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2-Oxo-1,2-dihydroquinoline-4-carboxylic acid monohydrate

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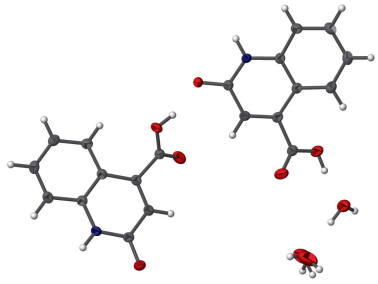
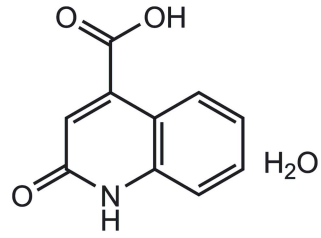
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{10}H_7NO_3\cdot H_2O$, O—H···O hydrogen bonds involving the carboxyl groups, the keto groups and the lattice water molecules form stepped sheets approximately parallel to {010} which are tied together by pairwise N—H···O interactions. The asymmetric unit contains two independent quinolone derivatives and two water molecules, one of which is disordered over two positions, of equal occupancy.

3D view



Chemical scheme



Structure description

Quinolone derivatives are a classical division of organic chemistry; many of these molecules have shown remarkable biological properties, including exceptional antibacterial activity (Beena & Rawat, 2013; Chai *et al.*, 2011; Hoshino *et al.*, 2008). Quinolone derivatives are frequently associated with medicinal applications, such as anti-fungal (Musiol *et al.*, 2010), anti-tumoral (Bergh *et al.*, 1997) and anti-cancer drugs (Elderfield & LeVon, 1960).

The asymmetric unit contains two independent molecules, which differ primarily in the orientation of the carboxyl group. O—H···O hydrogen bonds involving the carboxyl groups, the keto groups and the lattice water molecules (Table 1 and Fig. 1) form stepped sheets approximately parallel to {010} in the crystal. These layers are tied together by pairwise N—H···O interactions (Table 1 and Fig. 2).

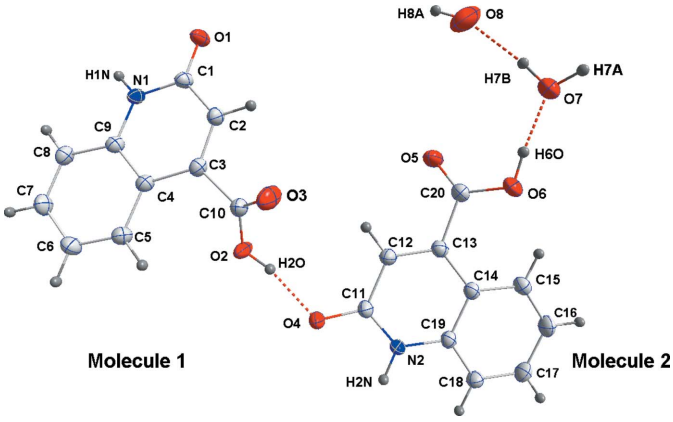


Figure 1
The asymmetric unit of the title compound with 50% probability ellipsoids. Only one site for the disordered water molecule (O8) is shown, and O—H···O hydrogen bonds are depicted as dotted lines.

Synthesis and crystallization

To a solution of isatin (2 g, 13.6 mmol) and malonic acid (1.4 g, 13.6 mmol) in 30 ml of acetic acid was added sodium acetate (0.11 g, 1.36 mmol). The reaction mixture was refluxed for 24 h. and after cooling, 100 ml of water–ice was added. The precipitate obtained was recrystallized from water to afford colourless crystals of the title hydrate in 90% yield.

