Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

9-(5-Bromo-2-hydroxyphenyl)-10-(2-hydroxypropyl)-3,3,6,6-tetramethyl-1,2,3,4,5,6,7,8,9,10-decahydroacridine-1,8-dione

Ali N. Khalilov,[a] Antar A. Abdelhamid,[a] Atash V. Gurbanov[b] and Seik Weng Ng[c]*

[a]Department of Organic Chemistry, Baku State University, Baku, Azerbaijan, [b]Chemistry & Environmental Science Division, School of Science, Manchester Metropolitan University, England, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

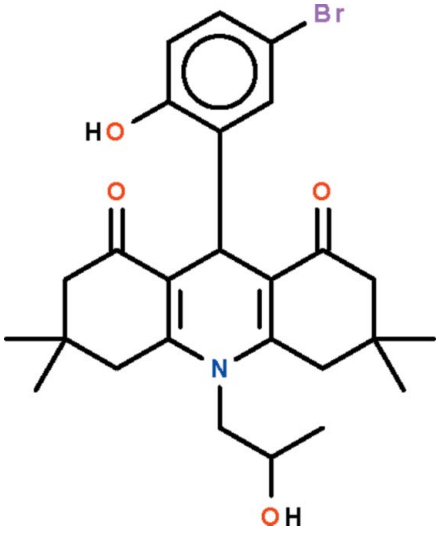
Received 10 April 2011; accepted 11 April 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.053; wR factor = 0.135; data-to-parameter ratio = 17.9.

The dihydropyridine ring in the title compound, $C_{26}H_{32}BrNO_4$, adopts an envelope conformation with the methine C atom representing the flap. The cyclohexenone rings also adopt envelope conformations. The phenolic hydroxy group forms an intramolecular hydrogen bond to one of the two keto O atoms. Intermolecular weak C—H···O hydrogen bonding is present in the crystal structure. The hydroxypropyl group is disordered over two sets of sites with an occupancy ratio of 0.636 (6):0.364 (6).

Related literature

For a related structure, see: Abdelhamid *et al.* (2011).



Experimental

Crystal data

$C_{26}H_{32}BrNO_4$
M_r = 502.44
Monoclinic, $P2_1/n$
a = 10.6685 (4) Å
b = 16.8190 (5) Å
c = 14.1260 (5) Å
β = 106.303 (3)°
V = 2432.76 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.72 mm^{-1}
T = 100 K
0.20 × 0.10 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.725, T_{max} = 0.919
11939 measured reflections
5402 independent reflections
3939 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.135
S = 1.03
5402 reflections
302 parameters
24 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.84	1.78	2.621 (4)	176
C10—H10A···O1^{i}	0.99	2.54	3.417 (5)	147

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Manchester Metropolitan University, Baku State University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5192).

References

Abdelhamid, A. A., Mohamed, S. K., Khalilov, A. N., Gurbanov, A. V. & Ng, S. W. (2011). *Acta Cryst.* E**67**, o744.
Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2011). E**67**, o1146 [doi:10.1107/S1600536811013481]

9-(5-Bromo-2-hydroxyphenyl)-10-(2-hydroxypropyl)-3,3,6,6-tetramethyl-1,2,3,4,5,6,7,8,9,10-decahydroacridine-1,8-dione

Ali N. Khalilov, Antar A. Abdelhamid, Atash V. Gurbanov and Seik Weng Ng

S1. Comment

In an earlier study, we reported 10-(2-hydroxyethyl)-9-(2-hydroxyphenyl)-3,3,6,6-tetramethyl-1,2,3,4,5,6,7,8,9,10-decahydroacridine-1,8-dione, which was synthesized by the reaction of dimedone, salicyladehyde and 2-aminoethanol (Abdelhamid *et al.*, 2011). In the present study, we replaced 2-aminoethanol by 1-amino-2-propanol and also used a bromine-subsituted salicyladehyde to form the title analog (Scheme I). The dihydropyridine ring in the $C_{26}H_{32}BrNO_4$ adopts an envelope conformation with the methine C atom representing the flap. The cyclohexenone rings also adopt envelope conformations with the C atoms bearing the methyl C atoms representing the flaps. The phenolic hydroxy group forms an intramolecular hydrogen bond to one of the two keto O atoms (Fig. 1).

