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(*E*)-*N*′-[1-(4-Hydroxyphenyl)ethylidene]-2-(quinolin-8-yloxy)acetohydrazide methanol solvate

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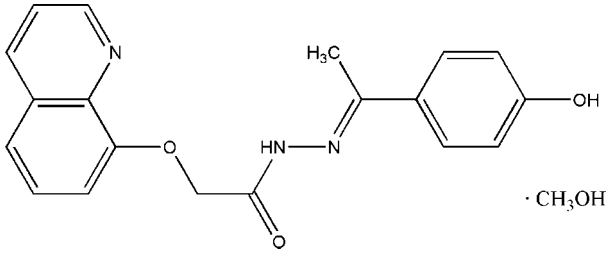
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.143; data-to-parameter ratio = 13.3.

In the title compound, $C_{19}H_{17}N_3O_3\cdot CH_4O$, the mean planes of the benzene ring and the quinoline rings make a dihedral angle of 75.5 (2)°. The acetohydrazide molecules are connected *via* pairs of intermolecular O—H···O hydrogen bonds into inversion dimers, and the methanol solvent molecule is linked to the acetohydrazide molecule *via* intermolecular N—H···O and bifurcated O—H···(N,O) hydrogen bonds.

Related literature

For background on the coordination chemistry of 8-hydroxyquinoline and its derivatives, see: Chen & Shi (1998). For related structures, see: Wen *et al.* (2005). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{19}H_{17}N_3O_3\cdot CH_4O$
M_r = 367.40
Triclinic, $P\overline{1}$
a = 9.552 (3) Å
b = 10.622 (2) Å
c = 10.665 (4) Å
α = 70.055 (5)°
β = 83.033 (4)°
γ = 65.845 (4)°
V = 927.9 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.20 × 0.18 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.986
4927 measured reflections
3261 independent reflections
2430 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.143
S = 1.08
3261 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 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
O3—H3···O2^{i}	0.82	1.85	2.647 (3)	165
O4—H4···N1	0.82	1.96	2.773 (3)	174
O4—H4···O1	0.82	2.60	3.036 (3)	115
N2—H2···O4	0.86	2.10	2.856 (3)	146

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2916).

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supporting information

Acta Cryst. (2009). E**65**, o651 [doi:10.1107/S1600536809006461]

(*E*)-*N*′-[1-(4-Hydroxyphenyl)ethylidene]-2-(quinolin-8-yloxy)acetohydrazide methanol solvate

Jun Tan

S1. Comment

8-Hydroxyquinoline and its derivatives constitute well known ligands in coordination chemistry (Chen & Shi, 1998). In our search for new extractants of metal ions and biologically active materials, the title compound, (I), has been synthesized. We report here its crystal structure. All bond lengths and angles are normal (Allen *et al.*, 1987), and are comparable to those in the related compound *N*′-(2-Fluorobenzylidene) -2-(quinolin-8-yloxy)-acetohydrazide methanol solvate (Wen *et al.*, 2005). The mean planes of the benzene ring and the quinoline rings make a dihedral angle of 75.5 (2)°. In the crystal structure, the methanol molecule is linked to the $C_{19}H_{17}N_3O_3$ molecule *via* intermolecular O—H···O, N—H···O and O—H···N hydrogen bonds (Fig. 1), intermolecular O—H···O hydrogen bonds (Table 1) link the molecules into centrosymmetric dimers (Fig. 2).

S2. Experimental

2-(Quinolin-8-yloxy)acetohydrazide (2.18 g, 10 mmol), 1-(4-hydroxyphenyl)ethanone (1.36 g, 10 mmol), ethanol (40 ml) and some drops of acetic acid were added to a 100 ml flask, and refluxed for 3 h. After cooling to room temperature, the mixture was filtered. Pale yellow blocks of (I) were obtained by slow evaporation of a acetone-methanol (1:2, *v*/*v*) solution over a period of 3 d. Analysis calculated for $C_{20}H_{21}N_3O_4$: C 65.38, H 5.76, N 11.43%; found: C 65.76, H 5.47, N 11.67%.

S3. Refinement

All H atoms were initially located in a difference Fourier map. The methylene H atoms were constrained to an ideal geometry, with C—H = 0.93 Å for aryl, 0.97 Å for the methylene, and 0.96 Å for the methyl H atoms, O—H = 0.82 Å and N—H = 0.86 Å. U_{iso}(H) = 1.2U_{eq}(C,*N*), or 1.5U_{eq}(C) for the methyl groups, and 1.5U_{eq}(O).

