (13)	0.37905 (4)	0.0317 (2)
O6	0.5808 (2)	0.31430 (16)	0.46977 (5)	0.0409 (3)
O7	0.1851 (2)	0.22790 (15)	0.50923 (4)	0.0370 (3)
N1	0.7797 (2)	0.45027 (15)	0.19139 (5)	0.0264 (3)
C1	0.6133 (3)	0.56258 (17)	0.21529 (5)	0.0253 (3)
C2	0.5848 (3)	0.71671 (19)	0.18733 (6)	0.0322 (3)
H2	0.691 (4)	0.735 (2)	0.1526 (8)	0.041 (5)*
C3	0.4194 (3)	0.83331 (19)	0.20776 (6)	0.0348 (3)
H3	0.403 (4)	0.937 (3)	0.1890 (8)	0.043 (5)*
C4	0.2734 (3)	0.80006 (19)	0.25639 (6)	0.0341 (3)
H4	0.157 (4)	0.883 (3)	0.2708 (8)	0.046 (5)*
C5	0.2999 (3)	0.65216 (19)	0.28472 (6)	0.0304 (3)
H5	0.198 (4)	0.632 (2)	0.3188 (8)	0.042 (5)*
C6	0.4736 (3)	0.53005 (17)	0.26569 (5)	0.0250 (3)
C7	0.5175 (3)	0.37093 (17)	0.29200 (5)	0.0258 (3)
C8	0.6876 (3)	0.26321 (18)	0.26838 (6)	0.0266 (3)
H8	0.720 (3)	0.155 (2)	0.2853 (7)	0.035 (4)*
C9	0.8144 (3)	0.31020 (17)	0.21775 (5)	0.0246 (3)
C10	1.0894 (3)	0.2362 (2)	0.14312 (6)	0.0291 (3)
H10A	1.229 (4)	0.163 (2)	0.1374 (7)	0.040 (5)*
H10B	1.164 (3)	0.363 (2)	0.1426 (7)	0.032 (4)*
C11	0.8761 (3)	0.18459 (17)	0.09398 (6)	0.0257 (3)
C12	0.7954 (3)	0.1969 (2)	−0.00618 (6)	0.0393 (4)
H12A	0.743 (4)	0.062 (3)	−0.0114 (8)	0.052 (5)*
H12B	0.632 (4)	0.253 (3)	−0.0010 (8)	0.052 (5)*
C13	0.9522 (4)	0.2659 (3)	−0.05472 (7)	0.0476 (4)
H13A	1.130 (5)	0.207 (3)	−0.0576 (10)	0.072 (7)*
H13B	0.832 (5)	0.235 (3)	−0.0907 (10)	0.070 (7)*
H13C	1.009 (5)	0.394 (3)	−0.0492 (10)	0.066 (6)*
C14	0.3772 (3)	0.30534 (19)	0.34306 (6)	0.0309 (3)
C15	0.1559 (3)	0.3732 (2)	0.42636 (6)	0.0339 (3)

