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9-(5-Bromo-2-hydroxyphenyl)-10-(2-hydroxyethyl)-3,4,6,7-tetrahydroacridine-1,8(2*H*,5*H*,9*H*,10*H*)-dione

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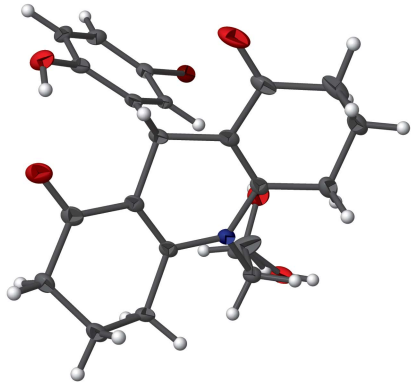
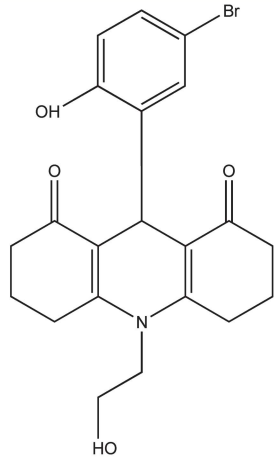
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{21}H_{22}BrNO_4$, the tetrahydroacridine-1,8-dione unit has a bromohydroxyphenyl-substituent on the central carbon atom of the dihydropyridine ring and a 2-hydroxyethyl substituent on the nitrogen atom. An intramolecular O—H···O hydrogen bond forms between the hydroxyl substituent on the benzene ring and a carbonyl oxygen from the acridinedione, forming an *S*(8) ring. The hydroxyl group of the 2-hydroxyethyl residue is disordered over two sites with an occupancy ratio of 0.572 (6):0.428 (6). In the crystal structure O—H···O and C—H···O hydrogen bonds together with Br···O halogen bonds stack the molecules along the *b*-axis direction.

3D view



Chemical scheme



Structure description

Acridine/acridone analogs are known anticancer drugs and cytotoxic agents. They represent an interesting class of compounds, displaying various forms of bioactivity (Antonini, 2002; Sebestík *et al.*, 2007). The title compound, $C_{21}H_{22}BrNO_4$, Fig. 1, comprises a central tetrahydroacridine-1,8-dione core with a bromohydroxyphenyl-substituent on the central C9 carbon atom of the dihydropyridine ring and a 2-hydroxyethyl substituent at N10. Both substituents point away from the same face of the acridine unit. The two cyclohexen-2-one rings of the acridinedione ring system each adopt envelope conformations with C3 and C6 respectively at the flaps while the dihydropyridine ring is a flattened boat. An intramolecular O2′—H2′···O8 hydrogen bond forms between the hydroxyl substituent on the benzene ring and a carbonyl oxygen from the acridinedione, forming an *S*(8) ring. The hydroxyl group of the 2-hydroxyethyl residue is disordered over two sites with an occupancy ratio of 0.572 (6):0.428 (6). In the

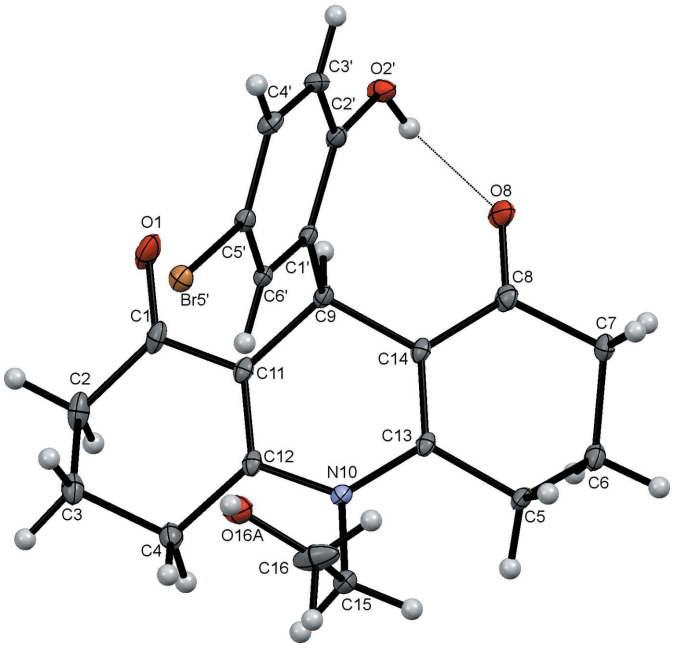


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. The O—H···O hydrogen bond is shown as a dashed line (see Table 1). Only one conformation shown for O16.

