Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-*N*′-(4-Bromobenzylidene)-2-(8-quinolyloxy)acetohydrazide monohydrate

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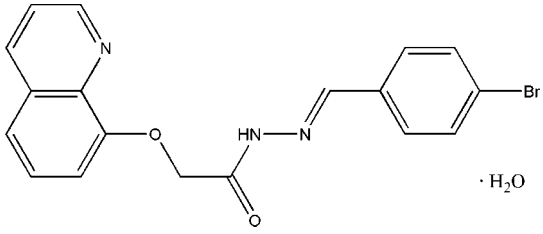
Received 22 May 2009; accepted 28 May 2009

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.011 Å; R factor = 0.070; wR factor = 0.178; data-to-parameter ratio = 13.2.

In the title compound, $C_{18}H_{14}BrN_3O_2\cdot H_2O$, the dihedral angle between the mean planes of the benzene ring and the quinoline ring system is 34.2 (3)°. In the crystal, the constituents are linked into chains by O—H···O, N—H···O and O—H···N hydrogen bonds.

Related literature

For a related structure, see: Tan (2009). For background to the coordination chemistry of 8-hydroxyquinoline and its derivatives, see: Chen & Shi (1998); Mona & Wageih (2002). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{14}BrN_3O_2\cdot H_2O$
M_r = 402.25
Monoclinic, $C2/c$
a = 21.95 (2) Å
b = 11.841 (8) Å
c = 13.057 (9) Å
β = 93.70 (2)°
V = 3387 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.45 mm^{-1}
T = 295 K
0.20 × 0.18 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
T_{min} = 0.640, T_{max} = 0.710
8378 measured reflections
2988 independent reflections
1334 reflections with $I > 2\sigma(I)$
R_{int} = 0.141

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.178
S = 1.04
2988 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3	0.86	2.04	2.860 (8)	160
O3—H19···N1	0.85	1.97	2.806 (8)	170
O3—H20···O2^{i}	0.85	2.11	2.783 (7)	136

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

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*.

This project was supported by the Natural Science Foundation of Zhejiang Province for Distinguished Young Students (No. 2008R40G2190024) and the Scientific Research Fund of the Zhejiang Provincial Education Department (No. Y200803569).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2981).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Chen, C. H. & Shi, J. M. (1998). *Coord. Chem. Rev.* **171**, 161—174.
Mona, M. M. & Wageih, G. H. (2002). *J. Coord. Chem.* **55**, 439–457.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART*, *SAINT* and *SADABS*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Tan, J. (2009). *Acta Cryst.* E**65**, o651.

supporting information

Acta Cryst. (2009). E**65**, o1474 [doi:10.1107/S1600536809020418]

(*E*)-*N*′-(4-Bromobenzylidene)-2-(8-quinolyloxy)acetohydrazide monohydrate

Jun Tan

S1. Comment

8-Hydroxyquinoline and its derivatives constitute well known ligands in coordination chemistry (Chen & Shi, 1998; Mona & Wageih, 2002). 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 (*E*)-*N*′-[1-(4-Hydroxyphenyl)ethylidene]-2-(quinolin-8- yloxy)acetohydrazide methanol solvate (Tan, 2009). The mean planes of the benzene ring and the quinoline rings make a dihedral angle of 34.2 (3)°. In the crystal structure, the $C_{18}H_{14}BrN_3O_2$ molecules and the water molecules are linked into chains by O—H···O, N—H···O and O—H···N hydrogen bonds.

S2. Experimental

2-(quinolin-8-yloxy)acetohydrazide (2.18 g, 10 mmol), 4-bromobenzaldehyde (1.85 g, 10 mmol), ethanol (40 ml) and some drops of acetic acid were added to a 100 ml flask, and refluxed for 5 h. After cooling to room temperature, the mixture was filtered. Colourless blocks of (I) were obtained by slow evaporation of a acetone-methanol (1:2, *v*/*v*) solution over a period of 3 d.

S3. Refinement

The H atoms were initially located in a difference Fourier map, then relocated in idealised positions (C—H = 0.93–0.97Å O—H = 0.85 Å and N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C,*N*) or 1.5U_{eq}(O).

