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2-Amino-4-(4-methoxyphenyl)-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile 1,4-dioxane hemisolvate

Shaaban K. Mohamed,[a] Mehmet Akkurt,[b]* Muhammad N. Tahir,[c] Antar A. Abdelhamid[a] and Sabry H. H. Younes[d]

[a]Chemistry and Environmental Division, Manchester Metropolitan University, Manchester M1 5GD, England, [b]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [c]University of Sargodha, Department of Physics, Sargodha, Pakistan, and [d]Chemistry Department, Faculty of Science, Sohag University, Sohag 82524, Egypt
Correspondence e-mail: akkurt@erciyes.edu.tr

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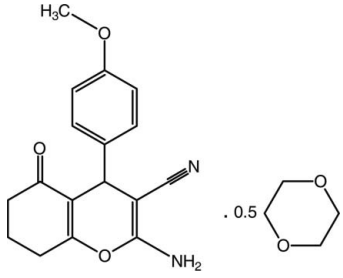
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.059; wR factor = 0.194; data-to-parameter ratio = 18.1.

In the crystal structure of the title compound, $C_{17}H_{16}N_2O_3\cdot 0.5C_4H_8O_2$, pairs of N—H···N hydrogen bonds link molecules into dimers with $R_2^2(12)$ motifs, which are connected by N—H···O hydrogen bonds, forming a supramolecular array in the *ab* plane. The 1,4-dioxane ring, which lies about an inversion center, adopts a chair conformation.

Related literature

For the biological activity of pyran and fused-pyran molecules, see: Bargagna *et al.* (1992); Symeonidis *et al.* (2009); Narender & Gupta (2009); Alvey *et al.* (2009); Gorlitzer *et al.* (1984); Han *et al.* (2008); Martinez & Marco (1997); Smith *et al.* (1998); Taylor *et al.* (1998). For related structures, see: Gourdeau *et al.* (2004); Foroumadi *et al.* (2007); Mohamed *et al.* (2012). For puckering parameters, see: Cremer & Pople (1975). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{17}H_{16}N_2O_3\cdot 0.5C_4H_8O_2$
M_r = 340.37
Triclinic, $P\overline{1}$
a = 8.0876 (4) Å
b = 9.2013 (4) Å
c = 12.1613 (6) Å
α = 94.376 (2)°
β = 102.827 (1)°
γ = 95.972 (2)°
V = 873.01 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.35 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.973, T_{max} = 0.980
14186 measured reflections
4108 independent reflections
3134 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.194
S = 1.07
4108 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^{i}	0.86	2.27	3.123 (3)	171
N1—H1B···O3^{ii}	0.86	2.10	2.945 (2)	167

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x+1, y, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5115).

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supplementary materials

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2-Amino-4-(4-methoxyphenyl)-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile 1,4-dioxane hemisolvate

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Comment

Pyran and fused pyran ring systems are biologically interesting compounds known for their antimicrobial and antifungal (Alvey, *et al.*, 2009), antioxidant (Symeonidis *et al.*, 2009), antileishmanial (Narender *et al.*, 2009), antitumor (Han *et al.*, 2008). In addition, fused chromene ring systems have platelet antiaggregating, local anesthetic (Bargagna *et al.* 1992) and antihistaminic activities (Gorlitzer *et al.* 1984). They also exhibit inhibitory effects on influenza virus sialidases (Smith *et al.* 1998; Taylor *et al.* 1998) and antiviral activities (Martinez & Marco, 1997). Such observations prompted us to report the synthesis and crystal structure of the title compound (I).

In (I), Fig. 1, the O2/C8—C10/C12/C13 4*H*-pyran and C12–C17 cyclohexene rings are puckered with puckering parameters (Cremer & Pople, 1975) of Q_T = 0.187 (2) Å, θ = 72.2 (5) °, φ = 175.7 (6) ° and Q_T = 0.455 (2) ° A, θ = 122.9 (3) °, φ = 48.5 (3) °, respectively. The centroid of the solvent 1,4-dioxane ring (O4/C18/C19/O4a/C18*a*/C19*a*) lies about an inversion center. The 1,4-dioxane ring adopts a chair conformation [puckering parameters Q_T = 0.560 (5) Å, θ = 3.46 (3) °, φ = 0.00 °]. The values of the bond lengths and angles in (I) are in normal ranges and are comparable with those of related structures (Gourdeau *et al.*, 2004; Foroumadi *et al.*, 2007; Mohamed *et al.*, 2012).