crystal structure, O16*A*–H16*C*···O8 hydrogen bonds together with Br···O halogen bonds (Desiraju *et al.*, 2013) [Br5′···O2′ = 3.1657 (19) Å] form chains of molecules along *a*. Additional C—H···O hydrogen bonds, Table 1, further stabilize the structure, linking these chains and forming stacks along the *b*-axis direction, Fig. 2.

The Cambridge Structural Database (Groom & Allen, 2014) reveals only six discrete structures of acridinediones with phenyl substituents at the 9-position (see for example, Feng *et al.*, 2005; Hua *et al.*, 2005; Tu *et al.*, 2005; Sivaraman *et al.*, 1996). Of these only 9-(3-bromo-5-chloro-2-hydroxyphenyl)-10-(2-hydroxyethyl)-3,4,6,7,9,10-hexahydroacridine-1,8(2*H*,5*H*)-dione (Mohamed *et al.*, 2013) has a 2-hydroxyethyl substituent on the nitrogen atom.

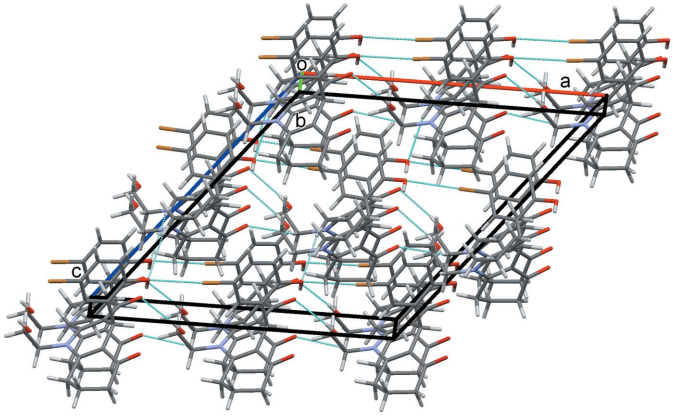


Figure 2
A view along the *b* axis of the crystal packing of the title compound with hydrogen bonds (see Table 1) and Br···O halogen bonds shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2′—H2′···O8	0.76 (4)	1.89 (5)	2.639 (3)	167 (5)
O16*A*—H16*C*···O8^{i}	0.84	2.29	3.119 (5)	170
C5—H5*A*···O2′^{ii}	0.99	2.55	3.514 (3)	165
C15—H15*A*···O1^{iii}	0.99	2.56	3.206 (4)	123

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

Synthesis and crystallization

A mixture of 1 mmol (201 mg) of 5-bromo-2-hydroxybenzaldehyde, 1 mmol (112 mg) of cyclohexane-1,3-dione and 1 mmol (61 mg) of 2-aminoethanol in 20 mL ethanol was refluxed for 4 h. The excess solvent was evaporated under vacuum and the residual solid product was collected, washed

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{22}BrNO_4$
M_r	432.30
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	100
a, *b*, *c* (Å)	16.0067 (4), 8.9455 (1), 16.1617 (4)
β (°)	128.853 (4)
V (Å^3)	1802.17 (10)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	3.35
Crystal size (mm)	0.36 × 0.26 × 0.23
Data collection	
Diffractometer	Agilent SuperNova Dual Source diffractometer with an Atlas detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min}, T_{max}	0.719, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7428, 2804, 2800
R_{int}	0.018
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.631
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.018, 0.047, 1.06
No. of reflections	2804
No. of parameters	259
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.33
Absolute structure	Flack *x* determined using 907 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter	−0.001 (10)

