organic compounds

(E)-N-Butyl-3-(3,4-dihydroxyphenyl)-acrylamide hemihydrate

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In the title compound, $C_{13}H_{17}NO_3 \cdot 0.5H_2O$, a new caffeic acid amide derivative, the solvent water molecule lies on a twofold axis and the terminal ethyl group appears disordered with occupancy factors of 0.525 (6) and 0.475 (6). The benzene ring makes an angle of 17.3 (2)° with the C=C—C—O linker. The presence of an ethylenic spacer in the caffeic acid amide molecule allows the formation of a conjugated system, strongly stabilized through π-electron delocalization. The C=C double bond in the linker is *trans*, similar to those previously reported in caffeic esters. The crystal is stabilized by O—H···O, N—H···O and C—H···O hydrogen bonds. The molecules of the caffeic acid amide form a supermolecular planar structure through O—H···O hydrogen bonds between a hydroxy group of one caffeic acid molecule and a carbonyl O atom of another. These planes interact *via* C—H···O, O—H···O and N—H···O hydrogen bonds to form a three-dimensional network.

Related literature

For phenolic acid compounds used in biology and medicine, see: Altuğ *et al.* (2008). For synthetic work on the similar compounds, see: Bylov *et al.* (1999). For compounds with similar properties, see: Son & Lewis (2002); Menezes *et al.* (2001); Lee *et al.* (2005). For the structure analysis of a similar compound, see: Xia *et al.* (2008).
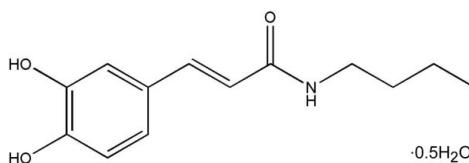
Experimental

Crystal data

$C_{13}H_{17}NO_3 \cdot 0.5H_2O$	V = 2634 (3) Å^3
M_r = 244.29	Z = 8
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 12.860 (7) Å	μ = 0.09 mm^{-1}
b = 14.928 (8) Å	T = 296 K
c = 15.015 (11) Å	$0.28 \times 0.22 \times 0.19$ mm
β = 113.967 (6)°	

Data collection

Bruker SMART APEX CCD diffractometer	7822 measured reflections
	2581 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)	1895 reflections with $I > 2\sigma(I)$
T_{min} = 0.977, T_{max} = 0.983	R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042	180 parameters
$wR(F^2)$ = 0.120	H-atom parameters constrained
S = 1.04	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
2581 reflections	$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···O3^i	0.85	1.91	2.7402 (19)	165
O4—H4B···O3^{ii}	0.85	1.91	2.7402 (19)	165
N1—H1B···O2^{iii}	0.86	2.29	3.129 (2)	165
N1—H1B···O1^{iii}	0.86	2.58	3.143 (3)	124
O1—H1A···O3^{iv}	0.82	1.94	2.7378 (19)	162
O2—H2A···O4^v	0.82	2.00	2.8217 (18)	177
C7—H7···O3	0.93	2.48	2.837 (2)	103
C8—H8···O2^{iii}	0.93	2.55	3.330 (2)	142

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

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); 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: BG2440).

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supplementary materials

(*E*)-*N*-Butyl-3-(3,4-dihydroxyphenyl)acrylamide hemihydrate

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Comment

Phenolic acids and their derivatives (esters, amides) are widely distributed in plants and can be present in considerable amounts in the human diet, which attract much attention in biology and medicine (Altuğ *et al.*, 2008). Phenolic acid amides, is a large class of organic compounds formed by the condensation reaction of aromatic acid and amine (Bylov *et al.*, 1999). The –CO—NH– backbone makes amides have the pharmacological functionality such as anti-proliferative, antiviral, antimalarial, general anesthetics and antimicrobials. Therefore, more and more phenolic acid amides have already been researched purposively and developed as potential anti-proliferative, antiviral, antimalarial, and antimicrobials drugs in recent years (Son & Lewis, 2002; Menezes *et al.*, 2001; Lee *et al.*, 2005). So in this paper, we synthesized and report on the structure of a new caffeic acid amide derivative, (*E*)-*N*-butyl-3-(3,4-dihydroxyphenyl)acrylamide monohydrate.