In the crystal, molecules are linked by the pairs of N—H···N hydrogen bonds, forming dimers, with an $R^2_2(12)$ motif (Bernstein *et al.*, 1995; Table 1, Fig. 2). These dimers are connected through the N—H···O hydrogen bonds with each other (Table 1, Fig. 2).

Experimental

A mixture of (4-methoxybenzylidene)propanedinitrile (184 mg, 1 mmol), cyclohexane-1,3-dione (112 mg, 1 mmol) in presence of ethanolamine (61 mg) as catalyst was refluxed in ethanol (50 ml). The reaction mixture was monitored by TLC until completion after 7 h. A solid product was deposited on cooling at ambient temperature and collected by filtration. The crude product was washed with dioxane and recrystallized from ethanol/drops of dioxane to afford the title compound in 78% yield. Single crystals suitable for X-ray analysis were grown up on slow evaporation of its mixed solvent ethanol/dioxane (9:1) solution at room temperature over three days. *M*.pt: 435 K.

Refinement

All H atoms were positioned geometrically and refined by using a riding model, with N—H = 0.86 Å and C—H = 0.93 Å (aromatic), 0.96 Å (methyl), 0.97 Å (methylene) and 0.98 Å (methine), with U_{iso}(H) = 1.5U_{eq}(C) for methyl-H and U_{iso}(H) = 1.2U_{eq}(C, N) for other H-atoms.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