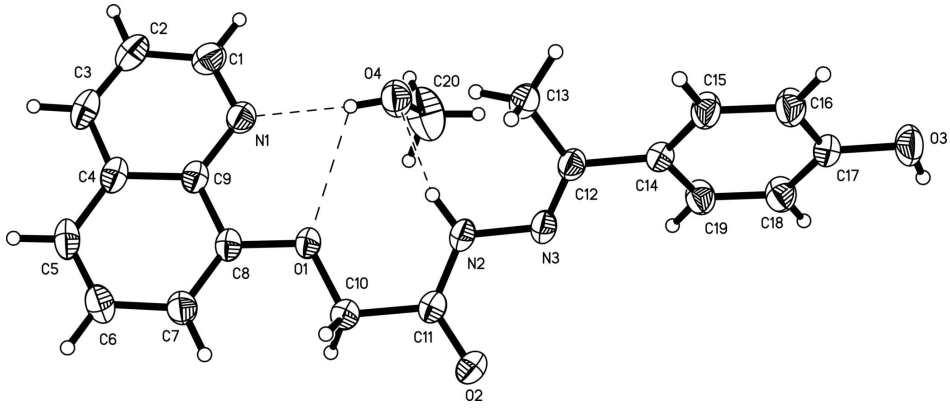

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. The dashed lines indicate hydrogen bonds.

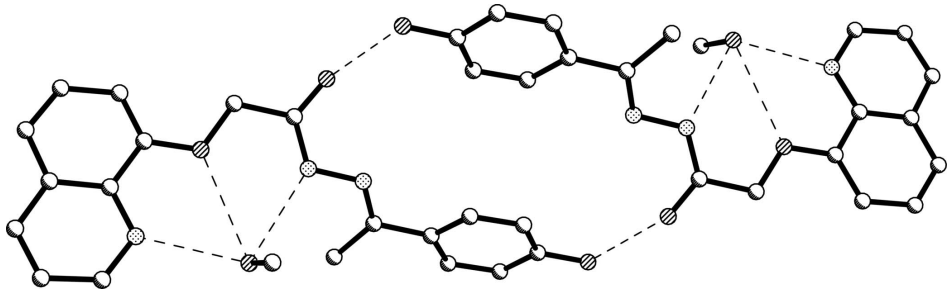

Figure 2

The structure of the dimers formed *via* hydrogen bonds, H atoms have been omitted for clarity. The dashed lines indicate hydrogen bonds.

(*E*)-*N*′-[1-(4-Hydroxyphenyl)ethylidene]-2-(quinolin-8- yloxy)acetohydrazide methanol solvate

Crystal data

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$\beta = 83.033\ (4)°$
$\gamma = 65.845\ (4)°$
$V = 927.9\ (5)$ Å^3
$Z = 2$
$F(000) = 388$
$D_x = 1.315$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1866 reflections
$\theta = 2.5–26.5°$
$\mu = 0.09$ mm^{-1}
$T = 295$ K
Block, light yellow
0.20 × 0.18 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.982$, $T_{max} = 0.986$
4927 measured reflections
3261 independent reflections
2430 reflections with $I > 2\sigma(I)$

R_{int} = 0.021
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −11→8
k = −12→7
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.143
S = 1.08
3261 reflections
246 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.5262P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	0.32959 (17)	0.65533 (18)	0.12916 (16)	0.0512 (4)
O2	0.0115 (2)	0.8800 (2)	−0.09376 (17)	0.0620 (5)
O3	−0.83771 (19)	1.1439 (3)	0.2526 (2)	0.0726 (6)
H3	−0.8762	1.1285	0.1977	0.109*
O4	0.1513 (2)	0.5644 (2)	0.3745 (2)	0.0666 (5)
H4	0.2444	0.5347	0.3643	0.100*
N1	0.4677 (2)	0.4420 (2)	0.3533 (2)	0.0523 (5)
N2	0.0236 (2)	0.7950 (2)	0.1324 (2)	0.0516 (5)
H2	0.0807	0.7494	0.2034	0.062*
N3	−0.1361 (2)	0.8523 (2)	0.1406 (2)	0.0509 (5)
C1	0.5370 (3)	0.3362 (3)	0.4623 (3)	0.0624 (7)
H1	0.4761	0.3085	0.5321	0.075*
C2	0.6963 (3)	0.2631 (3)	0.4795 (3)	0.0694 (8)
H2A	0.7393	0.1882	0.5581	0.083*
C3	0.7866 (3)	0.3033 (3)	0.3797 (3)	0.0672 (8)
H3A	0.8928	0.2558	0.3895	0.081*
C4	0.7203 (3)	0.4173 (3)	0.2607 (3)	0.0528 (6)
C5	0.8077 (3)	0.4653 (3)	0.1532 (3)	0.0638 (8)
H5	0.9143	0.4225	0.1589	0.077*
C6	0.7356 (3)	0.5740 (3)	0.0418 (3)	0.0646 (8)
H6	0.7940	0.6059	−0.0282	0.078*
C7	0.5749 (3)	0.6397 (3)	0.0292 (3)	0.0540 (6)