S2. Experimental

5-Bromo-2-hydroxybenzaldehyde (10 mmol), 1-amino-2-propanol (10 mol) and 20 dimedone (20 mmol) were heated in pyridine (50 ml) for 5 h. The solid that was isolated from the cool solution was collected and recrystallized from ethano; m.p. 508 K.

S3. Refinement

H-atoms were placed in calculated positions [C–H 0.95 to 0.99, O–H 0.84 Å; U(H) 1.2 to 1.5U(C,O)] and were included in the refinement in the riding model approximation.

The hydroxypropyl group is disordered over two positions in respect of three of the four non-hydrogen atoms; the C atom connected to the dihydropyridine ring is ordered. The carbon–carbon distances were restrained to 1.54±0.01Å and the carbon–oxygen distances to 1.45±0.01 Å. The temperature factors of the primed atoms were set to those of the unprimed atoms, and the anisotropic temperature factors were restrained to be nearly isotropic. The disorder refined to a 63.6 (1): 36.4 ratio.

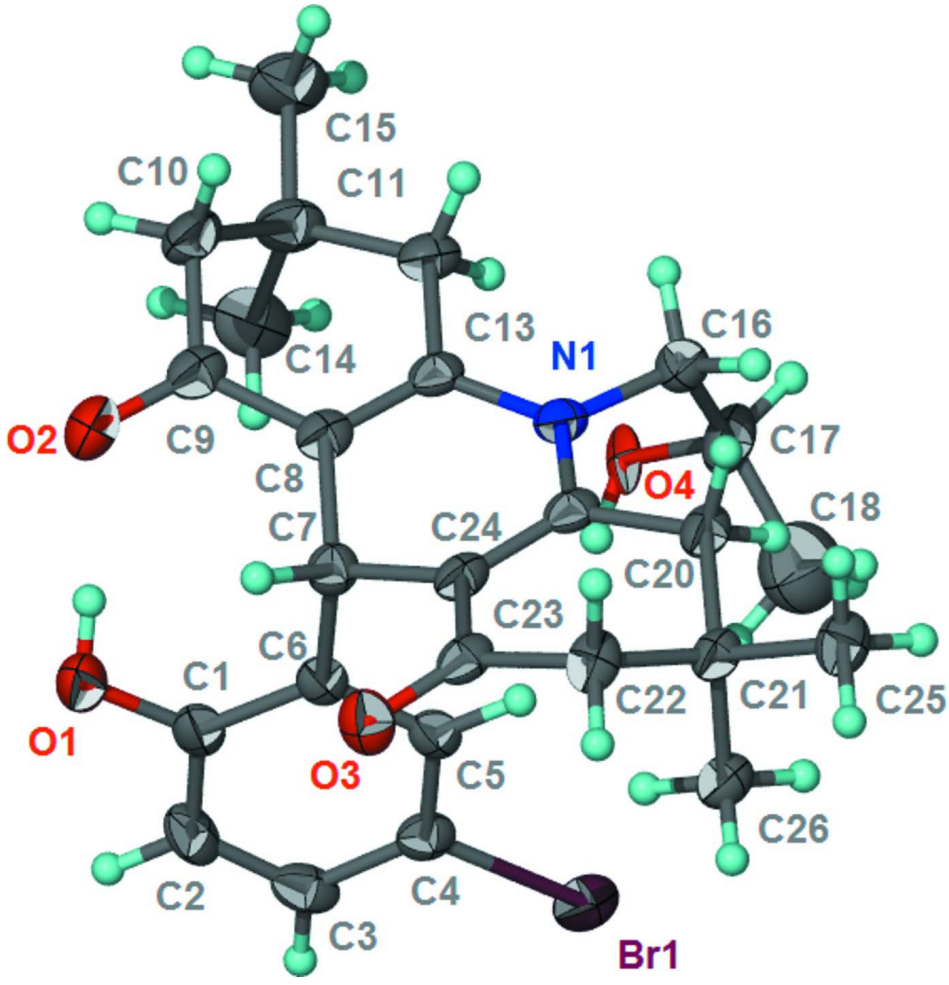


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{26}H_{32}BrNO_4$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder is not shown.