In the title compound (Fig. 1), all values of the geometric parameters are normal, the terminal C12—C13 group being disorderd with occupation factors of 0.525/0.475 (6) for both moieties. The benzene ring is planar within experimental observation (r.m.s. deviation: 0.005Å) and it makes an angle of 17.3 (2)° to the (C7—C8—C9—O3) linker. In the case of caffeic amide, the presence of an ethylenic spacer allows the formation of a conjugated system, strongly stabilized through π-electron delocalization. The C7═C8 bond is a *trans*-double bond, the same as in caffeic esters reported before (Xia *et al.*, 2008).

The crystal is stabilized by intermolecular O—H···O, N—H···O, O—H···N and C—H···O hydrogen bonds (Fig. 2). The molecules of the caffeic acid amide form a supermolecule plane structure through O—H···O hydrogen bonds between a hydroxyl of a caffeic acid and carbonyl O atom from another caffeic acid molecule. The supermolecule plane interacts with the another plane with C—H···O, O—H···O, N—H···O and O—H···N hydrogen bonds to form a three-dimensional network.

Experimental

To a stirred THF solution (15 ml) of commercial caffeic acid (0.179 g, 1 mmol) was added DCC (1.5 mmol) in THF (5 ml) at 0°C. The reaction mixture was stirred for 2 h at 0°C and *n*-butylamine (0.088 g, 1.2 mmol) was added for reacting overnight at room temperature, and then the precipitated dicyclohexylurea was filtered and washed with tetrahydrofuran. The combined filtrates were evaporated, the residue was extracted with EtOAc, and the extract was washed with 1 N NaHCO$_3$, H$_2$O, and 1 N HCl, dried over Na$_2$SO$_4$, and evaporated. The title compound was obtained by elution of the column with 25% petrole:EtOAc and recrystallized to give the pale yellow block crystal.

Refinement

All the H atoms were seen in a difference map but repositioned geometrically (C—H = 0.93–0.97, N—H = 0.86 and O—H = 0.85 Å) and refined as riding with U_{iso} = 1.2Ueq. The C12—C13 pair is disordered into two moieties with

occupancies of 0.525/0.475 (6).

Computing details

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); 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* (Sheldrick, 2008).
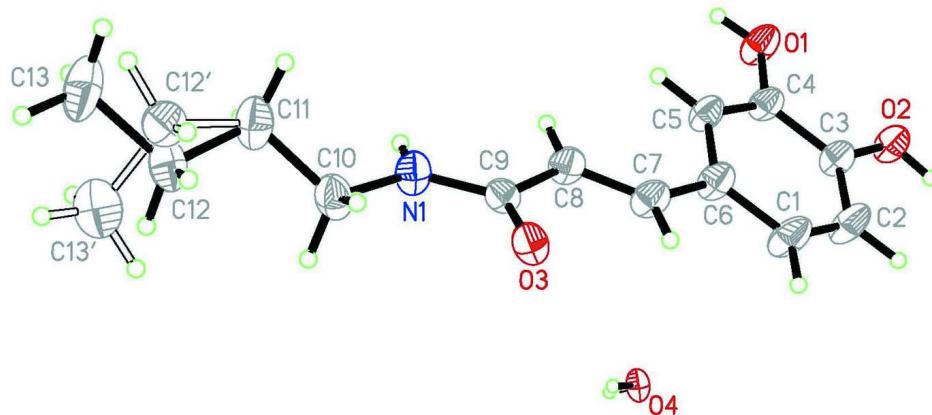