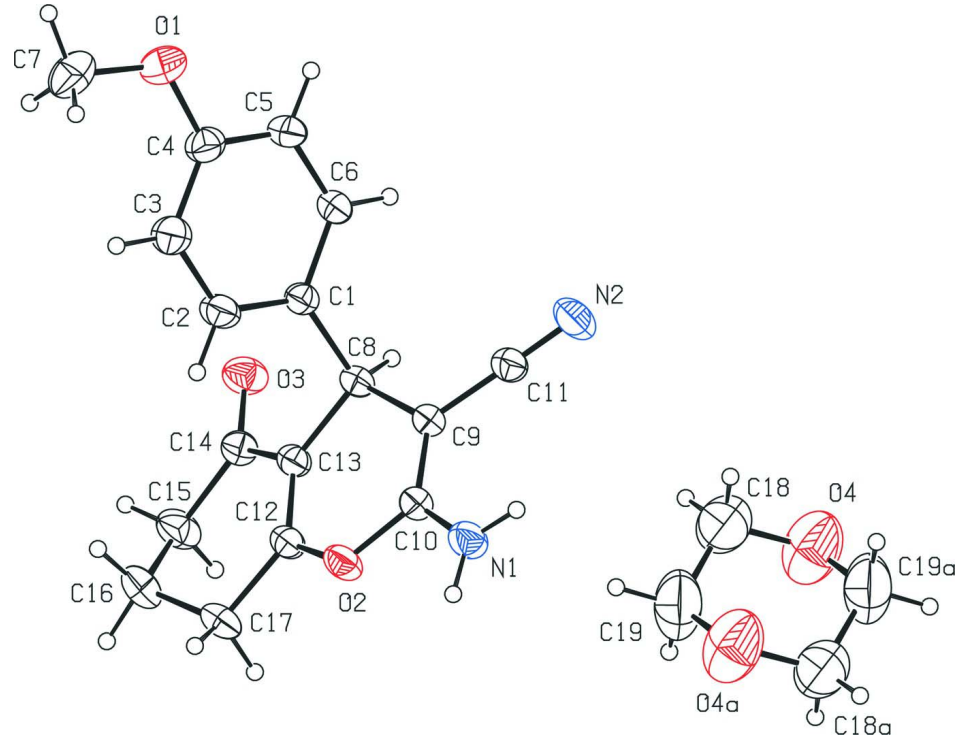

Figure 1

View of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

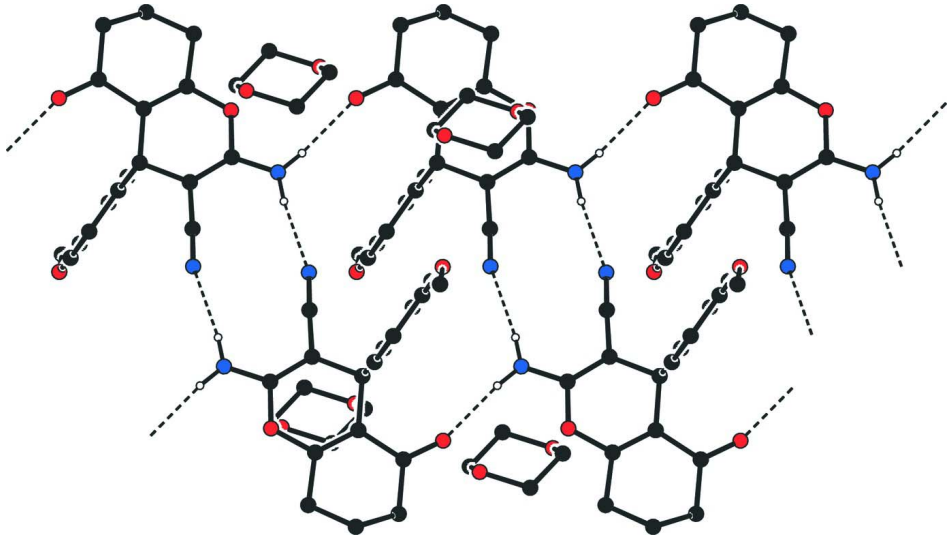

Figure 2

View of the dimers formed by pairs of N—H···N hydrogen bonds (dashed lines), with an $R^2_2(12)$ motif, and the N—H···O hydrogen bonds (dashed lines) which connect the dimers with each other, forming a two-dimensional array. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (*a*) 2 - *x*, 2 - *y*, 2 - *z*].

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Crystal data

$C_{17}H_{16}N_2O_3 \cdot 0.5C_4H_8O_2$
$M_r = 340.37$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.0876$ (4) Å
$b = 9.2013$ (4) Å
$c = 12.1613$ (6) Å
$\alpha = 94.376$ (2)°
$\beta = 102.827$ (1)°
$\gamma = 95.972$ (2)°
$V = 873.01$ (7) Å^3
$Z = 2$
$F(000) = 360$
$D_x = 1.295$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 420 reflections
$\theta = 3.6$–22.5°
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Prism, light-yellow
0.35 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0.81 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.973$, $T_{max} = 0.980$
14186 measured reflections
4108 independent reflections
3134 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.9°$, $\theta_{min} = 1.7°$
$h = -10 \rightarrow 10$
$k = -12 \rightarrow 8$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.194$
$S = 1.07$
4108 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
$w = 1/[\sigma^2(F_o^2) + (0.0997P)^2 + 0.273P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	0.1813 (2)	0.42680 (19)	0.00491 (15)	0.0760 (6)
O2	0.93204 (16)	0.95097 (14)	0.33842 (12)	0.0512 (4)
O3	0.36871 (18)	0.99158 (15)	0.37001 (14)	0.0595 (5)
N1	1.0877 (2)	0.77420 (19)	0.39337 (15)	0.0563 (6)
N2	0.8057 (3)	0.5088 (2)	0.49805 (19)	0.0712 (7)
C1	0.5009 (2)	0.70436 (17)	0.26984 (14)	0.0389 (5)
C2	0.4984 (3)	0.7302 (2)	0.15944 (17)	0.0531 (6)
C3	0.3939 (3)	0.6405 (2)	0.06812 (18)	0.0583 (7)
C4	0.2893 (3)	0.5219 (2)	0.08782 (18)	0.0537 (6)
C5	0.2917 (3)	0.4941 (2)	0.19793 (19)	0.0563 (7)
C6	0.3951 (2)	0.58441 (19)	0.28771 (17)	0.0476 (6)
C7	0.1568 (4)	0.4634 (3)	−0.1082 (2)	0.0809 (9)
C8	0.6180 (2)	0.79962 (17)	0.37058 (14)	0.0387 (5)
C9	0.7912 (2)	0.74660 (18)	0.40311 (14)	0.0405 (5)
C10	0.9333 (2)	0.81758 (19)	0.38054 (14)	0.0420 (5)
C11	0.8019 (2)	0.6148 (2)	0.45477 (17)	0.0487 (6)
C12	0.7895 (2)	1.02140 (18)	0.33096 (14)	0.0422 (5)
C13	0.6429 (2)	0.95783 (18)	0.34927 (14)	0.0403 (5)
C14	0.5022 (2)	1.04491 (19)	0.35100 (15)	0.0461 (6)
C15	0.5308 (3)	1.2042 (2)	0.3328 (2)	0.0634 (8)
C16	0.6528 (3)	1.2323 (2)	0.2563 (2)	0.0660 (8)
C17	0.8203 (3)	1.1737 (2)	0.29963 (18)	0.0537 (6)
O4	0.8992 (4)	0.9746 (4)	1.0758 (2)	0.1475 (16)
C18	0.8279 (5)	0.9756 (5)	0.9615 (4)	0.1243 (19)
C19	0.9322 (6)	1.0707 (6)	0.9113 (4)	0.138 (2)
H1A	1.10620	0.69140	0.41900	0.0680*
H1B	1.16900	0.82900	0.37610	0.0680*
H2	0.56870	0.81000	0.14570	0.0640*
H3	0.39450	0.66020	−0.00570	0.0700*
H5	0.22270	0.41340	0.21170	0.0680*
H6	0.39390	0.56470	0.36140	0.0570*

