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1,2-Bis(pyridin-4-yl)ethene–4-hydroxy-3-methoxybenzoic acid (1/1)

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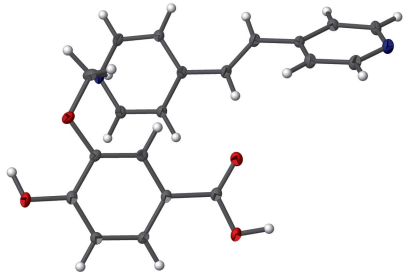
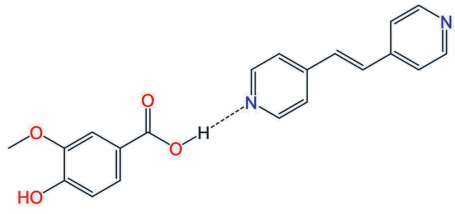
Structural data: full structural data are available from iucrdata.iucr.org

In the title 1:1 co-crystal [alternatively called bipyridine ethylene–*p*-vanillic acid (1/1)], $C_{12}H_{10}N_2{\cdot}C_8H_8O_4$, the dihedral angle between the pyridine rings is 59.51 (5)°. In the crystal, the molecules are linked by O—H···N hydrogen bonds, generating [401] chains of alternating $C_{12}H_{10}N_2$ and $C_8H_8O_4$ molecules.

3D view



Chemical scheme



Structure description

4-Hydroxy-3-methoxybenzoic acid, $C_8H_8O_4$, known commonly as *p*-vanillic acid, is used as a flavoring agent and naturally found in a variety of fruits and edible plants (Ingole *et al.*, 2021). In addition, *p*-vanillic acid is currently being investigated for its inflammatory pain-inhibiting properties (Calixto-Campos *et al.*, 2015). Despite the prevalence of the molecule in our foods and its potential medicinal benefits, structural information on vanillic acid is sparse with few crystal structures being reported thus far. As such it is crucial to expand the number of structures containing vanillic acid in order to better understand the non-covalent interactions involving this molecule. Bipyridine ethylene ($C_{12}H_{10}N_2$; BPyE) was selected as a suitable coformer for the present study because of its ability to form both simple and complex hydrogen-bonded networks with organic acids (Delori *et al.*, 2013; Bhattacharya *et al.*, 2013).

When *p*-vanillic acid is combined with BPyE in a 1:1 molar ratio, the resulting 1:1 co-crystal possesses monoclinic ($P2_1/c$) symmetry at 90 K. The vanillic acid has two distinct O—H···N-type hydrogen-bonding interactions (Table 1); one of these involves the carboxylic acid group and a BPyE N atom acceptor and resulting in a 2.6295 (12) Å distance between heteroatoms (Fig. 1). The other hydrogen bond occurs between the *para*-position hydroxyl group and the other pyridine N atom of a BPyE molecule resulting in a 2.6868 (13) Å distance between heteroatoms (Fig. 2). The co-crystal structure may be described as dimolecular units made up of one acid plus one coformer, which form $C_2^2(19)$ chain motifs. These chains propagate in the [401] direction, forming

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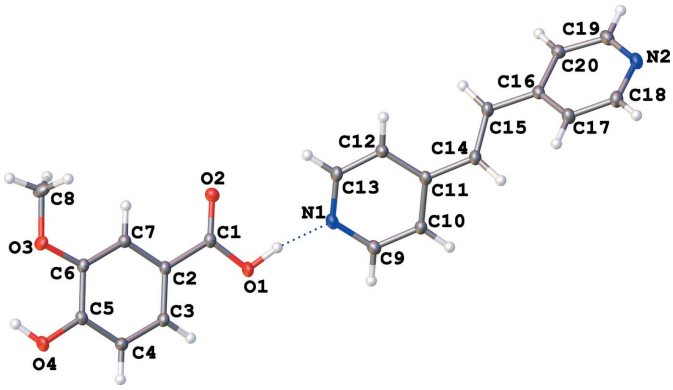

Figure 1
A bimolecular unit consisting of *p*-vanillic acid and BPyE with the hydrogen bond depicted as a blue dashed line. The BPyE molecule illustrated is generated by the symmetry operation $x-1, y, z$ from the asymmetric molecule.

twisting wires (Fig. 3). The wires stack along [010], forming sheets, which subsequently form layers parallel to (10$\overline{4}$), with every other sheet being rotated 180° about [010]. Two weak C—H···O contacts are also observed (Table 1).