Refinement

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

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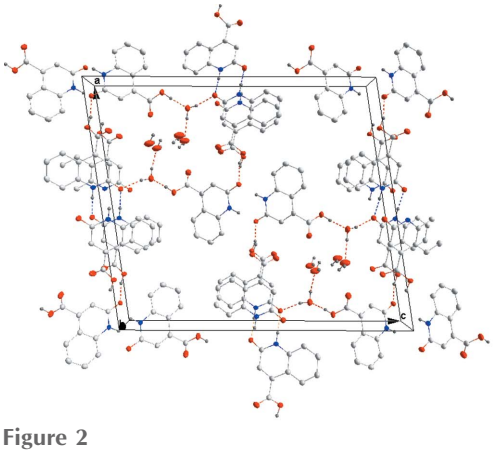

Figure 2
Packing structure viewed along the *b* axis, with O—H···O and N—H···O hydrogen bonds shown as red and blue dotted lines, respectively.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O4	0.87	1.73	2.5734 (15)	162
N1—H1···O1^{i}	0.91	1.91	2.8100 (17)	169
O6—H6*A*···O7	0.87	1.68	2.5423 (17)	172
N2—H2*B*···O4^{ii}	0.91	1.92	2.8229 (16)	171
O7—H7*A*···O1^{iii}	0.87	1.88	2.7336 (16)	165
O7—H7*B*···O8	0.87	2.01	2.841 (5)	159
O7—H7*B*···O8*A*	0.87	1.85	2.713 (4)	172

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$; (iii) $-x+\frac{1}{2}, y, -z+\frac{3}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_7NO_3·H_2O$
M_r	207.18
Crystal system, space group	Monoclinic, *P*2/*n*
Temperature (K)	150
a, *b*, *c* (Å)	20.7884 (8), 3.7215 (1), 23.8849 (9)
β (°)	98.582 (2)
V (Å^3)	1827.14 (11)
Z	8
Radiation type	Cu *K*α
μ (mm^{-1})	1.00
Crystal size (mm)	0.18 × 0.15 × 0.04
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.85, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12922, 3541, 2964
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.041, 0.110, 1.04
No. of reflections	3541
No. of parameters	281
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.25

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2016). **1**, x160997 [doi:10.1107/S2414314616009974]

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Crystal data

$C_{10}H_7NO_3·H_2O$
M_r = 207.18
Monoclinic, $P2/n$
a = 20.7884 (8) Å
b = 3.7215 (1) Å
c = 23.8849 (9) Å
β = 98.582 (2)°
V = 1827.14 (11) Å^3
Z = 8
$F(000)$ = 864
D_x = 1.506 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 8389 reflections
θ = 2.6–72.2°
μ = 1.00 mm^{-1}
T = 150 K
Plate, colourless
0.18 × 0.15 × 0.04 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*; Bruker, 2016)
T_{min} = 0.85, T_{max} = 0.96
12922 measured reflections
3541 independent reflections
2964 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 72.2°, θ_{min} = 3.1°
h = −24→20
k = −4→4
l = −29→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.110
S = 1.04
3541 reflections
281 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 0.7256P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.05828 (5)	0.4566 (3)	0.55972 (4)	0.0263 (3)	