Computer programs: *CrysAlis PRO* (Agilent, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *TITAN* (Hunter & Simpson, 1999), *Mercury* (Macrae *et al.*, 2008), *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009), *publCIF* (Westrip 2010) and *WinGX* (Farrugia, 2012).

with cold ethanol and dried under vacuum. The crude product was crystallized from ethanol to afford good quality crystals suitable for x-ray diffraction. M.p. 523 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydroxyl oxygen atom of the 2-hydroxyethyl substituent was disordered over two sites and refined as O16*A* and O16*B* with occupancies that sum to unity. Their hydrogen atoms were placed in calculated positions with d(O—H) = 0.84 Å and $U_{iso} = 1.5U_{eq}$(O). This disorder model converged with an occupancy ratio 0.572 (6):0.428 (6). One reflection with $F_o >>> F_c$ was omitted from the final refinement cycles.

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full crystallographic data

IUCrData (2016). **1**, x152425 [doi:10.1107/S2414314615024256]

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9-(5-Bromo-2-hydroxyphenyl)-10-(2-hydroxyethyl)-3,4,6,7-tetrahydroacridine-1,8(2*H*,5*H*,9*H*,10*H*)-dione

Crystal data

$C_{21}H_{22}BrNO_4$
M_r = 432.30
Monoclinic, *Cc*
a = 16.0067 (4) Å
b = 8.9455 (1) Å
c = 16.1617 (4) Å
β = 128.853 (4)°
V = 1802.17 (10) Å^3
Z = 4
F(000) = 888
D_x = 1.593 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 7090 reflections
θ = 3.6–76.5°
μ = 3.35 mm^{-1}
T = 100 K
Irregular block, yellow
0.36 × 0.26 × 0.23 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Mirror monochromator
Detector resolution: 5.1725 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.719, T_{max} = 1.000
7428 measured reflections
2804 independent reflections
2800 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 76.7°, θ_{min} = 5.8°
h = −19→19
k = −10→11
l = −20→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.047
S = 1.06
2804 reflections
259 parameters
2 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 1.182P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack *x* determined using 907 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter: −0.001 (10)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.7420 (2)	0.0715 (2)	0.6087 (2)	0.0378 (6)	
C1	0.7063 (2)	0.1074 (3)	0.6546 (3)	0.0231 (6)	
C2	0.7476 (2)	0.0391 (3)	0.7592 (3)	0.0289 (6)	
H2A	0.8067	0.1014	0.8180	0.035*	
H2B	0.7767	−0.0616	0.7655	0.035*	
C3	0.6597 (2)	0.0267 (3)	0.7692 (2)	0.0248 (6)	
H3A	0.6909	−0.0106	0.8410	0.030*	
H3B	0.6055	−0.0467	0.7167	0.030*	
C4	0.6053 (2)	0.1766 (3)	0.7510 (2)	0.0239 (6)	
H4A	0.5388	0.1600	0.7419	0.029*	
H4B	0.6535	0.2404	0.8144	0.029*	
C5	0.4704 (2)	0.6415 (3)	0.5530 (2)	0.0193 (5)	
H5A	0.4830	0.6610	0.6204	0.023*	
H5B	0.3922	0.6467	0.4942	0.023*	
C6	0.5275 (2)	0.7609 (3)	0.5368 (2)	0.0222 (6)	
H6A	0.4926	0.8589	0.5247	0.027*	
H6B	0.6031	0.7689	0.6020	0.027*	
C7	0.5246 (2)	0.7251 (3)	0.4435 (2)	0.0224 (6)	
H7A	0.4499	0.7332	0.3767	0.027*	
H7B	0.5687	0.7989	0.4405	0.027*	
C8	0.5665 (2)	0.5695 (3)	0.4525 (2)	0.0205 (6)	
O8	0.6077 (2)	0.5422 (3)	0.4105 (2)	0.0315 (5)	
C9	0.5888 (2)	0.2967 (3)	0.5088 (2)	0.0161 (5)	
H9	0.6530	0.3034	0.5117	0.019*	
N10	0.50788 (18)	0.3786 (2)	0.61618 (17)	0.0159 (4)	
C11	0.6232 (2)	0.2210 (3)	0.6090 (2)	0.0167 (5)	
C12	0.5778 (2)	0.2568 (3)	0.6548 (2)	0.0163 (5)	
C13	0.5111 (2)	0.4871 (3)	0.5565 (2)	0.0156 (5)	
C14	0.5538 (2)	0.4555 (3)	0.5078 (2)	0.0165 (5)	
C15	0.4331 (2)	0.3910 (3)	0.6399 (2)	0.0211 (6)	
H15A	0.4102	0.4964	0.6320	0.025*	
H15B	0.4701	0.3606	0.7144	0.025*	
C16	0.3354 (3)	0.2935 (4)	0.5665 (4)	0.0439 (10)	
H16A	0.2934	0.2970	0.5923	0.053*	
H16B	0.2911	0.3421	0.4958	0.053*	
O16A	0.3443 (3)	0.1546 (4)	0.5516 (3)	0.0277 (11)	0.572 (6)
H16C	0.2832	0.1154	0.5118	0.042*	0.572 (6)
O16B	0.2844 (4)	0.2789 (5)	0.6132 (5)	0.0271 (14)	0.428 (6)
H16D	0.3310	0.2655	0.6789	0.041*	0.428 (6)