9-(5-Bromo-2-hydroxyphenyl)-10-(2-hydroxypropyl)-3,3,6,6-tetramethyl- 1,2,3,4,5,6,7,8,9,10-decahydroacridine-1,8-dione

Crystal data

$C_{26}H_{32}BrNO_4$
M_r = 502.44
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 10.6685 (4) Å
b = 16.8190 (5) Å
c = 14.1260 (5) Å
β = 106.303 (3)°
V = 2432.76 (14) Å^3
Z = 4
$F(000)$ = 1048
D_x = 1.372 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3308 reflections
θ = 2.3–29.4°
μ = 1.72 mm^{-1}
T = 100 K
Prism, colorless
0.20 × 0.10 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.725, T_{max} = 0.919
11939 measured reflections
5402 independent reflections
3939 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −13→13
k = −21→19
l = −13→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.135
S = 1.03
5402 reflections
302 parameters
24 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
$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 1.4767P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	1.00011 (3)	0.07288 (2)	0.84090 (3)	0.02822 (14)	
O1	0.6038 (2)	0.22434 (18)	1.01434 (16)	0.0322 (6)	
H1	0.5337	0.2333	0.9706	0.039*	
O2	0.3796 (2)	0.25478 (16)	0.88504 (17)	0.0306 (6)	
O3	0.7557 (3)	0.41222 (15)	0.86062 (17)	0.0284 (6)	
O4	0.6148 (10)	0.0597 (4)	0.6070 (6)	0.0224 (9)	0.636 (6)
H4	0.6748	0.0648	0.6598	0.027*	0.636 (6)
O4′	0.6669 (7)	0.0829 (4)	0.4503 (4)	0.0224 (9)	0.364
H4′	0.7173	0.0435	0.4608	0.027*	0.364 (6)
N1	0.5582 (3)	0.22319 (18)	0.61661 (19)	0.0209 (6)	
C1	0.6924 (4)	0.1925 (2)	0.9722 (2)	0.0253 (8)	
C2	0.7829 (4)	0.1395 (2)	1.0291 (2)	0.0291 (9)	
H2	0.7803	0.1273	1.0942	0.035*	
C3	0.8759 (4)	0.1044 (2)	0.9923 (2)	0.0274 (8)	
H3	0.9380	0.0686	1.0315	0.033*	
C4	0.8772 (3)	0.1223 (2)	0.8975 (2)	0.0231 (8)	
C5	0.7896 (3)	0.1759 (2)	0.8406 (2)	0.0206 (7)	
H5	0.7928	0.1873	0.7754	0.025*	
C6	0.6975 (3)	0.2134 (2)	0.8771 (2)	0.0195 (7)	
C7	0.6024 (3)	0.2741 (2)	0.8146 (2)	0.0218 (7)	
H7	0.5812	0.3146	0.8595	0.026*	
C8	0.4774 (3)	0.2344 (2)	0.7571 (2)	0.0214 (7)	
C9	0.3703 (3)	0.2291 (2)	0.8002 (2)	0.0245 (8)	
C10	0.2455 (4)	0.1933 (2)	0.7402 (3)	0.0316 (9)	
H10A	0.1952	0.2335	0.6935	0.038*	