O2	0.30022 (5)	0.0876 (3)	0.48988 (4)	0.0271 (3)	
H2	0.3400	0.0624	0.5069	0.032*	
O3	0.28157 (6)	−0.1782 (4)	0.57018 (5)	0.0341 (3)	
N1	0.06261 (6)	0.2096 (4)	0.47364 (5)	0.0203 (3)	
H1	0.0213	0.2875	0.4620	0.024*	
C1	0.09018 (7)	0.2917 (4)	0.52711 (6)	0.0208 (3)	
C2	0.15720 (7)	0.1848 (4)	0.54320 (6)	0.0216 (3)	
H2A	0.1777	0.2205	0.5811	0.026*	
C3	0.19130 (7)	0.0348 (4)	0.50521 (6)	0.0199 (3)	
C4	0.16090 (7)	−0.0446 (4)	0.44812 (6)	0.0195 (3)	
C5	0.19256 (8)	−0.2098 (4)	0.40645 (6)	0.0226 (3)	
H5	0.2373	−0.2721	0.4150	0.027*	
C6	0.15898 (8)	−0.2811 (4)	0.35347 (6)	0.0244 (3)	
H6	0.1809	−0.3876	0.3255	0.029*	
C7	0.09275 (8)	−0.1973 (4)	0.34063 (6)	0.0241 (3)	
H7	0.0699	−0.2517	0.3041	0.029*	
C8	0.06040 (8)	−0.0374 (4)	0.38018 (6)	0.0221 (3)	
H8	0.0154	0.0180	0.3713	0.027*	
C9	0.09468 (7)	0.0431 (4)	0.43393 (6)	0.0197 (3)	
C10	0.26237 (7)	−0.0371 (4)	0.52540 (6)	0.0217 (3)	
O4	0.42412 (5)	0.0548 (3)	0.52056 (4)	0.0251 (3)	
O5	0.37123 (6)	0.7177 (4)	0.69734 (5)	0.0375 (3)	
O6	0.45531 (6)	0.4850 (4)	0.75528 (5)	0.0347 (3)	
H6A	0.4327	0.5472	0.7816	0.042*	
N2	0.51852 (6)	0.2797 (4)	0.56588 (5)	0.0197 (3)	
H2B	0.5374	0.1958	0.5365	0.024*	
C11	0.45441 (7)	0.2135 (4)	0.56345 (6)	0.0203 (3)	
C12	0.42424 (7)	0.3275 (4)	0.61097 (6)	0.0221 (3)	
H12	0.3787	0.2959	0.6100	0.026*	
C13	0.46007 (8)	0.4797 (4)	0.65710 (6)	0.0209 (3)	
C14	0.52881 (7)	0.5455 (4)	0.65896 (6)	0.0197 (3)	
C15	0.56950 (8)	0.7117 (4)	0.70415 (6)	0.0231 (3)	
H15	0.5519	0.7850	0.7368	0.028*	
C16	0.63443 (8)	0.7692 (4)	0.70153 (7)	0.0260 (4)	
H16	0.6613	0.8780	0.7326	0.031*	
C17	0.66096 (8)	0.6681 (5)	0.65332 (7)	0.0254 (3)	
H17	0.7057	0.7105	0.6518	0.030*	
C18	0.62274 (8)	0.5076 (4)	0.60813 (6)	0.0226 (3)	
H18	0.6408	0.4413	0.5753	0.027*	
C19	0.55683 (7)	0.4432 (4)	0.61111 (6)	0.0196 (3)	
C20	0.42396 (8)	0.5753 (5)	0.70562 (6)	0.0245 (3)	
O7	0.39711 (6)	0.7156 (4)	0.83450 (5)	0.0389 (3)	
H7A	0.4043	0.6144	0.8677	0.058*	
H7B	0.3549	0.7252	0.8268	0.058*	
O8	0.26582 (17)	0.934 (2)	0.80246 (18)	0.0619 (19)	0.494 (12)
H8A	0.2609	1.1497	0.8152	0.093*	0.494 (12)
H8B	0.2407	0.7859	0.8173	0.093*	0.494 (12)
O8A	0.26537 (17)	0.681 (3)	0.8129 (2)	0.071 (2)	0.506 (12)