H7	0.5283	0.7127	−0.0493	0.065*
C8	0.4869 (3)	0.5969 (3)	0.1319 (2)	0.0451 (6)
C9	0.5576 (3)	0.4842 (3)	0.2515 (2)	0.0449 (6)
C10	0.2571 (3)	0.7563 (3)	0.0056 (2)	0.0486 (6)
H10A	0.2909	0.7093	−0.0627	0.058*
H10B	0.2884	0.8376	−0.0199	0.058*
C11	0.0854 (3)	0.8127 (3)	0.0119 (2)	0.0455 (6)
C12	−0.1908 (3)	0.8900 (3)	0.2445 (2)	0.0463 (6)
C13	−0.0992 (3)	0.8864 (3)	0.3513 (3)	0.0587 (7)
H13A	−0.0081	0.7983	0.3722	0.088*
H13B	−0.1597	0.8897	0.4298	0.088*
H13C	−0.0712	0.9689	0.3203	0.088*
C14	−0.3614 (3)	0.9510 (3)	0.2510 (2)	0.0447 (6)
C15	−0.4388 (3)	1.0446 (3)	0.3227 (3)	0.0577 (7)
H15	−0.3831	1.0654	0.3729	0.069*
C16	−0.5971 (3)	1.1082 (3)	0.3218 (3)	0.0640 (8)
H16	−0.6464	1.1716	0.3705	0.077*
C17	−0.6820 (3)	1.0784 (3)	0.2495 (2)	0.0508 (6)
C18	−0.6079 (3)	0.9839 (3)	0.1787 (3)	0.0578 (7)
H18	−0.6644	0.9622	0.1300	0.069*
C19	−0.4494 (3)	0.9211 (3)	0.1796 (3)	0.0554 (7)
H19	−0.4006	0.8573	0.1313	0.067*
C20	0.0957 (4)	0.4729 (4)	0.3498 (5)	0.1075 (14)
H20A	0.1292	0.3811	0.4202	0.161*
H20B	0.1338	0.4576	0.2664	0.161*
H20C	−0.0144	0.5168	0.3456	0.161*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0323 (9)	0.0558 (10)	0.0498 (10)	−0.0091 (7)	−0.0026 (7)	−0.0074 (8)
O2	0.0498 (11)	0.0737 (13)	0.0533 (11)	−0.0199 (9)	−0.0132 (9)	−0.0100 (9)
O3	0.0358 (10)	0.0972 (16)	0.0839 (15)	−0.0128 (10)	−0.0033 (9)	−0.0429 (12)
O4	0.0499 (11)	0.0642 (12)	0.0743 (13)	−0.0161 (10)	0.0034 (10)	−0.0174 (10)
N1	0.0471 (12)	0.0523 (12)	0.0533 (12)	−0.0163 (10)	−0.0040 (10)	−0.0142 (10)
N2	0.0341 (11)	0.0552 (13)	0.0525 (13)	−0.0051 (9)	−0.0079 (9)	−0.0144 (10)
N3	0.0346 (11)	0.0521 (12)	0.0560 (13)	−0.0064 (9)	−0.0049 (9)	−0.0166 (10)
C1	0.0664 (18)	0.0619 (17)	0.0547 (16)	−0.0257 (15)	−0.0087 (13)	−0.0096 (14)
C2	0.0640 (19)	0.0627 (18)	0.0703 (19)	−0.0161 (15)	−0.0258 (16)	−0.0099 (15)
C3	0.0456 (16)	0.0624 (18)	0.085 (2)	−0.0084 (13)	−0.0224 (15)	−0.0211 (16)
C4	0.0409 (14)	0.0533 (15)	0.0679 (17)	−0.0133 (12)	−0.0092 (12)	−0.0268 (13)
C5	0.0331 (13)	0.0740 (19)	0.086 (2)	−0.0173 (13)	0.0023 (14)	−0.0330 (17)
C6	0.0447 (15)	0.0720 (19)	0.077 (2)	−0.0245 (14)	0.0125 (14)	−0.0252 (16)
C7	0.0457 (14)	0.0550 (15)	0.0571 (16)	−0.0182 (12)	0.0020 (12)	−0.0152 (12)
C8	0.0355 (12)	0.0448 (13)	0.0546 (14)	−0.0122 (10)	−0.0009 (11)	−0.0194 (11)
C9	0.0383 (13)	0.0446 (13)	0.0544 (15)	−0.0132 (11)	−0.0038 (11)	−0.0211 (11)
C10	0.0424 (13)	0.0505 (14)	0.0477 (14)	−0.0162 (11)	−0.0022 (11)	−0.0114 (11)
C11	0.0408 (13)	0.0409 (13)	0.0514 (14)	−0.0118 (10)	−0.0062 (11)	−0.0134 (11)