C1′	0.5024 (2)	0.2082 (3)	0.4092 (2)	0.0154 (5)
C2′	0.4972 (2)	0.2052 (3)	0.3189 (2)	0.0185 (5)
O2′	0.56623 (18)	0.2837 (2)	0.31285 (18)	0.0242 (4)
H2′	0.586 (4)	0.352 (5)	0.349 (3)	0.036*
C3′	0.4210 (2)	0.1174 (4)	0.2317 (2)	0.0208 (5)
H3′	0.4191	0.1156	0.1718	0.025*
C4′	0.3475 (2)	0.0325 (3)	0.2304 (2)	0.0201 (5)
H4′	0.2961	−0.0281	0.1709	0.024*
C5′	0.3516 (2)	0.0389 (3)	0.3183 (2)	0.0161 (5)
Br5′	0.25219 (2)	−0.07675 (2)	0.31963 (2)	0.01879 (8)
C6′	0.4270 (2)	0.1244 (3)	0.4064 (2)	0.0150 (5)
H6′	0.4275	0.1262	0.4655	0.018*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0449 (15)	0.0213 (11)	0.0662 (18)	0.0117 (9)	0.0440 (15)	0.0075 (10)
C1	0.0216 (14)	0.0108 (11)	0.0358 (17)	−0.0004 (10)	0.0174 (13)	0.0004 (12)
C2	0.0208 (15)	0.0168 (13)	0.0359 (17)	0.0035 (11)	0.0113 (14)	0.0060 (13)
C3	0.0265 (15)	0.0160 (13)	0.0216 (14)	−0.0004 (11)	0.0100 (13)	0.0017 (11)
C4	0.0286 (15)	0.0186 (14)	0.0194 (13)	0.0023 (11)	0.0126 (12)	0.0023 (11)
C5	0.0236 (14)	0.0140 (13)	0.0200 (13)	0.0052 (10)	0.0135 (12)	−0.0004 (10)
C6	0.0265 (15)	0.0129 (12)	0.0233 (14)	0.0015 (11)	0.0137 (12)	0.0001 (11)
C7	0.0308 (15)	0.0124 (12)	0.0256 (14)	0.0002 (11)	0.0184 (13)	0.0017 (11)
C8	0.0233 (15)	0.0133 (13)	0.0255 (15)	−0.0042 (10)	0.0156 (13)	−0.0032 (10)
O8	0.0535 (16)	0.0149 (9)	0.0491 (15)	−0.0047 (11)	0.0433 (14)	−0.0027 (11)
C9	0.0184 (13)	0.0109 (11)	0.0225 (13)	0.0006 (9)	0.0146 (12)	−0.0004 (10)
N10	0.0186 (11)	0.0134 (10)	0.0163 (11)	0.0011 (8)	0.0112 (10)	−0.0008 (9)
C11	0.0162 (12)	0.0111 (11)	0.0193 (13)	−0.0026 (9)	0.0094 (11)	−0.0032 (10)
C12	0.0157 (12)	0.0112 (11)	0.0154 (12)	−0.0016 (9)	0.0066 (10)	−0.0017 (10)
C13	0.0148 (11)	0.0117 (12)	0.0142 (12)	−0.0003 (10)	0.0061 (10)	−0.0021 (10)
C14	0.0173 (12)	0.0109 (11)	0.0187 (13)	−0.0020 (9)	0.0101 (11)	−0.0022 (10)
C15	0.0279 (15)	0.0173 (12)	0.0235 (14)	0.0038 (11)	0.0187 (13)	0.0014 (11)
C16	0.054 (2)	0.045 (2)	0.064 (3)	−0.0270 (18)	0.052 (2)	−0.0283 (19)
O16A	0.029 (2)	0.027 (2)	0.030 (2)	−0.0033 (16)	0.0202 (19)	−0.0022 (16)
O16B	0.035 (3)	0.017 (2)	0.053 (3)	0.002 (2)	0.039 (3)	0.004 (2)
C1′	0.0189 (12)	0.0091 (11)	0.0198 (13)	0.0006 (9)	0.0129 (11)	−0.0008 (9)
C2′	0.0241 (13)	0.0130 (12)	0.0276 (13)	0.0008 (10)	0.0207 (12)	0.0001 (11)
O2′	0.0338 (12)	0.0201 (10)	0.0328 (11)	−0.0096 (8)	0.0278 (10)	−0.0076 (9)
C3′	0.0297 (16)	0.0198 (13)	0.0222 (14)	0.0004 (13)	0.0207 (13)	−0.0017 (12)
C4′	0.0216 (14)	0.0168 (12)	0.0222 (14)	−0.0016 (11)	0.0138 (12)	−0.0052 (11)
C5′	0.0156 (12)	0.0130 (11)	0.0214 (13)	0.0004 (9)	0.0125 (11)	0.0005 (10)
Br5′	0.01627 (12)	0.01734 (12)	0.02339 (13)	−0.00335 (12)	0.01274 (10)	−0.00167 (12)
C6′	0.0197 (12)	0.0105 (11)	0.0181 (12)	0.0017 (10)	0.0135 (11)	0.0003 (10)