H10B	0.1923	0.1768	0.7841	0.038*	
C11	0.2724 (4)	0.1208 (2)	0.6826 (3)	0.0320 (9)	
C12	0.3568 (3)	0.1482 (2)	0.6168 (2)	0.0260 (8)	
H12A	0.3945	0.1007	0.5937	0.031*	
H12B	0.2999	0.1750	0.5580	0.031*	
C13	0.4664 (3)	0.2038 (2)	0.6662 (2)	0.0213 (8)	
C14	0.3435 (4)	0.0568 (2)	0.7541 (3)	0.0392 (10)	
H14A	0.3604	0.0108	0.7169	0.059*	
H14B	0.2893	0.0404	0.7964	0.059*	
H14C	0.4266	0.0780	0.7951	0.059*	
C15	0.1428 (4)	0.0876 (3)	0.6174 (3)	0.0461 (12)	
H15A	0.1603	0.0414	0.5808	0.069*	
H15B	0.0980	0.1286	0.5709	0.069*	
H15C	0.0876	0.0715	0.6590	0.069*	
C16	0.5558 (3)	0.1821 (2)	0.5232 (2)	0.0253 (8)	
H16A	0.5847	0.2201	0.4799	0.030*	0.636 (6)
H16B	0.4645	0.1671	0.4893	0.030*	0.636 (6)
H16C	0.5683	0.2211	0.4740	0.030*	0.364 (6)
H16D	0.4706	0.1554	0.4958	0.030*	0.364 (6)
C17	0.6394 (8)	0.1092 (5)	0.5351 (6)	0.035 (2)	0.636 (6)
H17	0.6079	0.0794	0.4715	0.042*	0.636 (6)
C17′	0.6674 (17)	0.1202 (11)	0.5460 (9)	0.035 (2)	0.364
H17′	0.7542	0.1415	0.5846	0.042*	0.364 (6)
C18	0.7835 (8)	0.1139 (5)	0.5556 (6)	0.064 (3)	0.636 (6)
H18A	0.8061	0.1579	0.5180	0.096*	0.636 (6)
H18B	0.8165	0.0639	0.5361	0.096*	0.636 (6)
H18C	0.8230	0.1229	0.6262	0.096*	0.636 (6)
C18′	0.613 (4)	0.0541 (18)	0.598 (2)	0.064 (3)	0.364
H18D	0.6726	0.0085	0.6100	0.096*	0.364 (6)
H18E	0.5270	0.0377	0.5569	0.096*	0.364 (6)
H18F	0.6050	0.0740	0.6615	0.096*	0.364 (6)
C19	0.6444 (3)	0.2861 (2)	0.6502 (2)	0.0207 (7)	
C20	0.7162 (3)	0.3212 (2)	0.5820 (2)	0.0221 (7)	
H20A	0.6538	0.3531	0.5310	0.027*	
H20B	0.7475	0.2772	0.5480	0.027*	
C21	0.8325 (3)	0.3738 (2)	0.6323 (2)	0.0208 (7)	
C22	0.7910 (4)	0.4311 (2)	0.7019 (2)	0.0241 (8)	
H22A	0.8672	0.4633	0.7376	0.029*	
H22B	0.7236	0.4677	0.6628	0.029*	
C23	0.7371 (3)	0.3877 (2)	0.7761 (2)	0.0222 (8)	
C24	0.6607 (3)	0.3159 (2)	0.7426 (2)	0.0208 (7)	
C25	0.8732 (4)	0.4213 (2)	0.5529 (3)	0.0273 (8)	
H25A	0.9004	0.3846	0.5085	0.041*	
H25B	0.9460	0.4566	0.5845	0.041*	
H25C	0.7991	0.4531	0.5150	0.041*	
C26	0.9486 (3)	0.3234 (2)	0.6901 (2)	0.0258 (8)	
H26A	0.9746	0.2869	0.6449	0.039*	
H26B	0.9233	0.2928	0.7409	0.039*	