Synthesis and crystallization

A 1:1 molar ratio of bipyridine ethylene (182.2 mg, 1 mmol) and *p*-vanillic acid (168.1 mg, 1 mmol) was added to a 25 ml scintillation vial to which methanol was added until both compounds dissolved (approximately 20 ml). The resulting solution was vortexed for 30 s at 3000 rpm on a VWR Mini Vortexer MV I. The solution was then stored in the dark uncapped to allow for crystal formation while the solvent slowly evaporated.

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.99 (2)	1.65 (2)	2.6295 (12)	169 (2)
O4—H4···N2^{ii}	0.92 (2)	1.84 (2)	2.6868 (13)	154 (2)
C4—H4A···O2^{iii}	0.95	2.53	3.2341 (14)	132
C9—H9···O3^{iv}	0.95	2.45	3.3520 (14)	158

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{10}N_2{\cdot}C_8H_8O_4$
M_r	350.36
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	90
a, b, c (Å)	9.1486 (5), 9.2114 (5), 20.3429 (12)
β (°)	98.416 (1)
V (Å^3)	1695.86 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.54 × 0.22 × 0.02
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.648, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33598, 5958, 4683
R_{int}	0.084
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.748
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.131, 1.03
No. of reflections	5958
No. of parameters	245
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.40, −0.26

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick 2015*b*), and *OLEX2* (Dolomanov *et al.*, 2009).

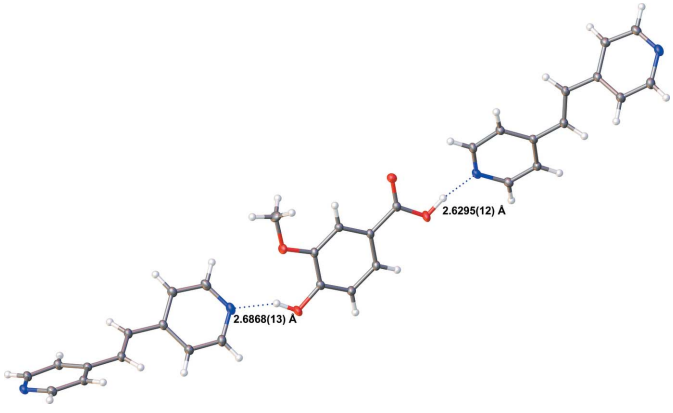

Figure 2
Part of a [401] hydrogen-bonded chain of *p*-vanillic acid and BPyE molecules. The O···N distances are shown for each O—H···N hydrogen-bonding interaction.

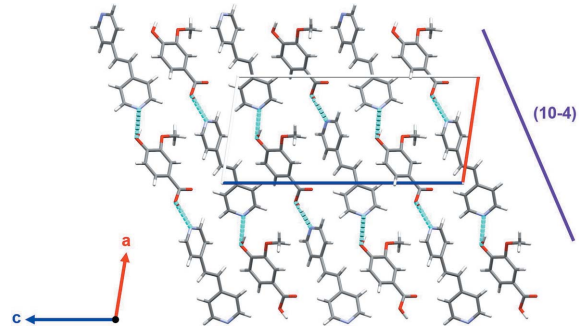

Figure 3
plane depicting twisting hydrogen-bonded wires running approximately parallel to (10$\overline{4}$). Hydrogen-bonding interactions are depicted as bright-blue dashed lines.