C12	0.0388 (13)	0.0423 (13)	0.0495 (14)	−0.0100 (10)	−0.0044 (11)	−0.0104 (11)
C13	0.0438 (14)	0.0680 (18)	0.0578 (16)	−0.0124 (13)	−0.0077 (12)	−0.0215 (14)
C14	0.0385 (12)	0.0462 (13)	0.0431 (13)	−0.0127 (10)	−0.0031 (10)	−0.0103 (11)
C15	0.0410 (14)	0.0717 (18)	0.0655 (17)	−0.0133 (13)	−0.0071 (12)	−0.0362 (15)
C16	0.0456 (15)	0.0753 (19)	0.0713 (18)	−0.0074 (13)	−0.0030 (13)	−0.0427 (16)
C17	0.0358 (13)	0.0590 (16)	0.0503 (14)	−0.0131 (11)	−0.0026 (11)	−0.0147 (12)
C18	0.0463 (15)	0.0756 (19)	0.0649 (17)	−0.0263 (14)	−0.0011 (12)	−0.0349 (15)
C19	0.0450 (15)	0.0657 (17)	0.0630 (16)	−0.0187 (13)	0.0031 (12)	−0.0341 (14)
C20	0.088 (3)	0.082 (3)	0.168 (4)	−0.045 (2)	0.025 (3)	−0.052 (3)

Geometric parameters (Å, º)

O1—C8	1.371 (3)	C7—C8	1.364 (3)
O1—C10	1.420 (3)	C7—H7	0.9300
O2—C11	1.229 (3)	C8—C9	1.423 (3)
O3—C17	1.361 (3)	C10—C11	1.501 (3)
O3—H3	0.8200	C10—H10A	0.9700
O4—C20	1.389 (4)	C10—H10B	0.9700
O4—H4	0.8200	C12—C14	1.490 (3)
N1—C1	1.319 (3)	C12—C13	1.501 (3)
N1—C9	1.369 (3)	C13—H13A	0.9600
N2—C11	1.333 (3)	C13—H13B	0.9600
N2—N3	1.396 (3)	C13—H13C	0.9600
N2—H2	0.8600	C14—C15	1.379 (3)
N3—C12	1.286 (3)	C14—C19	1.387 (3)
C1—C2	1.399 (4)	C15—C16	1.380 (4)
C1—H1	0.9300	C15—H15	0.9300
C2—C3	1.352 (4)	C16—C17	1.372 (4)
C2—H2A	0.9300	C16—H16	0.9300
C3—C4	1.413 (4)	C17—C18	1.372 (4)
C3—H3A	0.9300	C18—C19	1.382 (4)
C4—C5	1.410 (4)	C18—H18	0.9300
C4—C9	1.420 (3)	C19—H19	0.9300
C5—C6	1.353 (4)	C20—H20A	0.9600
C5—H5	0.9300	C20—H20B	0.9600
C6—C7	1.404 (4)	C20—H20C	0.9600
C6—H6	0.9300		
C8—O1—C10	116.27 (18)	C11—C10—H10B	109.1
C17—O3—H3	109.5	H10A—C10—H10B	107.9
C20—O4—H4	109.5	O2—C11—N2	124.5 (2)
C1—N1—C9	117.8 (2)	O2—C11—C10	117.8 (2)
C11—N2—N3	118.39 (19)	N2—C11—C10	117.4 (2)
C11—N2—H2	120.8	N3—C12—C14	115.1 (2)
N3—N2—H2	120.8	N3—C12—C13	125.8 (2)
C12—N3—N2	116.1 (2)	C14—C12—C13	118.9 (2)
N1—C1—C2	124.1 (3)	C12—C13—H13A	109.5
N1—C1—H1	117.9	C12—C13—H13B	109.5