H26C	1.0220	0.3584	0.7214	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0228 (2)	0.0251 (2)	0.0361 (2)	0.00032 (17)	0.00727 (15)	0.00592 (15)
O1	0.0261 (15)	0.0483 (19)	0.0246 (13)	−0.0083 (14)	0.0109 (10)	−0.0029 (12)
O2	0.0265 (15)	0.0350 (17)	0.0343 (14)	−0.0001 (13)	0.0150 (11)	0.0000 (12)
O3	0.0345 (15)	0.0256 (15)	0.0268 (13)	−0.0060 (12)	0.0116 (11)	−0.0040 (10)
O4	0.036 (2)	0.017 (2)	0.021 (2)	0.0144 (17)	0.0188 (16)	0.0029 (14)
O4′	0.036 (2)	0.017 (2)	0.021 (2)	0.0144 (17)	0.0188 (16)	0.0029 (14)
N1	0.0162 (15)	0.0231 (17)	0.0220 (14)	−0.0008 (13)	0.0029 (11)	0.0031 (12)
C1	0.023 (2)	0.032 (2)	0.0206 (17)	−0.0126 (17)	0.0060 (14)	−0.0035 (15)
C2	0.036 (2)	0.032 (2)	0.0185 (17)	−0.0117 (19)	0.0072 (15)	0.0053 (15)
C3	0.027 (2)	0.025 (2)	0.0243 (18)	−0.0072 (17)	−0.0018 (14)	0.0073 (15)
C4	0.0187 (19)	0.022 (2)	0.0266 (18)	−0.0048 (16)	0.0040 (14)	0.0021 (14)
C5	0.0211 (18)	0.0206 (19)	0.0192 (16)	−0.0067 (15)	0.0039 (13)	−0.0003 (13)
C6	0.0202 (19)	0.0179 (19)	0.0197 (16)	−0.0072 (15)	0.0047 (13)	−0.0003 (13)
C7	0.0217 (19)	0.0215 (19)	0.0230 (17)	−0.0027 (16)	0.0076 (13)	0.0000 (14)
C8	0.0202 (18)	0.0174 (19)	0.0258 (18)	0.0021 (15)	0.0052 (13)	0.0057 (14)
C9	0.0205 (19)	0.022 (2)	0.0307 (19)	0.0015 (16)	0.0070 (14)	0.0067 (15)
C10	0.020 (2)	0.042 (3)	0.034 (2)	−0.0015 (18)	0.0095 (15)	0.0067 (17)
C11	0.024 (2)	0.034 (2)	0.035 (2)	−0.0081 (18)	0.0030 (15)	0.0056 (17)
C12	0.0193 (19)	0.027 (2)	0.0292 (19)	−0.0010 (17)	0.0025 (14)	0.0030 (15)
C13	0.0149 (17)	0.024 (2)	0.0242 (18)	0.0024 (15)	0.0033 (13)	0.0066 (14)
C14	0.044 (3)	0.030 (2)	0.041 (2)	−0.011 (2)	0.0076 (18)	0.0081 (17)
C15	0.033 (2)	0.059 (3)	0.042 (2)	−0.023 (2)	0.0049 (18)	0.006 (2)
C16	0.0224 (19)	0.029 (2)	0.0244 (18)	0.0014 (17)	0.0072 (14)	0.0023 (15)
C17	0.031 (5)	0.042 (4)	0.038 (3)	0.010 (4)	0.020 (3)	0.016 (2)
C17′	0.031 (5)	0.042 (4)	0.038 (3)	0.010 (4)	0.020 (3)	0.016 (2)
C18	0.066 (5)	0.069 (5)	0.058 (4)	0.001 (4)	0.021 (4)	0.013 (4)
C18′	0.066 (5)	0.069 (5)	0.058 (4)	0.001 (4)	0.021 (4)	0.013 (4)
C19	0.0142 (17)	0.0214 (19)	0.0256 (17)	0.0034 (15)	0.0041 (13)	0.0065 (14)
C20	0.0202 (18)	0.023 (2)	0.0253 (17)	0.0049 (16)	0.0091 (13)	0.0072 (14)
C21	0.0193 (18)	0.0197 (19)	0.0252 (17)	0.0019 (15)	0.0092 (13)	0.0040 (14)
C22	0.028 (2)	0.0162 (19)	0.0308 (19)	0.0032 (16)	0.0136 (15)	0.0049 (14)
C23	0.0170 (18)	0.020 (2)	0.0299 (19)	0.0031 (15)	0.0075 (14)	0.0055 (14)
C24	0.0155 (17)	0.0199 (19)	0.0270 (18)	−0.0001 (15)	0.0061 (13)	0.0053 (14)
C25	0.030 (2)	0.024 (2)	0.0312 (19)	0.0009 (17)	0.0142 (15)	0.0045 (15)
C26	0.0206 (19)	0.027 (2)	0.0304 (19)	0.0010 (17)	0.0088 (14)	0.0023 (15)

Geometric parameters (Å, º)