Geometric parameters (Å, º)

O1—C1	1.230 (4)	N10—C13	1.391 (3)
C1—C11	1.454 (4)	N10—C12	1.398 (3)
C1—C2	1.506 (4)	N10—C15	1.473 (3)
C2—C3	1.518 (4)	C11—C12	1.361 (4)
C2—H2A	0.9900	C13—C14	1.358 (4)
C2—H2B	0.9900	C15—C16	1.511 (5)
C3—C4	1.524 (4)	C15—H15A	0.9900
C3—H3A	0.9900	C15—H15B	0.9900
C3—H3B	0.9900	C16—O16A	1.290 (5)
C4—C12	1.506 (4)	C16—O16B	1.425 (5)
C4—H4A	0.9900	C16—H16A	0.9900
C4—H4B	0.9900	C16—H16B	0.9900
C5—C13	1.513 (3)	O16A—H16C	0.8400
C5—C6	1.532 (4)	O16B—H16D	0.8400
C5—H5A	0.9900	C1′—C6′	1.398 (3)
C5—H5B	0.9900	C1′—C2′	1.408 (4)
C6—C7	1.513 (4)	C2′—O2′	1.363 (3)
C6—H6A	0.9900	C2′—C3′	1.391 (4)
C6—H6B	0.9900	O2′—H2′	0.76 (4)
C7—C8	1.512 (4)	C3′—C4′	1.389 (4)
C7—H7A	0.9900	C3′—H3′	0.9500
C7—H7B	0.9900	C4′—C5′	1.382 (4)
C8—O8	1.232 (4)	C4′—H4′	0.9500
C8—C14	1.452 (4)	C5′—C6′	1.384 (4)
C9—C11	1.506 (4)	C5′—Br5′	1.909 (2)
C9—C14	1.524 (3)	Br5′—O2′^{i}	3.1657 (19)
C9—C1′	1.529 (4)	C6′—H6′	0.9500
C9—H9	1.0000		
O1—C1—C11	120.1 (3)	C13—N10—C15	121.1 (2)
O1—C1—C2	121.9 (3)	C12—N10—C15	119.8 (2)
C11—C1—C2	118.0 (3)	C12—C11—C1	121.4 (2)
C1—C2—C3	111.5 (2)	C12—C11—C9	121.3 (2)
C1—C2—H2A	109.3	C1—C11—C9	117.4 (2)
C3—C2—H2A	109.3	C11—C12—N10	119.5 (2)
C1—C2—H2B	109.3	C11—C12—C4	122.6 (2)
C3—C2—H2B	109.3	N10—C12—C4	117.8 (2)
H2A—C2—H2B	108.0	C14—C13—N10	120.5 (2)
C2—C3—C4	111.7 (2)	C14—C13—C5	122.0 (2)
C2—C3—H3A	109.3	N10—C13—C5	117.5 (2)
C4—C3—H3A	109.3	C13—C14—C8	121.8 (2)