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full crystallographic data

IUCrData (2022). **7**, x220304 [https://doi.org/10.1107/S2414314622003042]

1,2-Bis(pyridin-4-yl)ethene–4-hydroxy-3-methoxybenzoic acid (1/1)

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1,2-Bis(pyridin-4-yl)ethene; 4-hydroxy-3-methoxybenzoic acid

Crystal data

$C_{12}H_{10}N_2·C_8H_8O_4$
M_r = 350.36
Monoclinic, $P2_1/c$
a = 9.1486 (5) Å
b = 9.2114 (5) Å
c = 20.3429 (12) Å
β = 98.416 (1)°
V = 1695.86 (16) Å^3
Z = 4
$F(000)$ = 736
D_x = 1.372 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5974 reflections
θ = 2.4–32.1°
μ = 0.10 mm^{-1}
T = 90 K
Plate, clear colourless
0.54 × 0.22 × 0.02 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.648, T_{max} = 0.746
33598 measured reflections
5958 independent reflections
4683 reflections with $I > 2\sigma(I)$
R_{int} = 0.084
θ_{max} = 32.1°, θ_{min} = 2.0°
h = −13→13
k = −13→13
l = −30→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.131
S = 1.03
5958 reflections
245 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.6347P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Extinction correction: *SHELXL2018/3* (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0070 (15)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The O-bound H atoms were located in difference maps and their positions were freely refined. The C-bound H atoms were placed geometrically (C—H = 0.95–0.98 Å) and refined as riding atoms with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.43471 (9)	0.32423 (9)	0.77939 (4)	0.01865 (17)
O2	−0.05986 (9)	0.39976 (10)	0.62580 (4)	0.01877 (17)
O4	0.41561 (9)	0.50304 (10)	0.88365 (4)	0.02072 (18)
O1	−0.17538 (9)	0.55862 (10)	0.68391 (4)	0.02055 (18)
N1	0.58124 (10)	0.49305 (11)	0.60383 (5)	0.01647 (18)
N2	−0.30499 (10)	0.09310 (11)	0.39212 (5)	0.0198 (2)
C11	0.30840 (11)	0.38151 (12)	0.54449 (5)	0.01433 (19)
C5	0.30531 (11)	0.49848 (12)	0.83165 (5)	0.01447 (19)
C1	−0.06039 (11)	0.47842 (12)	0.67408 (5)	0.01454 (19)
C2	0.06755 (11)	0.49121 (12)	0.72818 (5)	0.01337 (19)
C3	0.06593 (11)	0.58633 (12)	0.78115 (5)	0.01466 (19)
H3	−0.016259	0.648781	0.782394	0.018*
C7	0.19036 (11)	0.40137 (12)	0.72604 (5)	0.01356 (19)
H7	0.192506	0.337576	0.689504	0.016*
C16	−0.01655 (11)	0.18988 (12)	0.43775 (5)	0.01485 (19)
C12	0.44140 (11)	0.31630 (12)	0.53464 (5)	0.0158 (2)
H12	0.441106	0.232395	0.507463	0.019*
C6	0.30870 (11)	0.40521 (12)	0.77703 (5)	0.01375 (19)
C9	0.45404 (12)	0.55722 (13)	0.61287 (5)	0.0171 (2)
H9	0.458134	0.641952	0.639702	0.021*
C10	0.31694 (11)	0.50520 (12)	0.58473 (5)	0.0154 (2)
H10	0.229348	0.553233	0.592721	0.019*
C13	0.57369 (11)	0.37518 (13)	0.56488 (5)	0.0164 (2)
H13	0.663253	0.329869	0.557653	0.020*
C15	0.13307 (11)	0.24385 (13)	0.46164 (5)	0.0163 (2)