Br1—C4	1.908 (4)	C14—H14C	0.9800
O1—C1	1.360 (4)	C15—H15A	0.9800
O1—H1	0.8400	C15—H15B	0.9800
O2—C9	1.251 (4)	C15—H15C	0.9800
O3—C23	1.226 (4)	C16—C17	1.499 (7)

O4—C17	1.394 (7)	C16—C17′	1.547 (9)
O4—H4	0.8400	C16—H16A	0.9900
O4′—C17′	1.488 (10)	C16—H16B	0.9900
O4′—H4′	0.8400	C16—H16C	0.9900
N1—C13	1.393 (4)	C16—H16D	0.9900
N1—C19	1.394 (4)	C17—C18	1.484 (8)
N1—C16	1.483 (4)	C17—H17	1.0000
C1—C2	1.391 (5)	C17′—C18′	1.535 (10)
C1—C6	1.405 (5)	C17′—H17′	1.0000
C2—C3	1.376 (5)	C18—H18A	0.9800
C2—H2	0.9500	C18—H18B	0.9800
C3—C4	1.376 (5)	C18—H18C	0.9800
C3—H3	0.9500	C18′—H18D	0.9800
C4—C5	1.382 (5)	C18′—H18E	0.9800
C5—C6	1.383 (5)	C18′—H18F	0.9800
C5—H5	0.9500	C19—C24	1.364 (5)
C6—C7	1.532 (5)	C19—C20	1.509 (4)
C7—C24	1.507 (4)	C20—C21	1.526 (5)
C7—C8	1.509 (5)	C20—H20A	0.9900
C7—H7	1.0000	C20—H20B	0.9900
C8—C13	1.357 (5)	C21—C22	1.529 (5)
C8—C9	1.440 (5)	C21—C26	1.533 (5)
C9—C10	1.490 (5)	C21—C25	1.536 (5)
C10—C11	1.538 (6)	C22—C23	1.516 (5)
C10—H10A	0.9900	C22—H22A	0.9900
C10—H10B	0.9900	C22—H22B	0.9900
C11—C14	1.525 (5)	C23—C24	1.459 (5)
C11—C12	1.535 (5)	C25—H25A	0.9800
C11—C15	1.535 (5)	C25—H25B	0.9800
C12—C13	1.507 (5)	C25—H25C	0.9800
C12—H12A	0.9900	C26—H26A	0.9800
C12—H12B	0.9900	C26—H26B	0.9800
C14—H14A	0.9800	C26—H26C	0.9800
C14—H14B	0.9800		

C1—O1—H1	109.5	C17′—C16—H16A	102.0
C17′—O4′—H4′	109.5	N1—C16—H16B	108.6
C13—N1—C19	119.7 (3)	C17—C16—H16B	108.6
C13—N1—C16	119.9 (3)	H16A—C16—H16B	107.5
C19—N1—C16	120.1 (3)	N1—C16—H16C	110.1
O1—C1—C2	117.0 (3)	C17—C16—H16C	115.3
O1—C1—C6	122.5 (3)	C17′—C16—H16C	110.1
C2—C1—C6	120.4 (3)	N1—C16—H16D	110.1
C3—C2—C1	120.9 (3)	C17′—C16—H16D	110.1
C3—C2—H2	119.5	H16C—C16—H16D	108.4
C1—C2—H2	119.5	O4—C17—C18	106.6 (7)
C2—C3—C4	118.6 (3)	O4—C17—C16	110.0 (6)
C2—C3—H3	120.7	C18—C17—C16	122.0 (8)