H7A	0.11860	0.55860	−0.11240	0.1210*
H7B	0.07240	0.39170	−0.15710	0.1210*
H7C	0.26270	0.46480	−0.13150	0.1210*
H8	0.56480	0.79380	0.43530	0.0460*
H15A	0.57660	1.26170	0.40550	0.0760*
H15B	0.42210	1.23650	0.29930	0.0760*
H16A	0.60040	1.18570	0.18050	0.0790*
H16B	0.67420	1.33710	0.25170	0.0790*
H17A	0.88530	1.17380	0.24150	0.0640*
H17B	0.88670	1.23700	0.36540	0.0640*
H18A	0.71550	1.00780	0.95170	0.1500*
H18B	0.81450	0.87690	0.92390	0.1500*
H19A	0.94160	1.17020	0.94680	0.1660*
H19B	0.87970	1.07000	0.83140	0.1660*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0761 (11)	0.0640 (10)	0.0702 (10)	−0.0133 (8)	−0.0058 (8)	−0.0056 (8)
O2	0.0475 (7)	0.0467 (7)	0.0657 (8)	0.0030 (5)	0.0229 (6)	0.0207 (6)
O3	0.0480 (8)	0.0506 (8)	0.0832 (10)	0.0060 (6)	0.0217 (7)	0.0084 (7)
N1	0.0429 (9)	0.0552 (10)	0.0748 (11)	0.0057 (7)	0.0169 (8)	0.0229 (8)
N2	0.0600 (11)	0.0595 (11)	0.1025 (16)	0.0096 (8)	0.0244 (10)	0.0413 (11)
C1	0.0359 (8)	0.0347 (8)	0.0472 (9)	0.0047 (6)	0.0112 (7)	0.0063 (6)
C2	0.0594 (12)	0.0473 (10)	0.0514 (10)	−0.0082 (8)	0.0170 (9)	0.0062 (8)
C3	0.0649 (13)	0.0591 (12)	0.0475 (10)	−0.0043 (10)	0.0117 (9)	0.0042 (9)
C4	0.0487 (11)	0.0441 (10)	0.0612 (12)	0.0022 (8)	0.0016 (9)	−0.0009 (8)
C5	0.0505 (11)	0.0417 (10)	0.0702 (13)	−0.0070 (8)	0.0040 (9)	0.0124 (9)
C6	0.0454 (10)	0.0423 (9)	0.0543 (10)	0.0002 (7)	0.0091 (8)	0.0148 (8)
C7	0.0762 (17)	0.0896 (18)	0.0618 (14)	0.0016 (13)	−0.0056 (12)	−0.0107 (13)
C8	0.0407 (8)	0.0354 (8)	0.0418 (8)	0.0004 (6)	0.0145 (7)	0.0071 (6)
C9	0.0423 (9)	0.0372 (8)	0.0413 (8)	0.0004 (6)	0.0085 (7)	0.0087 (6)
C10	0.0443 (9)	0.0398 (8)	0.0414 (8)	0.0015 (7)	0.0092 (7)	0.0082 (7)
C11	0.0413 (9)	0.0462 (10)	0.0586 (11)	0.0016 (7)	0.0104 (8)	0.0144 (8)
C12	0.0499 (10)	0.0354 (8)	0.0420 (9)	0.0005 (7)	0.0133 (7)	0.0070 (7)
C13	0.0460 (9)	0.0341 (8)	0.0407 (8)	0.0008 (7)	0.0114 (7)	0.0049 (6)
C14	0.0494 (10)	0.0393 (9)	0.0481 (10)	0.0031 (7)	0.0091 (8)	0.0041 (7)
C15	0.0664 (13)	0.0403 (10)	0.0882 (16)	0.0107 (9)	0.0234 (12)	0.0150 (10)
C16	0.0820 (16)	0.0462 (11)	0.0748 (14)	0.0089 (10)	0.0219 (12)	0.0245 (10)
C17	0.0659 (12)	0.0391 (9)	0.0605 (11)	−0.0019 (8)	0.0251 (10)	0.0135 (8)
O4	0.125 (2)	0.236 (4)	0.0879 (17)	0.028 (2)	0.0352 (16)	0.018 (2)
C18	0.105 (3)	0.152 (4)	0.107 (3)	0.002 (3)	0.010 (2)	0.020 (3)
C19	0.114 (3)	0.200 (5)	0.111 (3)	0.038 (3)	0.022 (2)	0.069 (3)