C2—C1—H1	117.9	H13A—C13—H13B	109.5
C3—C2—C1	118.7 (3)	C12—C13—H13C	109.5
C3—C2—H2A	120.6	H13A—C13—H13C	109.5
C1—C2—H2A	120.6	H13B—C13—H13C	109.5
C2—C3—C4	120.3 (3)	C15—C14—C19	117.1 (2)
C2—C3—H3A	119.9	C15—C14—C12	121.7 (2)
C4—C3—H3A	119.9	C19—C14—C12	121.1 (2)
C5—C4—C3	123.2 (2)	C14—C15—C16	121.5 (2)
C5—C4—C9	119.7 (2)	C14—C15—H15	119.2
C3—C4—C9	117.1 (3)	C16—C15—H15	119.2
C6—C5—C4	119.7 (2)	C17—C16—C15	120.4 (2)
C6—C5—H5	120.2	C17—C16—H16	119.8
C4—C5—H5	120.2	C15—C16—H16	119.8
C5—C6—C7	121.7 (3)	O3—C17—C18	122.9 (2)
C5—C6—H6	119.2	O3—C17—C16	117.8 (2)
C7—C6—H6	119.2	C18—C17—C16	119.3 (2)
C8—C7—C6	120.2 (3)	C17—C18—C19	120.0 (2)
C8—C7—H7	119.9	C17—C18—H18	120.0
C6—C7—H7	119.9	C19—C18—H18	120.0
C7—C8—O1	124.3 (2)	C18—C19—C14	121.6 (2)
C7—C8—C9	120.1 (2)	C18—C19—H19	119.2
O1—C8—C9	115.5 (2)	C14—C19—H19	119.2
N1—C9—C4	122.0 (2)	O4—C20—H20A	109.5
N1—C9—C8	119.4 (2)	O4—C20—H20B	109.5
C4—C9—C8	118.6 (2)	H20A—C20—H20B	109.5
O1—C10—C11	112.4 (2)	O4—C20—H20C	109.5
O1—C10—H10A	109.1	H20A—C20—H20C	109.5
C11—C10—H10A	109.1	H20B—C20—H20C	109.5
O1—C10—H10B	109.1		

C11—N2—N3—C12	−151.2 (2)	O1—C8—C9—C4	179.2 (2)
C9—N1—C1—C2	−1.0 (4)	C8—O1—C10—C11	179.3 (2)
N1—C1—C2—C3	0.9 (5)	N3—N2—C11—O2	2.2 (4)
C1—C2—C3—C4	0.0 (5)	N3—N2—C11—C10	177.3 (2)
C2—C3—C4—C5	179.6 (3)	O1—C10—C11—O2	−167.4 (2)
C2—C3—C4—C9	−0.7 (4)	O1—C10—C11—N2	17.2 (3)
C3—C4—C5—C6	179.2 (3)	N2—N3—C12—C14	179.9 (2)
C9—C4—C5—C6	−0.5 (4)	N2—N3—C12—C13	4.1 (4)
C4—C5—C6—C7	−0.8 (4)	N3—C12—C14—C15	−154.8 (3)
C5—C6—C7—C8	1.5 (4)	C13—C12—C14—C15	21.3 (4)
C6—C7—C8—O1	179.5 (2)	N3—C12—C14—C19	22.1 (3)
C6—C7—C8—C9	−0.7 (4)	C13—C12—C14—C19	−161.8 (2)
C10—O1—C8—C7	6.5 (3)	C19—C14—C15—C16	−1.2 (4)
C10—O1—C8—C9	−173.2 (2)	C12—C14—C15—C16	175.9 (3)
C1—N1—C9—C4	0.2 (4)	C14—C15—C16—C17	0.5 (5)
C1—N1—C9—C8	179.3 (2)	C15—C16—C17—O3	179.8 (3)
C5—C4—C9—N1	−179.7 (2)	C15—C16—C17—C18	0.4 (4)
C3—C4—C9—N1	0.6 (4)	O3—C17—C18—C19	180.0 (3)

C5—C4—C9—C8	1.2 (4)	C16—C17—C18—C19	−0.7 (4)
C3—C4—C9—C8	−178.5 (2)	C17—C18—C19—C14	0.0 (4)
C7—C8—C9—N1	−179.7 (2)	C15—C14—C19—C18	0.9 (4)
O1—C8—C9—N1	0.1 (3)	C12—C14—C19—C18	−176.1 (2)
C7—C8—C9—C4	−0.6 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2^{i}	0.82	1.85	2.647 (3)	165
O4—H4···N1	0.82	1.96	2.773 (3)	174
O4—H4···O1	0.82	2.60	3.036 (3)	115
N2—H2···O4	0.86	2.10	2.856 (3)	146

Symmetry code: (i) −*x*−1, −*y*+2, −*z*.