C4—C3—H3	120.7	O4—C17—H17	105.7
C3—C4—C5	121.3 (3)	C18—C17—H17	105.7
C3—C4—Br1	120.5 (3)	C16—C17—H17	105.7
C5—C4—Br1	118.2 (2)	O4′—C17′—C18′	103.1 (17)
C6—C5—C4	121.0 (3)	O4′—C17′—C16	106.7 (8)
C6—C5—H5	119.5	C18′—C17′—C16	102 (2)
C4—C5—H5	119.5	O4′—C17′—H17′	114.4
C5—C6—C1	117.7 (3)	C18′—C17′—H17′	114.4
C5—C6—C7	120.9 (3)	C16—C17′—H17′	114.4
C1—C6—C7	121.4 (3)	C17—C18—H18A	109.5
C24—C7—C8	108.3 (3)	C17—C18—H18B	109.5
C24—C7—C6	111.6 (3)	H18A—C18—H18B	109.5
C8—C7—C6	110.9 (3)	C17—C18—H18C	109.5
C24—C7—H7	108.7	H18A—C18—H18C	109.5
C8—C7—H7	108.7	H18B—C18—H18C	109.5
C6—C7—H7	108.7	C17′—C18′—H18D	109.5
C13—C8—C9	120.6 (3)	C17′—C18′—H18E	109.5
C13—C8—C7	120.3 (3)	H18D—C18′—H18E	109.5
C9—C8—C7	119.0 (3)	C17′—C18′—H18F	109.5
O2—C9—C8	121.7 (3)	H18D—C18′—H18F	109.5
O2—C9—C10	120.1 (3)	H18E—C18′—H18F	109.5
C8—C9—C10	118.2 (3)	C24—C19—N1	120.0 (3)
C9—C10—C11	110.6 (3)	C24—C19—C20	121.1 (3)
C9—C10—H10A	109.5	N1—C19—C20	119.0 (3)
C11—C10—H10A	109.5	C19—C20—C21	115.0 (3)
C9—C10—H10B	109.5	C19—C20—H20A	108.5
C11—C10—H10B	109.5	C21—C20—H20A	108.5
H10A—C10—H10B	108.1	C19—C20—H20B	108.5
C14—C11—C12	110.2 (3)	C21—C20—H20B	108.5
C14—C11—C15	109.7 (3)	H20A—C20—H20B	107.5
C12—C11—C15	109.2 (3)	C20—C21—C22	108.7 (3)
C14—C11—C10	110.0 (3)	C20—C21—C26	111.0 (3)
C12—C11—C10	108.2 (3)	C22—C21—C26	110.0 (3)
C15—C11—C10	109.6 (4)	C20—C21—C25	108.8 (3)
C13—C12—C11	114.6 (3)	C22—C21—C25	109.5 (3)
C13—C12—H12A	108.6	C26—C21—C25	109.0 (3)
C11—C12—H12A	108.6	C23—C22—C21	112.1 (3)
C13—C12—H12B	108.6	C23—C22—H22A	109.2
C11—C12—H12B	108.6	C21—C22—H22A	109.2
H12A—C12—H12B	107.6	C23—C22—H22B	109.2
C8—C13—N1	120.0 (3)	C21—C22—H22B	109.2
C8—C13—C12	121.5 (3)	H22A—C22—H22B	107.9
N1—C13—C12	118.5 (3)	O3—C23—C24	121.2 (3)
C11—C14—H14A	109.5	O3—C23—C22	121.5 (3)
C11—C14—H14B	109.5	C24—C23—C22	117.4 (3)
H14A—C14—H14B	109.5	C19—C24—C23	121.6 (3)
C11—C14—H14C	109.5	C19—C24—C7	120.6 (3)
H14A—C14—H14C	109.5	C23—C24—C7	117.8 (3)

H14B—C14—H14C	109.5	C21—C25—H25A	109.5
C11—C15—H15A	109.5	C21—C25—H25B	109.5
C11—C15—H15B	109.5	H25A—C25—H25B	109.5
H15A—C15—H15B	109.5	C21—C25—H25C	109.5
C11—C15—H15C	109.5	H25A—C25—H25C	109.5
H15A—C15—H15C	109.5	H25B—C25—H25C	109.5
H15B—C15—H15C	109.5	C21—C26—H26A	109.5
N1—C16—C17	114.8 (4)	C21—C26—H26B	109.5
N1—C16—C17′	107.9 (5)	H26A—C26—H26B	109.5
C17—C16—C17′	13.0 (11)	C21—C26—H26C	109.5
N1—C16—H16A	108.6	H26A—C26—H26C	109.5
C17—C16—H16A	108.6	H26B—C26—H26C	109.5