H15A	0.005 (4)	0.282 (3)	0.4126 (8)	0.042 (5)*
H15B	0.094 (4)	0.479 (3)	0.4439 (8)	0.043 (5)*
C16	0.3364 (3)	0.30131 (18)	0.46988 (6)	0.0273 (3)
C17	0.3261 (3)	0.1532 (2)	0.55576 (7)	0.0376 (4)
H17A	0.341 (4)	0.031 (3)	0.5435 (8)	0.052 (5)*
H17B	0.506 (4)	0.219 (3)	0.5618 (8)	0.047 (5)*
C18	0.1607 (4)	0.1651 (2)	0.60672 (7)	0.0403 (4)
H18A	0.249 (4)	0.113 (3)	0.6388 (9)	0.058 (6)*
H18B	−0.019 (4)	0.104 (3)	0.5980 (8)	0.050 (5)*
H18C	0.158 (5)	0.296 (3)	0.6203 (10)	0.069 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0316 (5)	0.0373 (5)	0.0231 (5)	0.0121 (4)	0.0057 (4)	0.0030 (4)
O2	0.0276 (5)	0.0424 (6)	0.0325 (5)	0.0004 (4)	0.0062 (4)	−0.0021 (4)
O3	0.0311 (5)	0.0395 (5)	0.0225 (5)	0.0015 (4)	0.0016 (4)	0.0026 (4)
O4	0.0931 (10)	0.0301 (6)	0.0388 (6)	−0.0094 (6)	0.0309 (6)	0.0011 (5)
O5	0.0359 (5)	0.0364 (5)	0.0256 (5)	0.0087 (4)	0.0141 (4)	0.0053 (4)
O6	0.0265 (5)	0.0575 (7)	0.0419 (6)	0.0097 (5)	0.0125 (4)	0.0108 (5)
O7	0.0269 (5)	0.0550 (7)	0.0322 (5)	0.0067 (4)	0.0076 (4)	0.0185 (5)
N1	0.0264 (5)	0.0309 (6)	0.0215 (5)	0.0026 (4)	0.0019 (4)	0.0021 (4)
C1	0.0249 (6)	0.0277 (6)	0.0218 (6)	0.0015 (5)	−0.0017 (5)	−0.0010 (5)
C2	0.0378 (8)	0.0332 (7)	0.0250 (7)	0.0013 (6)	0.0016 (6)	0.0061 (5)
C3	0.0440 (8)	0.0274 (7)	0.0322 (7)	0.0055 (6)	−0.0067 (6)	0.0039 (6)
C4	0.0369 (8)	0.0305 (7)	0.0339 (8)	0.0089 (6)	−0.0044 (6)	−0.0055 (6)
C5	0.0320 (7)	0.0331 (7)	0.0251 (7)	0.0032 (6)	0.0034 (6)	−0.0029 (5)
C6	0.0250 (6)	0.0261 (6)	0.0217 (6)	−0.0002 (5)	−0.0021 (5)	−0.0012 (5)
C7	0.0268 (6)	0.0278 (6)	0.0208 (6)	−0.0018 (5)	0.0019 (5)	−0.0007 (5)
C8	0.0310 (7)	0.0269 (6)	0.0213 (6)	0.0029 (5)	0.0011 (5)	0.0018 (5)
C9	0.0240 (6)	0.0292 (6)	0.0199 (6)	0.0033 (5)	−0.0001 (5)	−0.0004 (5)
C10	0.0245 (6)	0.0410 (8)	0.0230 (7)	0.0074 (6)	0.0057 (5)	0.0016 (5)
C11	0.0250 (6)	0.0275 (6)	0.0257 (7)	0.0079 (5)	0.0057 (5)	−0.0006 (5)
C12	0.0373 (8)	0.0537 (10)	0.0257 (7)	0.0070 (7)	−0.0040 (6)	−0.0009 (6)
C13	0.0662 (12)	0.0509 (10)	0.0253 (8)	0.0065 (9)	0.0009 (8)	0.0049 (7)
C14	0.0345 (7)	0.0309 (7)	0.0253 (7)	−0.0017 (6)	0.0064 (6)	−0.0013 (5)
C15	0.0299 (7)	0.0479 (9)	0.0264 (7)	0.0073 (6)	0.0128 (6)	0.0094 (6)
C16	0.0268 (7)	0.0290 (6)	0.0267 (7)	0.0046 (5)	0.0094 (5)	0.0001 (5)
C17	0.0367 (8)	0.0459 (9)	0.0349 (8)	0.0153 (7)	0.0064 (6)	0.0138 (7)
C18	0.0368 (8)	0.0522 (10)	0.0323 (8)	0.0047 (7)	0.0024 (7)	0.0097 (7)

Geometric parameters (Å, º)

O1—C9	1.3577 (15)	C6—C7	1.4401 (19)
O1—C10	1.4285 (16)	C7—C8	1.3633 (19)
O2—C11	1.2036 (17)	C7—C14	1.4988 (19)
O3—C11	1.3367 (16)	C8—C9	1.4180 (18)
O3—C12	1.4598 (17)	C8—H8	0.972 (18)

O4—C14	1.2035 (19)	C10—C11	1.5092 (19)
O5—C14	1.3399 (17)	C10—H10A	0.954 (19)
O5—C15	1.4405 (16)	C10—H10B	0.983 (17)
O6—C16	1.1978 (17)	C12—C13	1.498 (2)
O7—C16	1.3259 (17)	C12—H12A	1.02 (2)
O7—C17	1.4593 (18)	C12—H12B	0.97 (2)
N1—C9	1.3012 (17)	C13—H13A	1.05 (2)
N1—C1	1.3762 (17)	C13—H13B	1.00 (2)
C1—C2	1.4090 (19)	C13—H13C	0.97 (2)
C1—C6	1.4201 (19)	C15—C16	1.506 (2)
C2—C3	1.366 (2)	C15—H15A	0.96 (2)
C2—H2	1.001 (18)	C15—H15B	0.97 (2)
C3—C4	1.402 (2)	C17—C18	1.486 (2)
C3—H3	0.943 (19)	C17—H17A	0.97 (2)
C4—C5	1.370 (2)	C17—H17B	0.95 (2)
C4—H4	0.966 (19)	C18—H18A	0.99 (2)
C5—C6	1.4152 (19)	C18—H18B	0.95 (2)
C5—H5	0.978 (19)	C18—H18C	1.03 (3)