H8AA	0.2488	0.7914	0.7819	0.107*	0.506 (12)
H8AB	0.2466	0.7575	0.8408	0.107*	0.506 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0222 (6)	0.0375 (7)	0.0196 (5)	0.0065 (5)	0.0043 (4)	−0.0006 (5)
O2	0.0149 (5)	0.0434 (7)	0.0228 (5)	0.0000 (5)	0.0028 (4)	0.0026 (5)
O3	0.0236 (6)	0.0495 (8)	0.0279 (6)	0.0038 (5)	−0.0003 (5)	0.0117 (6)
N1	0.0154 (6)	0.0263 (7)	0.0192 (6)	0.0016 (5)	0.0024 (5)	0.0018 (5)
C1	0.0197 (8)	0.0250 (8)	0.0182 (7)	0.0008 (6)	0.0044 (6)	0.0030 (6)
C2	0.0193 (7)	0.0271 (8)	0.0178 (7)	−0.0001 (6)	0.0012 (5)	0.0024 (6)
C3	0.0185 (7)	0.0211 (7)	0.0195 (7)	0.0003 (6)	0.0014 (5)	0.0033 (6)
C4	0.0187 (7)	0.0204 (7)	0.0192 (7)	−0.0005 (6)	0.0025 (5)	0.0023 (6)
C5	0.0215 (8)	0.0239 (8)	0.0230 (7)	0.0014 (6)	0.0047 (6)	0.0010 (6)
C6	0.0285 (8)	0.0245 (8)	0.0209 (7)	0.0011 (6)	0.0059 (6)	−0.0002 (6)
C7	0.0286 (8)	0.0238 (8)	0.0186 (7)	−0.0021 (6)	−0.0007 (6)	0.0010 (6)
C8	0.0205 (7)	0.0240 (8)	0.0210 (7)	−0.0012 (6)	0.0002 (6)	0.0038 (6)
C9	0.0204 (7)	0.0205 (7)	0.0182 (7)	−0.0004 (6)	0.0032 (5)	0.0031 (6)
C10	0.0195 (8)	0.0256 (8)	0.0196 (7)	0.0010 (6)	0.0021 (6)	−0.0015 (6)
O4	0.0184 (5)	0.0376 (7)	0.0188 (5)	0.0002 (5)	0.0016 (4)	−0.0062 (5)
O5	0.0298 (7)	0.0586 (9)	0.0247 (6)	0.0155 (6)	0.0066 (5)	−0.0015 (6)
O6	0.0305 (7)	0.0586 (9)	0.0157 (5)	0.0077 (6)	0.0056 (5)	0.0029 (5)
N2	0.0184 (6)	0.0263 (7)	0.0150 (6)	0.0017 (5)	0.0039 (5)	−0.0008 (5)
C11	0.0196 (7)	0.0243 (8)	0.0166 (7)	0.0015 (6)	0.0017 (5)	0.0008 (6)
C12	0.0192 (7)	0.0285 (8)	0.0189 (7)	0.0024 (6)	0.0040 (6)	0.0009 (6)
C13	0.0232 (8)	0.0227 (8)	0.0169 (7)	0.0038 (6)	0.0033 (6)	0.0024 (6)
C14	0.0222 (8)	0.0192 (7)	0.0173 (7)	0.0027 (6)	0.0021 (5)	0.0020 (5)
C15	0.0281 (8)	0.0228 (8)	0.0183 (7)	0.0002 (6)	0.0031 (6)	0.0003 (6)
C16	0.0284 (9)	0.0239 (8)	0.0241 (8)	−0.0028 (6)	−0.0020 (6)	−0.0012 (6)
C17	0.0200 (8)	0.0272 (8)	0.0283 (8)	−0.0016 (6)	0.0013 (6)	0.0032 (7)
C18	0.0204 (8)	0.0257 (8)	0.0220 (7)	0.0019 (6)	0.0045 (6)	0.0012 (6)
C19	0.0213 (8)	0.0196 (7)	0.0173 (7)	0.0020 (6)	0.0014 (5)	0.0021 (6)
C20	0.0240 (8)	0.0309 (9)	0.0189 (7)	0.0007 (6)	0.0039 (6)	−0.0015 (6)
O7	0.0332 (7)	0.0630 (9)	0.0212 (6)	0.0031 (6)	0.0064 (5)	0.0029 (6)
O8	0.0327 (18)	0.080 (5)	0.075 (3)	−0.0015 (19)	0.0131 (15)	0.007 (2)
O8A	0.0355 (19)	0.098 (6)	0.080 (3)	0.009 (2)	0.0097 (17)	−0.006 (3)