Figure 1

View of the molecular structure of (*E*)-*N*-butyl-3-(3,4-dihydroxyphenyl)acrylamide monohydrate with displacement ellipsoids at the 30% probability level. In open bonds, the minor part of the disordered tail.
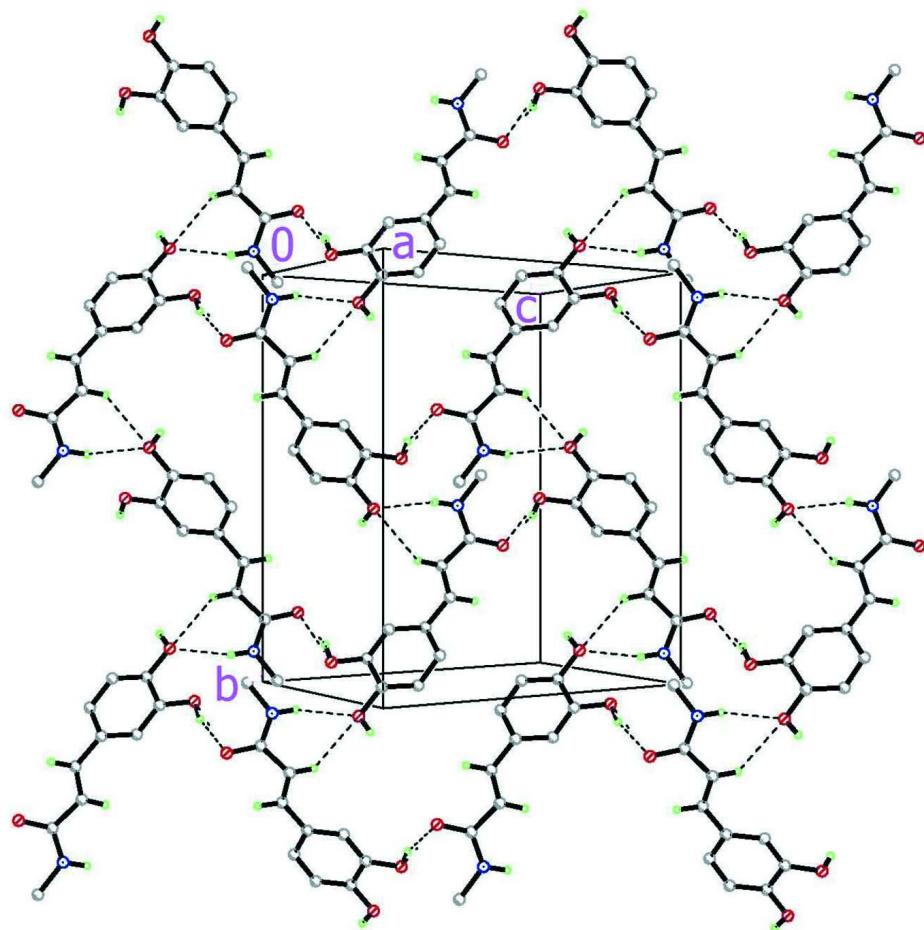
Figure 2

The two-dimensional plane formed by the hydrogen bonds of the molecules (Dashed lines represent hydrogen bonds, some of the H and C atoms have been omitted)

(*E*)-*N*-Butyl-3-(3,4-dihydroxyphenyl)acrylamide monohydrate

Crystal data

$C_{13}H_{17}NO_3 \cdot 0.5H_2O$	$F(000) = 1048$
$M_r = 244.29$	$D_x = 1.232$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 2581 reflections
$a = 12.860\ (7)$ Å	$\theta = 2.2–26.0°$
$b = 14.928\ (8)$ Å	$\mu = 0.09$ mm^{-1}
$c = 15.015\ (11)$ Å	$T = 296$ K
$\beta = 113.967\ (6)°$	Block, yellow
$V = 2634\ (3)$ Å^3	$0.28 \times 0.22 \times 0.19$ mm
$Z = 8$	

Data collection

Bruker SMART APEX CCD diffractometer	φ and ω scans
	Absorption correction: multi-scan
Radiation source: fine-focus sealed tube	(*SADABS*; Sheldrick, 2008)
Graphite monochromator	$T_{min} = 0.977$, $T_{max} = 0.983$