C2—C3—H3B	109.3	C13—C14—C9	120.3 (2)
C4—C3—H3B	109.3	C8—C14—C9	117.9 (2)
H3A—C3—H3B	107.9	N10—C15—C16	111.2 (2)
C12—C4—C3	112.4 (2)	N10—C15—H15A	109.4
C12—C4—H4A	109.1	C16—C15—H15A	109.4

C3—C4—H4A	109.1	N10—C15—H15B	109.4
C12—C4—H4B	109.1	C16—C15—H15B	109.4
C3—C4—H4B	109.1	H15A—C15—H15B	108.0
H4A—C4—H4B	107.9	O16A—C16—C15	121.4 (4)
C13—C5—C6	110.8 (2)	O16B—C16—C15	106.9 (3)
C13—C5—H5A	109.5	O16A—C16—H16A	107.0
C6—C5—H5A	109.5	C15—C16—H16A	107.0
C13—C5—H5B	109.5	O16A—C16—H16B	107.0
C6—C5—H5B	109.5	C15—C16—H16B	107.0
H5A—C5—H5B	108.1	H16A—C16—H16B	106.7
C7—C6—C5	112.0 (2)	C16—O16A—H16C	109.5
C7—C6—H6A	109.2	C16—O16B—H16D	109.5
C5—C6—H6A	109.2	C6′—C1′—C2′	117.9 (2)
C7—C6—H6B	109.2	C6′—C1′—C9	120.3 (2)
C5—C6—H6B	109.2	C2′—C1′—C9	121.8 (2)
H6A—C6—H6B	107.9	O2′—C2′—C3′	116.9 (2)
C8—C7—C6	111.4 (2)	O2′—C2′—C1′	122.7 (2)
C8—C7—H7A	109.4	C3′—C2′—C1′	120.3 (2)
C6—C7—H7A	109.4	C2′—O2′—H2′	110 (3)
C8—C7—H7B	109.4	C4′—C3′—C2′	121.3 (3)
C6—C7—H7B	109.4	C4′—C3′—H3′	119.3
H7A—C7—H7B	108.0	C2′—C3′—H3′	119.3
O8—C8—C14	122.0 (2)	C5′—C4′—C3′	117.9 (3)
O8—C8—C7	119.2 (3)	C5′—C4′—H4′	121.0
C14—C8—C7	118.8 (2)	C3′—C4′—H4′	121.0
C11—C9—C14	108.3 (2)	C4′—C5′—C6′	121.9 (2)
C11—C9—C1′	112.3 (2)	C4′—C5′—Br5′	119.2 (2)
C14—C9—C1′	112.8 (2)	C6′—C5′—Br5′	118.86 (19)
C11—C9—H9	107.8	C5′—Br5′—O2′^{i}	170.21 (9)
C14—C9—H9	107.8	C5′—C6′—C1′	120.5 (2)
C1′—C9—H9	107.8	C5′—C6′—H6′	119.7
C13—N10—C12	119.1 (2)	C1′—C6′—H6′	119.7