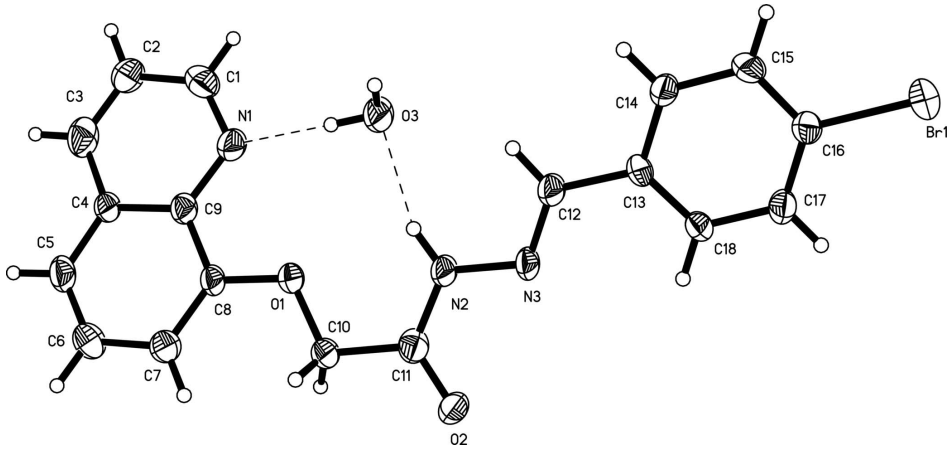


Figure 1

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

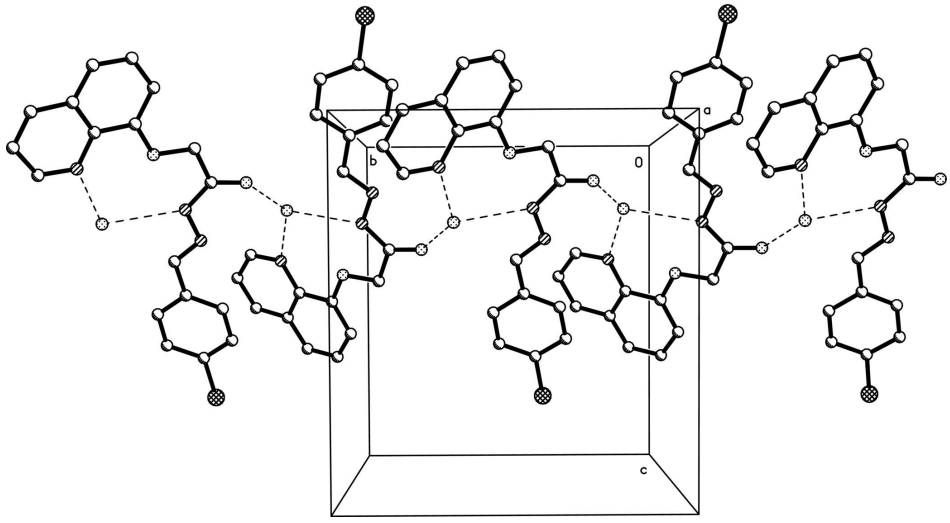


Figure 2

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

(*E*)-*N*′-(4-Bromobenzylidene)-2-(8-quinolyloxy)acetohydrazide monohydrate

Crystal data

$C_{18}H_{14}BrN_3O_2·H_2O$
M_r = 402.25
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 21.95 (2) Å
b = 11.841 (8) Å
c = 13.057 (9) Å
β = 93.70 (2)°
V = 3387 (4) Å^3
Z = 8
F(000) = 1632
D_x = 1.578 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1037 reflections
θ = 2.5–19.7°
μ = 2.45 mm^{-1}
T = 295 K
Block, colourless
0.20 × 0.18 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
T_{min} = 0.640, T_{max} = 0.710
8378 measured reflections
2988 independent reflections
1334 reflections with $I > 2\sigma(I)$
R_{int} = 0.141
θ_{max} = 25.1°, θ_{min} = 2.0°
h = −15→26
k = −14→13
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.178
S = 1.04
2988 reflections
227 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

$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 0.013P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.75$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0009 (2)