7822 measured reflections	$\theta_{max} = 26.0°$, $\theta_{min} = 2.2°$
2581 independent reflections	$h = -15 \rightarrow 15$
1895 reflections with $I > 2\sigma(I)$	$k = -18 \rightarrow 15$
$R_{int} = 0.025$	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.120$	
$S = 1.04$	H-atom parameters constrained
2581 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2 + 1.0544P]$ where $P = (F_o^2 + 2F_c^2)/3$
180 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.18$ e Å^{-3}
	$\Delta\rho_{min} = -0.21$ 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. The terminal C13 and methylene C12 have been treated disorderd.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O4	0.5000	0.79934 (9)	0.7500	0.0471 (4)	
H4A	0.5047	0.7659	0.7973	0.057*	0.50
H4B	0.4953	0.7659	0.7027	0.057*	0.50
N1	0.63571 (12)	0.56741 (9)	−0.01730 (9)	0.0517 (4)	
H1B	0.6878	0.5587	0.0401	0.062*	
O1	0.83466 (10)	0.95089 (8)	0.33417 (8)	0.0653 (4)	
H1A	0.8785	0.9099	0.3375	0.098*	
O2	0.67900 (9)	1.07499 (8)	0.30337 (8)	0.0558 (3)	
H2A	0.6254	1.1101	0.2869	0.084*	
O3	0.51295 (9)	0.66595 (7)	−0.12054 (7)	0.0493 (3)	
C1	0.53067 (15)	0.93015 (13)	0.09233 (13)	0.0656 (6)	
H1	0.4611	0.9268	0.0388	0.079*	
C2	0.55145 (15)	1.00043 (13)	0.15684 (13)	0.0638 (5)	
H2	0.4962	1.0443	0.1459	0.077*	
C3	0.65313 (13)	1.00632 (11)	0.23735 (11)	0.0491 (4)	
C4	0.73642 (13)	0.94036 (11)	0.25296 (11)	0.0479 (4)	
C5	0.71557 (13)	0.87094 (11)	0.18753 (11)	0.0498 (4)	
H5	0.7713	0.8277	0.1977	0.060*	
C6	0.61164 (14)	0.86440 (12)	0.10578 (11)	0.0522 (4)	
C7	0.58305 (13)	0.79218 (12)	0.03400 (12)	0.0520 (4)	
H7	0.5189	0.8017	−0.0233	0.062*	

C8	0.63569 (13)	0.71565 (11)	0.03940 (11)	0.0483 (4)	
H8	0.7026	0.7038	0.0935	0.058*	
C9	0.59066 (12)	0.64825 (10)	−0.03873 (10)	0.0410 (4)	
C10	0.60274 (16)	0.49214 (12)	−0.08466 (13)	0.0608 (5)	
H10A	0.5750	0.5145	−0.1509	0.073*	
H10B	0.5411	0.4598	−0.0776	0.073*	
C11	0.69973 (18)	0.42951 (12)	−0.06711 (14)	0.0678 (5)	
H11A	0.7326	0.4095	0.0002	0.081*	
H11B	0.7585	0.4582	−0.0819	0.081*	
C12	0.6467 (8)	0.3505 (6)	−0.1365 (8)	0.077 (2)	0.525 (6)
H12A	0.5909	0.3206	−0.1188	0.093*	0.525 (6)
H12B	0.6088	0.3720	−0.2029	0.093*	0.525 (6)
C13	0.7411 (5)	0.2857 (3)	−0.1286 (4)	0.097 (2)	0.525 (6)
H13A	0.7933	0.3148	−0.1503	0.146*	0.525 (6)
H13B	0.7089	0.2342	−0.1686	0.146*	0.525 (6)
H13C	0.7808	0.2673	−0.0620	0.146*	0.525 (6)
C12′	0.6881 (7)	0.3529 (8)	−0.1425 (9)	0.073 (2)	0.475 (6)
H12C	0.6553	0.3766	−0.2083	0.088*	0.475 (6)
H12D	0.7624	0.3283	−0.1305	0.088*	0.475 (6)
C13′	0.6133 (5)	0.2818 (4)	−0.1313 (4)	0.098 (2)	0.475 (6)
H13D	0.6453	0.2599	−0.0655	0.147*	0.475 (6)
H13E	0.6074	0.2334	−0.1752	0.147*	0.475 (6)
H13F	0.5391	0.3061	−0.1458	0.147*	0.475 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4	0.0635 (10)	0.0324 (8)	0.0410 (8)	0.000	0.0166 (7)	0.000
N1	0.0572 (8)	0.0449 (8)	0.0358 (7)	0.0049 (6)	0.0011 (6)	0.0003 (6)
O1	0.0455 (6)	0.0695 (9)	0.0532 (7)	0.0148 (6)	−0.0085 (5)	−0.0213 (6)
O2	0.0493 (6)	0.0568 (7)	0.0478 (7)	0.0099 (5)	0.0059 (5)	−0.0159 (5)
O3	0.0523 (6)	0.0427 (7)	0.0359 (6)	−0.0050 (5)	0.0005 (5)	0.0034 (5)
C1	0.0442 (9)	0.0799 (14)	0.0484 (10)	0.0186 (9)	−0.0062 (8)	−0.0193 (9)
C2	0.0478 (9)	0.0726 (13)	0.0521 (10)	0.0236 (9)	0.0006 (8)	−0.0175 (9)
C3	0.0446 (8)	0.0536 (10)	0.0400 (8)	0.0058 (7)	0.0079 (7)	−0.0120 (7)
C4	0.0378 (8)	0.0562 (10)	0.0373 (8)	0.0061 (7)	0.0024 (6)	−0.0053 (7)
C5	0.0412 (8)	0.0523 (10)	0.0447 (9)	0.0120 (7)	0.0060 (7)	−0.0071 (7)
C6	0.0457 (9)	0.0580 (11)	0.0399 (9)	0.0090 (7)	0.0042 (7)	−0.0110 (8)
C7	0.0413 (8)	0.0614 (11)	0.0389 (8)	0.0057 (7)	0.0015 (7)	−0.0087 (7)
C8	0.0424 (8)	0.0521 (10)	0.0372 (8)	0.0028 (7)	0.0025 (7)	−0.0036 (7)
C9	0.0393 (7)	0.0435 (9)	0.0344 (8)	−0.0038 (6)	0.0092 (6)	0.0020 (6)
C10	0.0609 (11)	0.0474 (11)	0.0547 (10)	−0.0030 (8)	0.0033 (9)	−0.0042 (8)
C11	0.0828 (14)	0.0510 (11)	0.0556 (11)	0.0111 (10)	0.0138 (10)	0.0000 (9)
C12	0.096 (6)	0.048 (4)	0.090 (4)	−0.003 (4)	0.040 (4)	−0.018 (3)
C13	0.141 (5)	0.061 (3)	0.106 (4)	0.029 (3)	0.067 (3)	−0.009 (2)
C12′	0.076 (5)	0.066 (5)	0.089 (4)	−0.003 (4)	0.044 (4)	−0.008 (3)
C13′	0.113 (5)	0.074 (4)	0.109 (4)	−0.002 (3)	0.046 (4)	0.001 (3)