O1—C1—C2—C3	180.0 (3)	C11—C12—C13—C8	−8.0 (5)
C6—C1—C2—C3	−2.3 (6)	C11—C12—C13—N1	171.6 (3)
C1—C2—C3—C4	−0.5 (6)	C13—N1—C16—C17	−91.6 (6)
C2—C3—C4—C5	1.8 (5)	C19—N1—C16—C17	94.3 (6)
C2—C3—C4—Br1	−177.9 (3)	C13—N1—C16—C17′	−103.5 (10)
C3—C4—C5—C6	−0.1 (5)	C19—N1—C16—C17′	82.4 (10)
Br1—C4—C5—C6	179.5 (3)	N1—C16—C17—O4	49.4 (8)
C4—C5—C6—C1	−2.6 (5)	C17′—C16—C17—O4	110 (4)
C4—C5—C6—C7	178.7 (3)	N1—C16—C17—C18	−76.5 (8)
O1—C1—C6—C5	−178.6 (3)	C17′—C16—C17—C18	−16 (3)
C2—C1—C6—C5	3.8 (5)	N1—C16—C17′—O4′	−177.2 (10)
O1—C1—C6—C7	0.1 (5)	C17—C16—C17′—O4′	59 (3)
C2—C1—C6—C7	−177.6 (3)	N1—C16—C17′—C18′	74.8 (16)
C5—C6—C7—C24	−28.8 (4)	C17—C16—C17′—C18′	−49 (4)
C1—C6—C7—C24	152.6 (3)	C13—N1—C19—C24	15.8 (5)
C5—C6—C7—C8	92.0 (4)	C16—N1—C19—C24	−170.1 (3)
C1—C6—C7—C8	−86.6 (4)	C13—N1—C19—C20	−163.1 (3)
C24—C7—C8—C13	34.3 (4)	C16—N1—C19—C20	11.1 (4)
C6—C7—C8—C13	−88.5 (4)	C24—C19—C20—C21	16.5 (5)
C24—C7—C8—C9	−146.0 (3)	N1—C19—C20—C21	−164.7 (3)
C6—C7—C8—C9	91.2 (4)	C19—C20—C21—C22	−46.6 (4)
C13—C8—C9—O2	177.8 (3)	C19—C20—C21—C26	74.4 (4)
C7—C8—C9—O2	−1.9 (5)	C19—C20—C21—C25	−165.8 (3)
C13—C8—C9—C10	−3.3 (5)	C20—C21—C22—C23	55.7 (4)
C7—C8—C9—C10	177.0 (3)	C26—C21—C22—C23	−65.9 (4)
O2—C9—C10—C11	−140.9 (3)	C25—C21—C22—C23	174.4 (3)
C8—C9—C10—C11	40.3 (4)	C21—C22—C23—O3	144.8 (3)
C9—C10—C11—C14	62.2 (4)	C21—C22—C23—C24	−35.9 (4)
C9—C10—C11—C12	−58.2 (4)	N1—C19—C24—C23	−172.3 (3)
C9—C10—C11—C15	−177.2 (3)	C20—C19—C24—C23	6.5 (5)
C14—C11—C12—C13	−77.2 (4)	N1—C19—C24—C7	9.1 (5)
C15—C11—C12—C13	162.3 (3)	C20—C19—C24—C7	−172.1 (3)
C10—C11—C12—C13	43.1 (4)	O3—C23—C24—C19	−177.0 (3)
C9—C8—C13—N1	166.7 (3)	C22—C23—C24—C19	3.7 (5)
C7—C8—C13—N1	−13.6 (5)	O3—C23—C24—C7	1.6 (5)

C9—C8—C13—C12	−13.7 (5)	C22—C23—C24—C7	−177.7 (3)
C7—C8—C13—C12	165.9 (3)	C8—C7—C24—C19	−31.9 (4)
C19—N1—C13—C8	−13.5 (5)	C6—C7—C24—C19	90.4 (4)
C16—N1—C13—C8	172.4 (3)	C8—C7—C24—C23	149.4 (3)
C19—N1—C13—C12	166.9 (3)	C6—C7—C24—C23	−88.2 (4)
C16—N1—C13—C12	−7.2 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.84	1.78	2.621 (4)	176
C10—H10*A*···O1^{i}	0.99	2.54	3.417 (5)	147

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