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}
Br1	0.90959 (4)	−0.09454 (8)	−0.24581 (7)	0.0744 (4)
O1	0.6370 (2)	0.0076 (4)	0.4059 (4)	0.0572 (15)
O2	0.7206 (2)	−0.2340 (5)	0.3387 (4)	0.0720 (18)
O3	0.6745 (2)	0.1677 (4)	0.2304 (4)	0.0709 (17)
H19	0.6501	0.1798	0.2773	0.106*
H20	0.7041	0.2133	0.2416	0.106*
N1	0.5826 (3)	0.2041 (6)	0.3665 (5)	0.0569 (18)
N2	0.7139 (2)	−0.0597 (5)	0.2679 (5)	0.0512 (17)
H2	0.7015	0.0089	0.2724	0.061*
N3	0.7481 (2)	−0.0944 (5)	0.1878 (4)	0.0498 (16)
C1	0.5556 (4)	0.3013 (8)	0.3491 (7)	0.071 (2)
H1	0.5638	0.3395	0.2893	0.085*
C2	0.5152 (4)	0.3521 (7)	0.4142 (7)	0.071 (3)
H2A	0.4977	0.4219	0.3980	0.085*
C3	0.5024 (3)	0.2977 (8)	0.5002 (7)	0.069 (3)
H3	0.4749	0.3292	0.5432	0.083*
C4	0.5300 (3)	0.1940 (6)	0.5264 (6)	0.0469 (19)
C5	0.5217 (4)	0.1349 (7)	0.6158 (6)	0.060 (2)
H5	0.4951	0.1631	0.6621	0.072*
C6	0.5512 (4)	0.0379 (8)	0.6369 (7)	0.067 (2)
H6	0.5448	0.0005	0.6979	0.081*
C7	0.5913 (3)	−0.0086 (7)	0.5699 (6)	0.060 (2)
H7	0.6115	−0.0760	0.5860	0.072*
C8	0.6007 (3)	0.0465 (6)	0.4799 (6)	0.0462 (19)
C9	0.5708 (3)	0.1502 (6)	0.4560 (6)	0.0459 (19)
C10	0.6614 (3)	−0.1020 (6)	0.4229 (6)	0.054 (2)
H10A	0.6283	−0.1556	0.4271	0.065*
H10B	0.6855	−0.1032	0.4879	0.065*
C11	0.7011 (3)	−0.1375 (7)	0.3383 (6)	0.053 (2)
C12	0.7666 (3)	−0.0121 (7)	0.1327 (6)	0.050 (2)
H12	0.7585	0.0621	0.1509	0.060*