Geometric parameters (Å, º)

O4—H4A	0.8501	C8—C9	1.474 (2)
O4—H4B	0.8501	C8—H8	0.9300
N1—C9	1.321 (2)	C10—C11	1.494 (3)
N1—C10	1.455 (2)	C10—H10A	0.9700
N1—H1B	0.8600	C10—H10B	0.9700
O1—C4	1.3624 (19)	C11—C12	1.537 (9)
O1—H1A	0.8200	C11—C12′	1.574 (11)
O2—C3	1.3699 (19)	C11—H11A	0.9700
O2—H2A	0.8200	C11—H11B	0.9700
O3—C9	1.2571 (18)	C12—C13	1.519 (10)
C1—C2	1.378 (2)	C12—H12A	0.9700
C1—C6	1.385 (2)	C12—H12B	0.9700
C1—H1	0.9300	C13—H13A	0.9600
C2—C3	1.377 (2)	C13—H13B	0.9600
C2—H2	0.9300	C13—H13C	0.9600
C3—C4	1.403 (2)	C12′—C13′	1.487 (11)
C4—C5	1.377 (2)	C12′—H12C	0.9700
C5—C6	1.403 (2)	C12′—H12D	0.9700
C5—H5	0.9300	C13′—H13D	0.9600
C6—C7	1.462 (2)	C13′—H13E	0.9600
C7—C8	1.314 (2)	C13′—H13F	0.9600
C7—H7	0.9300		
H4A—O4—H4B	108.0	N1—C10—C11	111.97 (15)
C9—N1—C10	124.15 (14)	N1—C10—H10A	109.2
C9—N1—H1B	117.9	C11—C10—H10A	109.2
C10—N1—H1B	117.9	N1—C10—H10B	109.2
C4—O1—H1A	109.5	C11—C10—H10B	109.2
C3—O2—H2A	109.5	H10A—C10—H10B	107.9
C2—C1—C6	121.15 (15)	C10—C11—C12	104.6 (4)
C2—C1—H1	119.4	C10—C11—C12′	120.0 (4)
C6—C1—H1	119.4	C10—C11—H11A	110.8
C3—C2—C1	120.63 (15)	C12—C11—H11A	110.8
C3—C2—H2	119.7	C12′—C11—H11A	113.6
C1—C2—H2	119.7	C10—C11—H11B	110.8
O2—C3—C2	123.23 (14)	C12—C11—H11B	110.8
O2—C3—C4	117.38 (14)	C12′—C11—H11B	90.6
C2—C3—C4	119.37 (15)	H11A—C11—H11B	108.9
O1—C4—C5	124.49 (14)	C13—C12—C11	108.4 (6)
O1—C4—C3	115.86 (14)	C13—C12—H12A	110.0
C5—C4—C3	119.65 (14)	C11—C12—H12A	110.0
C4—C5—C6	121.09 (14)	C13—C12—H12B	110.0
C4—C5—H5	119.5	C11—C12—H12B	110.0
C6—C5—H5	119.5	H12A—C12—H12B	108.4
C1—C6—C5	118.09 (15)	C13′—C12′—C11	108.3 (6)
C1—C6—C7	117.78 (15)	C13′—C12′—H12C	110.0
C5—C6—C7	124.13 (15)	C11—C12′—H12C	110.0
C8—C7—C6	128.82 (15)	C13′—C12′—H12D	110.0