Geometric parameters (Å, º)

O1—C4	1.364 (3)	C13—C14	1.461 (2)
O1—C7	1.417 (3)	C14—C15	1.501 (3)
O2—C10	1.366 (2)	C15—C16	1.516 (3)
O2—C12	1.369 (2)	C16—C17	1.511 (3)

O3—C14	1.216 (2)	C2—H2	0.9300
O4—C18	1.383 (5)	C3—H3	0.9300
O4—C19^{i}	1.446 (6)	C5—H5	0.9300
N1—C10	1.330 (2)	C6—H6	0.9300
N2—C11	1.143 (3)	C7—H7C	0.9600
N1—H1B	0.8600	C7—H7A	0.9600
N1—H1A	0.8600	C7—H7B	0.9600
C1—C2	1.377 (3)	C8—H8	0.9800
C1—C8	1.521 (2)	C15—H15B	0.9700
C1—C6	1.386 (2)	C15—H15A	0.9700
C2—C3	1.388 (3)	C16—H16A	0.9700
C3—C4	1.379 (3)	C16—H16B	0.9700
C4—C5	1.379 (3)	C17—H17B	0.9700
C5—C6	1.376 (3)	C17—H17A	0.9700
C8—C13	1.499 (2)	C18—C19	1.417 (7)
C8—C9	1.511 (2)	C18—H18A	0.9700
C9—C10	1.354 (2)	C18—H18B	0.9700
C9—C11	1.410 (3)	C19—H19A	0.9700
C12—C13	1.338 (2)	C19—H19B	0.9700
C12—C17	1.491 (3)		

C4—O1—C7	117.78 (19)	C2—C3—H3	120.00
C10—O2—C12	118.91 (14)	C6—C5—H5	120.00
C18—O4—C19^{i}	108.6 (3)	C4—C5—H5	120.00
H1A—N1—H1B	120.00	C1—C6—H6	120.00
C10—N1—H1B	120.00	C5—C6—H6	120.00
C10—N1—H1A	120.00	O1—C7—H7A	109.00
C2—C1—C6	117.77 (17)	O1—C7—H7B	109.00
C6—C1—C8	119.84 (15)	H7A—C7—H7B	109.00
C2—C1—C8	122.37 (15)	H7A—C7—H7C	109.00
C1—C2—C3	121.88 (19)	H7B—C7—H7C	110.00
C2—C3—C4	119.41 (19)	O1—C7—H7C	109.00
O1—C4—C5	116.23 (19)	C9—C8—H8	108.00
C3—C4—C5	119.3 (2)	C13—C8—H8	108.00
O1—C4—C3	124.49 (19)	C1—C8—H8	108.00
C4—C5—C6	120.73 (19)	C14—C15—H15B	109.00
C1—C6—C5	120.93 (18)	C16—C15—H15A	109.00
C9—C8—C13	108.63 (14)	C16—C15—H15B	109.00
C1—C8—C13	112.38 (14)	H15A—C15—H15B	108.00
C1—C8—C9	111.95 (13)	C14—C15—H15A	109.00
C8—C9—C10	122.54 (15)	C15—C16—H16B	109.00
C10—C9—C11	119.42 (16)	C17—C16—H16A	109.00
C8—C9—C11	118.00 (14)	C15—C16—H16A	109.00
O2—C10—N1	110.30 (15)	H16A—C16—H16B	108.00
N1—C10—C9	128.22 (17)	C17—C16—H16B	109.00
O2—C10—C9	121.48 (15)	C12—C17—H17A	110.00
N2—C11—C9	177.6 (2)	C12—C17—H17B	110.00
O2—C12—C13	122.91 (15)	C16—C17—H17B	110.00
C13—C12—C17	125.75 (17)	H17A—C17—H17B	108.00