C13	0.8002 (3)	−0.0349 (7)	0.0416 (5)	0.0441 (19)
C14	0.8235 (3)	0.0555 (6)	−0.0099 (6)	0.051 (2)
H14	0.8178	0.1285	0.0139	0.061*
C15	0.8551 (3)	0.0384 (7)	−0.0965 (6)	0.058 (2)
H15	0.8714	0.0993	−0.1304	0.069*
C16	0.8623 (3)	−0.0703 (7)	−0.1320 (6)	0.050 (2)
C17	0.8391 (3)	−0.1611 (7)	−0.0827 (6)	0.050 (2)
H17	0.8437	−0.2340	−0.1073	0.060*
C18	0.8085 (3)	−0.1412 (6)	0.0047 (5)	0.0459 (19)
H18	0.7932	−0.2023	0.0397	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0833 (7)	0.0776 (7)	0.0666 (6)	0.0062 (5)	0.0376 (5)	0.0007 (6)
O1	0.075 (4)	0.046 (3)	0.055 (3)	0.009 (3)	0.036 (3)	0.003 (3)
O2	0.096 (4)	0.037 (3)	0.089 (5)	0.008 (3)	0.056 (4)	0.004 (3)
O3	0.078 (4)	0.055 (4)	0.086 (4)	−0.008 (3)	0.050 (3)	−0.008 (3)
N1	0.060 (4)	0.048 (4)	0.066 (5)	0.004 (3)	0.025 (4)	−0.004 (4)
N2	0.053 (4)	0.041 (4)	0.063 (4)	0.001 (3)	0.033 (3)	−0.002 (3)
N3	0.053 (4)	0.045 (4)	0.055 (4)	−0.001 (3)	0.031 (3)	−0.007 (4)
C1	0.081 (6)	0.069 (7)	0.066 (6)	0.005 (5)	0.027 (5)	0.015 (5)
C2	0.076 (6)	0.059 (6)	0.080 (7)	0.027 (5)	0.023 (5)	0.004 (5)
C3	0.056 (6)	0.077 (7)	0.077 (7)	0.004 (5)	0.027 (5)	−0.014 (6)
C4	0.047 (5)	0.046 (5)	0.050 (5)	−0.001 (4)	0.024 (4)	−0.002 (4)
C5	0.069 (6)	0.064 (6)	0.051 (5)	−0.005 (5)	0.028 (4)	−0.011 (5)
C6	0.069 (6)	0.071 (7)	0.066 (6)	−0.004 (5)	0.037 (5)	0.007 (5)
C7	0.063 (5)	0.053 (5)	0.068 (6)	0.003 (4)	0.036 (5)	0.005 (5)
C8	0.053 (5)	0.044 (5)	0.045 (5)	−0.003 (4)	0.024 (4)	−0.004 (4)
C9	0.045 (5)	0.046 (5)	0.049 (5)	−0.003 (4)	0.016 (4)	−0.004 (4)
C10	0.064 (5)	0.044 (5)	0.058 (5)	−0.001 (4)	0.033 (4)	0.003 (4)
C11	0.053 (5)	0.046 (5)	0.062 (5)	−0.012 (4)	0.021 (4)	−0.008 (5)
C12	0.049 (5)	0.044 (5)	0.061 (5)	0.001 (4)	0.025 (4)	−0.004 (4)
C13	0.038 (4)	0.050 (5)	0.047 (5)	0.000 (4)	0.019 (4)	0.003 (4)
C14	0.052 (5)	0.040 (5)	0.063 (5)	0.002 (4)	0.023 (4)	−0.006 (4)
C15	0.055 (5)	0.049 (5)	0.072 (6)	0.000 (4)	0.027 (4)	0.015 (5)
C16	0.044 (4)	0.052 (6)	0.058 (5)	0.008 (4)	0.016 (4)	0.007 (4)
C17	0.054 (5)	0.049 (5)	0.047 (5)	0.003 (4)	0.013 (4)	−0.009 (4)
C18	0.053 (5)	0.041 (5)	0.045 (5)	−0.005 (4)	0.019 (4)	0.001 (4)

Geometric parameters (Å, º)

Br1—C16	1.889 (7)	C5—H5	0.9300
O1—C8	1.371 (7)	C6—C7	1.394 (9)
O1—C10	1.417 (8)	C6—H6	0.9300
O2—C11	1.220 (8)	C7—C8	1.371 (10)
O3—H19	0.8500	C7—H7	0.9300
O3—H20	0.8500	C8—C9	1.417 (10)

N1—C1	1.309 (9)	C10—C11	1.509 (9)
N1—C9	1.370 (9)	C10—H10A	0.9700
N2—C11	1.344 (9)	C10—H10B	0.9700
N2—N3	1.389 (7)	C12—C13	1.464 (9)
N2—H2	0.8600	C12—H12	0.9300
N3—C12	1.292 (8)	C13—C18	1.364 (9)
C1—C2	1.402 (11)	C13—C14	1.381 (9)
C1—H1	0.9300	C14—C15	1.379 (9)
C2—C3	1.341 (11)	C14—H14	0.9300
C2—H2A	0.9300	C15—C16	1.380 (10)
C3—C4	1.402 (10)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.368 (10)
C4—C5	1.383 (10)	C17—C18	1.380 (9)
C4—C9	1.422 (9)	C17—H17	0.9300
C5—C6	1.338 (10)	C18—H18	0.9300