Geometric parameters (Å, º)

O1—C1	1.2558 (19)	O6—H6A	0.8703
O2—C10	1.3242 (19)	N2—C11	1.348 (2)
O2—H2	0.8700	N2—C19	1.3836 (19)
O3—C10	1.2047 (19)	N2—H2B	0.9098
N1—C1	1.3545 (19)	C11—C12	1.440 (2)
N1—C9	1.3844 (19)	C12—C13	1.358 (2)
N1—H1	0.9101	C12—H12	0.9500
C1—C2	1.445 (2)	C13—C14	1.444 (2)

C2—C3	1.353 (2)	C13—C20	1.514 (2)
C2—H2A	0.9500	C14—C19	1.410 (2)
C3—C4	1.445 (2)	C14—C15	1.411 (2)
C3—C10	1.508 (2)	C15—C16	1.377 (2)
C4—C9	1.406 (2)	C15—H15	0.9500
C4—C5	1.413 (2)	C16—C17	1.400 (2)
C5—C6	1.377 (2)	C16—H16	0.9500
C5—H5	0.9500	C17—C18	1.377 (2)
C6—C7	1.400 (2)	C17—H17	0.9500
C6—H6	0.9500	C18—C19	1.403 (2)
C7—C8	1.374 (2)	C18—H18	0.9500
C7—H7	0.9500	O7—H7A	0.8700
C8—C9	1.405 (2)	O7—H7B	0.8701
C8—H8	0.9500	O8—H8A	0.8700
O4—C11	1.2661 (18)	O8—H8B	0.8702
O5—C20	1.207 (2)	O8A—H8AA	0.8699
O6—C20	1.3091 (19)	O8A—H8AB	0.8700

C10—O2—H2	106.1	C11—N2—H2B	116.2
C1—N1—C9	124.59 (13)	C19—N2—H2B	119.3
C1—N1—H1	117.5	O4—C11—N2	119.30 (14)
C9—N1—H1	117.6	O4—C11—C12	123.55 (14)
O1—C1—N1	120.45 (13)	N2—C11—C12	117.15 (13)
O1—C1—C2	123.16 (13)	C13—C12—C11	120.77 (14)
N1—C1—C2	116.37 (13)	C13—C12—H12	119.6
C3—C2—C1	121.09 (13)	C11—C12—H12	119.6
C3—C2—H2A	119.5	C12—C13—C14	121.06 (14)
C1—C2—H2A	119.5	C12—C13—C20	116.39 (14)
C2—C3—C4	121.21 (14)	C14—C13—C20	122.55 (13)
C2—C3—C10	116.44 (13)	C19—C14—C15	117.74 (14)
C4—C3—C10	122.35 (14)	C19—C14—C13	117.11 (13)
C9—C4—C5	118.25 (13)	C15—C14—C13	125.13 (14)
C9—C4—C3	117.03 (14)	C16—C15—C14	120.87 (15)
C5—C4—C3	124.70 (14)	C16—C15—H15	119.6
C6—C5—C4	120.36 (15)	C14—C15—H15	119.6
C6—C5—H5	119.8	C15—C16—C17	120.29 (14)
C4—C5—H5	119.8	C15—C16—H16	119.9
C5—C6—C7	120.38 (15)	C17—C16—H16	119.9
C5—C6—H6	119.8	C18—C17—C16	120.60 (15)
C7—C6—H6	119.8	C18—C17—H17	119.7
C8—C7—C6	120.79 (14)	C16—C17—H17	119.7
C8—C7—H7	119.6	C17—C18—C19	119.20 (15)
C6—C7—H7	119.6	C17—C18—H18	120.4
C7—C8—C9	119.15 (14)	C19—C18—H18	120.4
C7—C8—H8	120.4	N2—C19—C18	119.21 (13)
C9—C8—H8	120.4	N2—C19—C14	119.49 (14)
N1—C9—C8	119.41 (14)	C18—C19—C14	121.29 (14)
N1—C9—C4	119.54 (13)	O5—C20—O6	125.33 (15)