H15	0.210971	0.220751	0.437269	0.020*
C4	0.18456 (11)	0.58996 (12)	0.83222 (5)	0.0158 (2)
H4A	0.183227	0.655853	0.868048	0.019*
C20	−0.06769 (12)	0.17485 (13)	0.36998 (5)	0.0172 (2)
H20	−0.004731	0.196381	0.338053	0.021*
C14	0.16281 (11)	0.32450 (13)	0.51668 (5)	0.0163 (2)
H14	0.082548	0.346774	0.539750	0.020*
C17	−0.11344 (12)	0.15200 (13)	0.48206 (6)	0.0180 (2)
H17	−0.083003	0.159193	0.528642	0.022*
C18	−0.25442 (12)	0.10380 (13)	0.45737 (6)	0.0192 (2)
H18	−0.318447	0.077004	0.488118	0.023*
C19	−0.21164 (12)	0.12807 (13)	0.34974 (6)	0.0199 (2)
H19	−0.245544	0.120512	0.303447	0.024*
C8	0.44161 (13)	0.22430 (14)	0.72620 (6)	0.0221 (2)
H8A	0.430464	0.277176	0.683957	0.033*
H8B	0.361902	0.152884	0.725170	0.033*
H8C	0.537185	0.174302	0.732989	0.033*
H4	0.499 (2)	0.458 (3)	0.8743 (11)	0.055 (6)*
H1	−0.259 (3)	0.528 (3)	0.6504 (12)	0.066 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0149 (3)	0.0218 (4)	0.0183 (4)	0.0073 (3)	−0.0006 (3)	−0.0023 (3)
O2	0.0165 (4)	0.0236 (4)	0.0156 (4)	0.0004 (3)	0.0004 (3)	−0.0028 (3)
O4	0.0136 (4)	0.0285 (5)	0.0181 (4)	0.0034 (3)	−0.0043 (3)	−0.0043 (3)
O1	0.0116 (3)	0.0257 (4)	0.0226 (4)	0.0033 (3)	−0.0031 (3)	−0.0063 (3)
N1	0.0135 (4)	0.0191 (5)	0.0156 (4)	−0.0005 (3)	−0.0016 (3)	0.0012 (3)
N2	0.0141 (4)	0.0209 (5)	0.0229 (5)	−0.0007 (3)	−0.0020 (3)	−0.0022 (4)
C11	0.0129 (4)	0.0171 (5)	0.0125 (4)	0.0002 (4)	0.0003 (3)	0.0012 (4)
C5	0.0123 (4)	0.0158 (5)	0.0148 (4)	−0.0010 (3)	0.0006 (3)	0.0010 (4)
C1	0.0119 (4)	0.0158 (5)	0.0157 (4)	−0.0006 (3)	0.0012 (3)	0.0016 (4)
C2	0.0107 (4)	0.0147 (5)	0.0144 (4)	−0.0004 (3)	0.0005 (3)	0.0009 (3)
C3	0.0118 (4)	0.0152 (5)	0.0167 (4)	0.0017 (3)	0.0010 (3)	−0.0003 (4)
C7	0.0131 (4)	0.0142 (5)	0.0134 (4)	−0.0001 (3)	0.0021 (3)	0.0002 (3)
C16	0.0125 (4)	0.0154 (5)	0.0159 (4)	0.0013 (3)	−0.0004 (3)	−0.0015 (4)
C12	0.0138 (4)	0.0172 (5)	0.0156 (4)	0.0015 (4)	−0.0004 (3)	−0.0020 (4)
C6	0.0115 (4)	0.0142 (5)	0.0154 (4)	0.0018 (3)	0.0015 (3)	0.0016 (4)
C9	0.0164 (5)	0.0181 (5)	0.0158 (5)	0.0005 (4)	−0.0010 (4)	−0.0012 (4)
C10	0.0126 (4)	0.0189 (5)	0.0145 (4)	0.0015 (4)	0.0008 (3)	−0.0011 (4)
C13	0.0120 (4)	0.0199 (5)	0.0166 (5)	0.0021 (4)	0.0000 (3)	0.0009 (4)
C15	0.0119 (4)	0.0201 (5)	0.0164 (5)	0.0002 (4)	0.0008 (3)	0.0002 (4)
C4	0.0135 (4)	0.0176 (5)	0.0160 (4)	0.0002 (4)	0.0015 (3)	−0.0030 (4)
C20	0.0161 (5)	0.0187 (5)	0.0164 (5)	−0.0001 (4)	0.0010 (4)	−0.0027 (4)
C14	0.0117 (4)	0.0197 (5)	0.0169 (5)	0.0002 (4)	0.0008 (3)	−0.0007 (4)
C17	0.0146 (4)	0.0222 (5)	0.0165 (5)	−0.0008 (4)	0.0001 (4)	0.0001 (4)
C18	0.0135 (5)	0.0221 (5)	0.0218 (5)	−0.0008 (4)	0.0018 (4)	0.0000 (4)
C19	0.0174 (5)	0.0226 (6)	0.0180 (5)	−0.0005 (4)	−0.0029 (4)	−0.0035 (4)
C8	0.0230 (5)	0.0235 (6)	0.0198 (5)	0.0101 (4)	0.0031 (4)	−0.0025 (4)