C8—O1—C10	115.4 (5)	N1—C9—C4	122.9 (7)
H19—O3—H20	106.1	C8—C9—C4	118.3 (7)
C1—N1—C9	116.7 (7)	O1—C10—C11	111.8 (6)
C11—N2—N3	117.4 (6)	O1—C10—H10A	109.3
C11—N2—H2	121.3	C11—C10—H10A	109.3
N3—N2—H2	121.3	O1—C10—H10B	109.3
C12—N3—N2	113.6 (6)	C11—C10—H10B	109.3
N1—C1—C2	124.7 (8)	H10A—C10—H10B	107.9
N1—C1—H1	117.7	O2—C11—N2	123.8 (7)
C2—C1—H1	117.7	O2—C11—C10	118.4 (7)
C3—C2—C1	118.5 (8)	N2—C11—C10	117.8 (7)
C3—C2—H2A	120.8	N3—C12—C13	120.4 (7)
C1—C2—H2A	120.8	N3—C12—H12	119.8
C2—C3—C4	121.0 (8)	C13—C12—H12	119.8
C2—C3—H3	119.5	C18—C13—C14	118.7 (6)
C4—C3—H3	119.5	C18—C13—C12	122.9 (7)
C5—C4—C3	124.8 (7)	C14—C13—C12	118.3 (7)
C5—C4—C9	119.0 (7)	C15—C14—C13	120.5 (7)
C3—C4—C9	116.2 (7)	C15—C14—H14	119.7
C6—C5—C4	121.3 (7)	C13—C14—H14	119.7
C6—C5—H5	119.3	C14—C15—C16	119.1 (7)
C4—C5—H5	119.3	C14—C15—H15	120.4
C5—C6—C7	121.7 (8)	C16—C15—H15	120.4
C5—C6—H6	119.1	C17—C16—C15	121.4 (7)
C7—C6—H6	119.1	C17—C16—Br1	119.4 (6)
C8—C7—C6	119.1 (7)	C15—C16—Br1	119.1 (6)
C8—C7—H7	120.5	C16—C17—C18	118.1 (7)
C6—C7—H7	120.5	C16—C17—H17	121.0
C7—C8—O1	124.8 (7)	C18—C17—H17	121.0
C7—C8—C9	120.6 (7)	C13—C18—C17	122.2 (7)
O1—C8—C9	114.7 (6)	C13—C18—H18	118.9
N1—C9—C8	118.7 (6)	C17—C18—H18	118.9

C11—N2—N3—C12	−169.8 (7)	C3—C4—C9—N1	−0.8 (11)
C9—N1—C1—C2	−1.2 (13)	C5—C4—C9—C8	0.8 (11)
N1—C1—C2—C3	−0.6 (14)	C3—C4—C9—C8	178.9 (7)
C1—C2—C3—C4	1.8 (14)	C8—O1—C10—C11	−179.5 (6)
C2—C3—C4—C5	176.9 (8)	N3—N2—C11—O2	4.4 (12)
C2—C3—C4—C9	−1.1 (12)	N3—N2—C11—C10	−177.2 (6)
C3—C4—C5—C6	−177.9 (8)	O1—C10—C11—O2	−173.5 (7)
C9—C4—C5—C6	0.1 (12)	O1—C10—C11—N2	7.9 (10)
C4—C5—C6—C7	−0.4 (13)	N2—N3—C12—C13	−176.4 (6)
C5—C6—C7—C8	−0.1 (13)	N3—C12—C13—C18	6.5 (11)
C6—C7—C8—O1	−177.3 (7)	N3—C12—C13—C14	−174.6 (7)
C6—C7—C8—C9	1.0 (12)	C18—C13—C14—C15	−0.6 (11)
C10—O1—C8—C7	5.5 (11)	C12—C13—C14—C15	−179.6 (7)
C10—O1—C8—C9	−172.9 (6)	C13—C14—C15—C16	1.1 (12)
C1—N1—C9—C8	−177.8 (7)	C14—C15—C16—C17	−0.5 (11)
C1—N1—C9—C4	1.9 (11)	C14—C15—C16—Br1	−176.4 (6)
C7—C8—C9—N1	178.3 (7)	C15—C16—C17—C18	−0.6 (11)
O1—C8—C9—N1	−3.2 (10)	Br1—C16—C17—C18	175.3 (5)
C7—C8—C9—C4	−1.4 (11)	C14—C13—C18—C17	−0.6 (11)
O1—C8—C9—C4	177.1 (7)	C12—C13—C18—C17	178.4 (7)
C5—C4—C9—N1	−178.9 (7)	C16—C17—C18—C13	1.1 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3	0.86	2.04	2.860 (8)	160
O3—H19···N1	0.85	1.97	2.806 (8)	170
O3—H20···O2^{i}	0.85	2.11	2.783 (7)	136

Symmetry code: (i) −*x*+3/2, *y*+1/2, −*z*+1/2.