C9—O1—C10	115.23 (10)	O2—C11—C10	125.79 (12)
C11—O3—C12	116.03 (11)	O3—C11—C10	109.56 (11)
C14—O5—C15	115.02 (11)	O3—C12—C13	106.86 (13)
C16—O7—C17	117.59 (11)	O3—C12—H12A	108.1 (11)
C9—N1—C1	117.42 (11)	C13—C12—H12A	111.8 (11)
N1—C1—C2	116.81 (12)	O3—C12—H12B	108.2 (12)
N1—C1—C6	123.38 (12)	C13—C12—H12B	112.1 (12)
C2—C1—C6	119.81 (12)	H12A—C12—H12B	109.6 (16)
C3—C2—C1	120.40 (13)	C12—C13—H13A	109.5 (13)
C3—C2—H2	123.1 (10)	C12—C13—H13B	108.0 (13)
C1—C2—H2	116.5 (10)	H13A—C13—H13B	110.2 (18)
C2—C3—C4	120.43 (13)	C12—C13—H13C	112.1 (13)
C2—C3—H3	119.8 (11)	H13A—C13—H13C	107.2 (19)
C4—C3—H3	119.7 (11)	H13B—C13—H13C	109.8 (19)
C5—C4—C3	120.31 (13)	O4—C14—O5	122.56 (13)
C5—C4—H4	119.4 (11)	O4—C14—C7	123.18 (13)
C3—C4—H4	120.3 (11)	O5—C14—C7	114.25 (12)
C4—C5—C6	121.04 (13)	O5—C15—C16	111.47 (11)
C4—C5—H5	118.9 (11)	O5—C15—H15A	110.1 (11)
C6—C5—H5	120.0 (11)	C16—C15—H15A	109.7 (11)
C5—C6—C1	117.97 (12)	O5—C15—H15B	104.6 (11)
C5—C6—C7	125.85 (12)	C16—C15—H15B	108.7 (11)
C1—C6—C7	116.16 (12)	H15A—C15—H15B	112.2 (15)
C8—C7—C6	119.62 (12)	O6—C16—O7	125.43 (13)
C8—C7—C14	115.35 (12)	O6—C16—C15	124.80 (13)
C6—C7—C14	124.95 (12)	O7—C16—C15	109.73 (11)
C7—C8—C9	118.76 (12)	O7—C17—C18	107.62 (12)
C7—C8—H8	121.0 (10)	O7—C17—H17A	108.0 (12)
C9—C8—H8	120.2 (10)	C18—C17—H17A	111.4 (12)

N1—C9—O1	119.94 (11)	O7—C17—H17B	107.5 (12)
N1—C9—C8	124.63 (12)	C18—C17—H17B	113.4 (12)
O1—C9—C8	115.43 (11)	H17A—C17—H17B	108.7 (16)
O1—C10—C11	111.20 (11)	C17—C18—H18A	109.5 (12)
O1—C10—H10A	106.4 (11)	C17—C18—H18B	110.4 (12)
C11—C10—H10A	107.0 (11)	H18A—C18—H18B	109.9 (17)
O1—C10—H10B	112.6 (9)	C17—C18—H18C	109.8 (13)
C11—C10—H10B	109.0 (10)	H18A—C18—H18C	106.2 (18)
H10A—C10—H10B	110.5 (15)	H18B—C18—H18C	111.0 (17)
O2—C11—O3	124.61 (12)		

C9—N1—C1—C2	177.99 (12)	C10—O1—C9—C8	175.21 (11)
C9—N1—C1—C6	−1.91 (18)	C7—C8—C9—N1	−0.3 (2)
N1—C1—C2—C3	178.82 (13)	C7—C8—C9—O1	−179.63 (11)
C6—C1—C2—C3	−1.3 (2)	C9—O1—C10—C11	−76.01 (14)
C1—C2—C3—C4	−0.8 (2)	C12—O3—C11—O2	0.38 (19)
C2—C3—C4—C5	1.5 (2)	C12—O3—C11—C10	178.34 (12)
C3—C4—C5—C6	−0.1 (2)	O1—C10—C11—O2	−8.81 (19)
C4—C5—C6—C1	−1.89 (19)	O1—C10—C11—O3	173.25 (10)
C4—C5—C6—C7	179.92 (12)	C11—O3—C12—C13	−177.61 (13)
N1—C1—C6—C5	−177.54 (12)	C15—O5—C14—O4	−4.6 (2)
C2—C1—C6—C5	2.56 (18)	C15—O5—C14—C7	176.06 (11)
N1—C1—C6—C7	0.83 (18)	C8—C7—C14—O4	−25.5 (2)
C2—C1—C6—C7	−179.08 (12)	C6—C7—C14—O4	151.15 (16)
C5—C6—C7—C8	178.79 (12)	C8—C7—C14—O5	153.84 (12)
C1—C6—C7—C8	0.57 (18)	C6—C7—C14—O5	−29.51 (19)
C5—C6—C7—C14	2.3 (2)	C14—O5—C15—C16	72.46 (16)
C1—C6—C7—C14	−175.94 (12)	C17—O7—C16—O6	−1.3 (2)
C6—C7—C8—C9	−0.84 (19)	C17—O7—C16—C15	−178.99 (13)
C14—C7—C8—C9	175.99 (11)	O5—C15—C16—O6	9.4 (2)
C1—N1—C9—O1	−179.05 (11)	O5—C15—C16—O7	−172.89 (12)
C1—N1—C9—C8	1.65 (19)	C16—O7—C17—C18	151.56 (14)
C10—O1—C9—N1	−4.16 (17)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O5	0.977 (19)	2.244 (17)	2.8681 (17)	120.7 (14)
C10—H10*A*···O2^{i}	0.954 (19)	2.435 (19)	3.3079 (16)	152.1 (15)
C10—H10*B*···*Cg*2^{i}	0.983 (17)	3.249 (16)	4.0173 (14)	136.3 (15)

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