Geometric parameters (Å, º)

O3—C6	1.3680 (12)	C16—C15	1.4705 (15)
O3—C8	1.4292 (14)	C16—C20	1.3963 (15)
O2—C1	1.2211 (13)	C16—C17	1.3979 (15)
O4—C5	1.3516 (12)	C12—H12	0.9500
O4—H4	0.92 (2)	C12—C13	1.3854 (15)
O1—C1	1.3243 (13)	C9—H9	0.9500
O1—H1	0.99 (2)	C9—C10	1.3858 (15)
N1—C9	1.3417 (14)	C10—H10	0.9500
N1—C13	1.3400 (15)	C13—H13	0.9500
N2—C18	1.3439 (15)	C15—H15	0.9500
N2—C19	1.3386 (16)	C15—C14	1.3379 (15)
C11—C12	1.3975 (15)	C4—H4A	0.9500
C11—C10	1.3984 (15)	C20—H20	0.9500
C11—C14	1.4661 (14)	C20—C19	1.3895 (15)
C5—C6	1.4083 (15)	C14—H14	0.9500
C5—C4	1.3908 (15)	C17—H17	0.9500

C1—C2	1.4892 (14)	C17—C18	1.3869 (15)
C2—C3	1.3906 (15)	C18—H18	0.9500
C2—C7	1.4012 (14)	C19—H19	0.9500
C3—H3	0.9500	C8—H8A	0.9800
C3—C4	1.3886 (14)	C8—H8B	0.9800
C7—H7	0.9500	C8—H8C	0.9800
C7—C6	1.3858 (14)		