C8—C9—C4	121.05 (14)	O5—C20—C13	121.30 (14)
O3—C10—O2	124.87 (14)	O6—C20—C13	113.37 (14)
O3—C10—C3	122.70 (14)	H7A—O7—H7B	104.1
O2—C10—C3	112.36 (12)	H8A—O8—H8B	109.5
C20—O6—H6A	109.7	H8AA—O8A—H8AB	109.5
C11—N2—C19	124.34 (13)		

C9—N1—C1—O1	177.00 (14)	C19—N2—C11—O4	−178.38 (14)
C9—N1—C1—C2	−2.0 (2)	C19—N2—C11—C12	1.1 (2)
O1—C1—C2—C3	−174.35 (15)	O4—C11—C12—C13	176.50 (15)
N1—C1—C2—C3	4.6 (2)	N2—C11—C12—C13	−3.0 (2)
C1—C2—C3—C4	−3.9 (2)	C11—C12—C13—C14	2.6 (2)
C1—C2—C3—C10	174.98 (14)	C11—C12—C13—C20	−177.53 (14)
C2—C3—C4—C9	0.4 (2)	C12—C13—C14—C19	−0.4 (2)
C10—C3—C4—C9	−178.41 (14)	C20—C13—C14—C19	179.79 (14)
C2—C3—C4—C5	−178.18 (15)	C12—C13—C14—C15	177.96 (15)
C10—C3—C4—C5	3.0 (2)	C20—C13—C14—C15	−1.9 (2)
C9—C4—C5—C6	0.1 (2)	C19—C14—C15—C16	−0.4 (2)
C3—C4—C5—C6	178.66 (15)	C13—C14—C15—C16	−178.72 (15)
C4—C5—C6—C7	−1.3 (2)	C14—C15—C16—C17	1.0 (2)
C5—C6—C7—C8	1.1 (2)	C15—C16—C17—C18	−0.5 (2)
C6—C7—C8—C9	0.2 (2)	C16—C17—C18—C19	−0.6 (2)
C1—N1—C9—C8	178.27 (15)	C11—N2—C19—C18	−178.15 (14)
C1—N1—C9—C4	−1.4 (2)	C11—N2—C19—C14	1.1 (2)
C7—C8—C9—N1	178.94 (14)	C17—C18—C19—N2	−179.57 (14)
C7—C8—C9—C4	−1.4 (2)	C17—C18—C19—C14	1.2 (2)
C5—C4—C9—N1	−179.12 (14)	C15—C14—C19—N2	−179.93 (13)
C3—C4—C9—N1	2.2 (2)	C13—C14—C19—N2	−1.5 (2)
C5—C4—C9—C8	1.2 (2)	C15—C14—C19—C18	−0.7 (2)
C3—C4—C9—C8	−177.40 (14)	C13—C14—C19—C18	177.75 (14)
C2—C3—C10—O3	46.5 (2)	C12—C13—C20—O5	−43.5 (2)
C4—C3—C10—O3	−134.67 (17)	C14—C13—C20—O5	136.39 (18)
C2—C3—C10—O2	−130.40 (15)	C12—C13—C20—O6	135.88 (16)
C4—C3—C10—O2	48.4 (2)	C14—C13—C20—O6	−44.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O4	0.87	1.73	2.5734 (15)	162
N1—H1···O1^{i}	0.91	1.91	2.8100 (17)	169
O6—H6*A*···O7	0.87	1.68	2.5423 (17)	172
N2—H2*B*···O4^{ii}	0.91	1.92	2.8229 (16)	171
O7—H7*A*···O1^{iii}	0.87	1.88	2.7336 (16)	165
O7—H7*B*···O8	0.87	2.01	2.841 (5)	159
O7—H7*B*···O8*A*	0.87	1.85	2.713 (4)	172

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*+1/2, *y*, −*z*+3/2.