O2—C12—C17	111.34 (16)	C16—C17—H17A	110.00
C8—C13—C14	118.19 (14)	O4—C18—C19	110.9 (4)
C8—C13—C12	122.27 (15)	O4^{i}—C19—C18	110.8 (4)
C12—C13—C14	119.54 (15)	O4—C18—H18A	109.00
C13—C14—C15	117.57 (16)	O4—C18—H18B	109.00
O3—C14—C13	121.28 (16)	C19—C18—H18A	109.00
O3—C14—C15	121.11 (17)	C19—C18—H18B	109.00
C14—C15—C16	112.24 (17)	H18A—C18—H18B	108.00
C15—C16—C17	111.57 (18)	C18—C19—H19A	109.00
C12—C17—C16	110.51 (18)	C18—C19—H19B	109.00
C1—C2—H2	119.00	H19A—C19—H19B	108.00
C3—C2—H2	119.00	O4^{i}—C19—H19A	109.00
C4—C3—H3	120.00	O4^{i}—C19—H19B	110.00

C7—O1—C4—C3	−9.3 (3)	C1—C8—C9—C10	105.99 (18)
C7—O1—C4—C5	171.1 (2)	C1—C8—C9—C11	−71.4 (2)
C10—O2—C12—C17	171.59 (15)	C9—C8—C13—C14	−161.46 (15)
C12—O2—C10—N1	−172.95 (15)	C1—C8—C13—C14	74.12 (19)
C10—O2—C12—C13	−8.8 (2)	C9—C8—C13—C12	17.3 (2)
C12—O2—C10—C9	7.4 (2)	C11—C9—C10—N1	5.4 (3)
C18^{i}—O4^{i}—C19—C18	−58.0 (5)	C8—C9—C10—O2	7.6 (3)
C19^{i}—O4—C18—C19	−58.0 (5)	C8—C9—C10—N1	−172.00 (17)
C8—C1—C2—C3	178.46 (19)	C11—C9—C10—O2	−175.05 (16)
C8—C1—C6—C5	−178.09 (17)	C17—C12—C13—C8	174.55 (17)
C2—C1—C6—C5	0.2 (3)	C17—C12—C13—C14	−6.7 (3)
C2—C1—C8—C9	−87.6 (2)	O2—C12—C17—C16	162.26 (16)
C2—C1—C8—C13	34.9 (2)	C13—C12—C17—C16	−17.3 (3)
C6—C1—C8—C9	90.63 (19)	O2—C12—C13—C14	173.82 (15)
C6—C1—C8—C13	−146.80 (16)	O2—C12—C13—C8	−5.0 (3)
C6—C1—C2—C3	0.2 (3)	C12—C13—C14—O3	−178.26 (18)
C1—C2—C3—C4	0.0 (3)	C8—C13—C14—O3	0.6 (3)
C2—C3—C4—C5	−0.5 (3)	C12—C13—C14—C15	−0.5 (3)
C2—C3—C4—O1	179.8 (2)	C8—C13—C14—C15	178.31 (16)
O1—C4—C5—C6	−179.37 (19)	O3—C14—C15—C16	−151.3 (2)
C3—C4—C5—C6	1.0 (3)	C13—C14—C15—C16	31.0 (3)
C4—C5—C6—C1	−0.8 (3)	C14—C15—C16—C17	−54.6 (2)
C13—C8—C9—C11	163.92 (15)	C15—C16—C17—C12	46.9 (2)
C1—C8—C13—C12	−107.09 (18)	O4—C18—C19—O4^{i}	59.3 (5)
C13—C8—C9—C10	−18.7 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N2^{ii}	0.86	2.27	3.123 (3)	171
N1—H1*B*···O3^{iii}	0.86	2.10	2.945 (2)	167

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