O1—C1—C2—C3	−147.2 (3)	C5—C13—C14—C8	2.2 (4)
C11—C1—C2—C3	33.9 (4)	N10—C13—C14—C9	6.0 (4)
C1—C2—C3—C4	−54.2 (3)	C5—C13—C14—C9	−177.0 (2)
C2—C3—C4—C12	46.0 (3)	O8—C8—C14—C13	178.2 (3)
C13—C5—C6—C7	51.0 (3)	C7—C8—C14—C13	−3.8 (4)
C5—C6—C7—C8	−53.0 (3)	O8—C8—C14—C9	−2.6 (4)
C6—C7—C8—O8	−152.5 (3)	C7—C8—C14—C9	175.4 (2)
C6—C7—C8—C14	29.4 (4)	C11—C9—C14—C13	−29.8 (3)
O1—C1—C11—C12	176.1 (3)	C1′—C9—C14—C13	95.1 (3)
C2—C1—C11—C12	−5.0 (4)	C11—C9—C14—C8	151.0 (2)
O1—C1—C11—C9	−3.5 (4)	C1′—C9—C14—C8	−84.2 (3)
C2—C1—C11—C9	175.4 (2)	C13—N10—C15—C16	100.2 (3)
C14—C9—C11—C12	31.0 (3)	C12—N10—C15—C16	−80.4 (3)
C1′—C9—C11—C12	−94.3 (3)	N10—C15—C16—O16A	50.0 (5)
C14—C9—C11—C1	−149.4 (2)	N10—C15—C16—O16B	163.7 (3)

C1′—C9—C11—C1	85.4 (3)	C11—C9—C1′—C6′	32.8 (3)
C1—C11—C12—N10	172.3 (2)	C14—C9—C1′—C6′	−89.9 (3)
C9—C11—C12—N10	−8.1 (4)	C11—C9—C1′—C2′	−145.8 (2)
C1—C11—C12—C4	−3.6 (4)	C14—C9—C1′—C2′	91.5 (3)
C9—C11—C12—C4	176.0 (2)	C6′—C1′—C2′—O2′	179.4 (2)
C13—N10—C12—C11	−19.9 (4)	C9—C1′—C2′—O2′	−2.0 (4)
C15—N10—C12—C11	160.7 (2)	C6′—C1′—C2′—C3′	−1.9 (4)
C13—N10—C12—C4	156.2 (2)	C9—C1′—C2′—C3′	176.7 (2)
C15—N10—C12—C4	−23.2 (3)	O2′—C2′—C3′—C4′	179.6 (3)
C3—C4—C12—C11	−17.5 (4)	C1′—C2′—C3′—C4′	0.8 (4)
C3—C4—C12—N10	166.5 (2)	C2′—C3′—C4′—C5′	0.7 (4)
C12—N10—C13—C14	20.9 (4)	C3′—C4′—C5′—C6′	−1.1 (4)
C15—N10—C13—C14	−159.7 (3)	C3′—C4′—C5′—Br5′	−179.8 (2)
C12—N10—C13—C5	−156.2 (2)	C4′—C5′—C6′—C1′	0.0 (4)
C15—N10—C13—C5	23.2 (4)	Br5′—C5′—C6′—C1′	178.73 (19)
C6—C5—C13—C14	−25.8 (3)	C2′—C1′—C6′—C5′	1.5 (4)
C6—C5—C13—N10	151.2 (2)	C9—C1′—C6′—C5′	−177.1 (2)
N10—C13—C14—C8	−174.8 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2′—H2′···O8	0.76 (4)	1.89 (5)	2.639 (3)	167 (5)
O16*A*—H16*C*···O8^{i}	0.84	2.29	3.119 (5)	170
C5—H5*A*···O2′^{ii}	0.99	2.55	3.514 (3)	165
C15—H15*A*···O1^{iii}	0.99	2.56	3.206 (4)	123

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