C8—C7—H7	115.6	C11—C12′—H12D	110.0
C6—C7—H7	115.6	H12C—C12′—H12D	108.4
C7—C8—C9	121.24 (15)	C12′—C13′—H13D	109.5
C7—C8—H8	119.4	C12′—C13′—H13E	109.5
C9—C8—H8	119.4	H13D—C13′—H13E	109.5
O3—C9—N1	121.73 (14)	C12′—C13′—H13F	109.5
O3—C9—C8	122.27 (14)	H13D—C13′—H13F	109.5
N1—C9—C8	116.00 (13)	H13E—C13′—H13F	109.5
C6—C1—C2—C3	−0.9 (3)	C5—C6—C7—C8	12.7 (3)
C1—C2—C3—O2	179.32 (18)	C6—C7—C8—C9	176.70 (16)
C1—C2—C3—C4	0.6 (3)	C10—N1—C9—O3	1.0 (2)
O2—C3—C4—O1	1.2 (2)	C10—N1—C9—C8	−179.89 (15)
C2—C3—C4—O1	179.99 (17)	C7—C8—C9—O3	12.8 (2)
O2—C3—C4—C5	−178.59 (15)	C7—C8—C9—N1	−166.28 (16)
C2—C3—C4—C5	0.2 (3)	C9—N1—C10—C11	148.87 (17)
O1—C4—C5—C6	179.54 (17)	N1—C10—C11—C12	174.2 (4)
C3—C4—C5—C6	−0.7 (3)	N1—C10—C11—C12′	−169.8 (4)
C2—C1—C6—C5	0.4 (3)	C10—C11—C12—C13	176.3 (5)
C2—C1—C6—C7	−179.91 (18)	C12′—C11—C12—C13	37.4 (19)
C4—C5—C6—C1	0.4 (3)	C10—C11—C12′—C13′	−74.3 (8)
C4—C5—C6—C7	−179.25 (17)	C12—C11—C12′—C13′	−27.1 (17)
C1—C6—C7—C8	−166.91 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O3[i]	0.85	1.91	2.7402 (19)	165
O4—H4*B*···O3[ii]	0.85	1.91	2.7402 (19)	165
N1—H1*B*···O2[iii]	0.86	2.29	3.129 (2)	165
N1—H1*B*···O1[iii]	0.86	2.58	3.143 (3)	124
O1—H1*A*···O3[iv]	0.82	1.94	2.7378 (19)	162
O2—H2*A*···O4[v]	0.82	2.00	2.8217 (18)	177
C7—H7···O3	0.93	2.48	2.837 (2)	103
C8—H8···O2[iii]	0.93	2.55	3.330 (2)	142

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