C6—O3—C8	117.07 (9)	C10—C9—H9	118.6
C5—O4—H4	112.0 (14)	C11—C10—H10	120.2
C1—O1—H1	107.0 (14)	C9—C10—C11	119.55 (10)
C13—N1—C9	117.86 (9)	C9—C10—H10	120.2
C19—N2—C18	117.30 (10)	N1—C13—C12	123.09 (10)
C12—C11—C10	117.32 (10)	N1—C13—H13	118.5
C12—C11—C14	123.47 (10)	C12—C13—H13	118.5
C10—C11—C14	119.18 (9)	C16—C15—H15	119.0
O4—C5—C6	122.43 (9)	C14—C15—C16	121.99 (10)
O4—C5—C4	118.53 (10)	C14—C15—H15	119.0
C4—C5—C6	119.04 (9)	C5—C4—H4A	119.5
O2—C1—O1	123.31 (10)	C3—C4—C5	120.93 (10)
O2—C1—C2	123.10 (10)	C3—C4—H4A	119.5
O1—C1—C2	113.58 (9)	C16—C20—H20	120.4
C3—C2—C1	121.74 (9)	C19—C20—C16	119.30 (10)
C3—C2—C7	119.71 (9)	C19—C20—H20	120.4
C7—C2—C1	118.52 (9)	C11—C14—H14	117.1
C2—C3—H3	120.0	C15—C14—C11	125.72 (10)
C4—C3—C2	119.94 (10)	C15—C14—H14	117.1
C4—C3—H3	120.0	C16—C17—H17	120.3
C2—C7—H7	119.9	C18—C17—C16	119.35 (10)
C6—C7—C2	120.26 (10)	C18—C17—H17	120.3
C6—C7—H7	119.9	N2—C18—C17	123.28 (11)
C20—C16—C15	121.40 (10)	N2—C18—H18	118.4
C20—C16—C17	117.35 (10)	C17—C18—H18	118.4
C17—C16—C15	121.24 (10)	N2—C19—C20	123.38 (10)
C11—C12—H12	120.3	N2—C19—H19	118.3
C13—C12—C11	119.36 (10)	C20—C19—H19	118.3
C13—C12—H12	120.3	O3—C8—H8A	109.5
O3—C6—C5	114.87 (9)	O3—C8—H8B	109.5
O3—C6—C7	125.05 (10)	O3—C8—H8C	109.5
C7—C6—C5	120.07 (9)	H8A—C8—H8B	109.5
N1—C9—H9	118.6	H8A—C8—H8C	109.5
N1—C9—C10	122.81 (10)	H8B—C8—H8C	109.5

O2—C1—C2—C3	177.25 (11)	C12—C11—C14—C15	−26.50 (18)
O2—C1—C2—C7	−4.63 (16)	C6—C5—C4—C3	2.43 (16)
O4—C5—C6—O3	−2.61 (15)	C9—N1—C13—C12	−0.93 (16)
O4—C5—C6—C7	177.83 (10)	C10—C11—C12—C13	0.39 (16)
O4—C5—C4—C3	−177.84 (10)	C10—C11—C14—C15	155.42 (11)

O1—C1—C2—C3	−3.78 (15)	C13—N1—C9—C10	1.19 (16)
O1—C1—C2—C7	174.34 (10)	C15—C16—C20—C19	−177.84 (11)
N1—C9—C10—C11	−0.66 (17)	C15—C16—C17—C18	178.96 (11)
C11—C12—C13—N1	0.15 (17)	C4—C5—C6—O3	177.11 (9)
C1—C2—C3—C4	176.90 (10)	C4—C5—C6—C7	−2.45 (16)
C1—C2—C7—C6	−177.00 (9)	C20—C16—C15—C14	146.38 (12)
C2—C3—C4—C5	−0.61 (17)	C20—C16—C17—C18	−0.85 (17)
C2—C7—C6—O3	−178.84 (10)	C14—C11—C12—C13	−177.72 (10)
C2—C7—C6—C5	0.68 (16)	C14—C11—C10—C9	178.05 (10)
C3—C2—C7—C6	1.15 (16)	C17—C16—C15—C14	−33.42 (17)
C7—C2—C3—C4	−1.20 (16)	C17—C16—C20—C19	1.97 (17)
C16—C15—C14—C11	179.32 (10)	C18—N2—C19—C20	−0.37 (18)
C16—C20—C19—N2	−1.42 (19)	C19—N2—C18—C17	1.59 (18)
C16—C17—C18—N2	−0.98 (19)	C8—O3—C6—C5	177.99 (10)
C12—C11—C10—C9	−0.15 (16)	C8—O3—C6—C7	−2.47 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.99 (2)	1.65 (2)	2.6295 (12)	169 (2)
O4—H4···N2^{ii}	0.92 (2)	1.84 (2)	2.6868 (13)	154 (2)
C4—H4*A*···O2^{iii}	0.95	2.53	3.2341 (14)	132
C9—H9···O3^{iv}	0.95	2.45	3.3520 (14)	158

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