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(*Z*)-1-Benzoyl-5-benzylidene-2-hydroxy-4-oxo-4,5-dihydro-1*H*-pyrrole-3-carbonitrile

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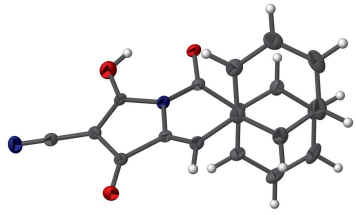
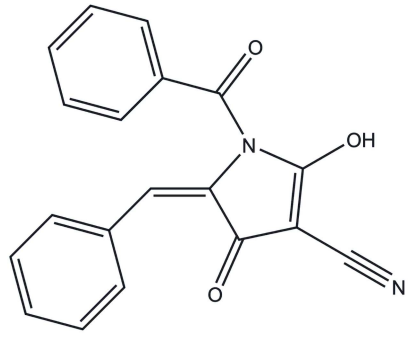
The title compound, $C_{19}H_{12}N_2O_3$, obtained as an intermediate in the synthesis of a pyrrole derivative, is composed of a five-membered heterocycle with substituted groups *via* double or triple bonds as well as single bonds, without an asymmetric carbon atom. An intramolecular O—H···O link occurs. In the crystal, O—H···N hydrogen bonds link the molecules.

3D view



Chemical scheme



Structure description

Pyrrole is widely known as a biologically active scaffold, which possesses a diverse nature of activities (Tzankova *et al.*, 2018). Pyrrole derivatives are biologically active and attract attention for the synthesis of new medicinal products (Guo *et al.*, 2015); Mokrov *et al.*, 2015). Here we report the crystal structure of (*Z*)-1-benzoyl-5-benzylidene-2-hydroxy-4-oxo-4,5-dihydro-1*H*-pyrrole-3-carbonitrile, which crystallizes in a chiral space group despite there being no apparent chiral moiety in the molecule (Koshima & Matsuura, 1998; Matsuura & Koshima, 2005).

The molecular structure of the title compound (Fig. 1) is composed of a planar [maximum deviation of 0.051 (3) Å for atom C12] five-membered (N1/C8/C9/C11/C12) pyrrole ring in the usual geometry (Gainsford *et al.*, 2013) and two phenyl rings (C1–C6 and C14–19) arranged approximately parallel to each other [dihedral angle = 15.2 (2)°; torsion angles N1—C12—C13—C14 = 2.9 (6) and C12—N1—C7—C6 = 23.0 (5)°]. Pyrroles can incorporate various types of substituent groups (Sun *et al.*, 2014; Polindara-García & Miranda, 2012) and in this compound all five atoms in the pyrrole ring are substituted. An intramolecular hydrogen bond (O2—H2···O1; Table 1) is observed.

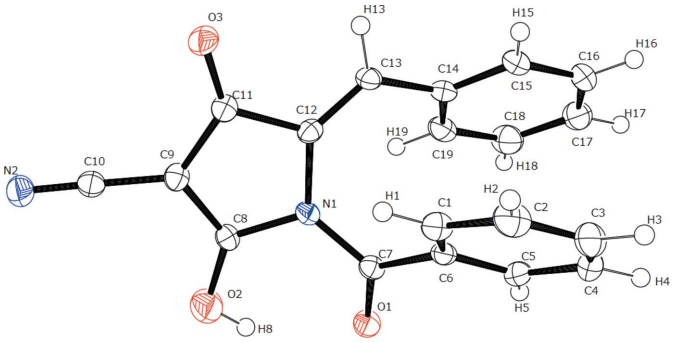


Figure 1
The title compound with 50% probability ellipsoids for non-hydrogen atoms.

In the crystal, O2—H2···N2^{i} hydrogen bonds (Fig. 2 and Table 1) link the molecules. In addition, the almost planar moieties of the molecules, namely the phenyl and pyrrole rings, afford a helical step-like conformation with neighboring molecules aligned along the *b*-axis direction (Fig. 3).

A similar compound 4-methyl-5-(4-nitrobenzylidene)-2-oxo-2,5-dihydro-1*H*-pyrrole-3-carbonitrile (Gainsford *et al.*, 2013) has already been reported and has a similar structure to the title compound. Narasegowda *et al.* (2005) reported a case of chiral crystallization in space group $P2_12_12_1$, the same space group as the title compound. In contrast, our recent examples of chiral crystals composed of achiral molecules both crystallize in space group $P2_1$ (Yagi *et al.*, 2018; Yamazaki *et al.*, 2018). To the best of our knowledge, this is the first crystal structure reported for chiral crystallization of a pyrrole of this type.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.82	2.10	2.769 (4)	138
O2—H2···N2^{i}	0.82	2.52	3.074 (5)	126

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$.

Synthesis and crystallization

The title compound was obtained as an intermediate in the synthesis of pyrrole derivatives, namely treatment of 1-acetyl-2-amino-4-oxo-4,5-dihydro-1*H*-pyrrole-3-carbonitrile, benzaldehyde and benzoyl chloride. X-ray quality crystals were obtained from slow evaporation of a methanol solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Since it is very difficult to determine the absolute structure reliably with Mo radiation, the choice of the absolute structure is arbitrary.

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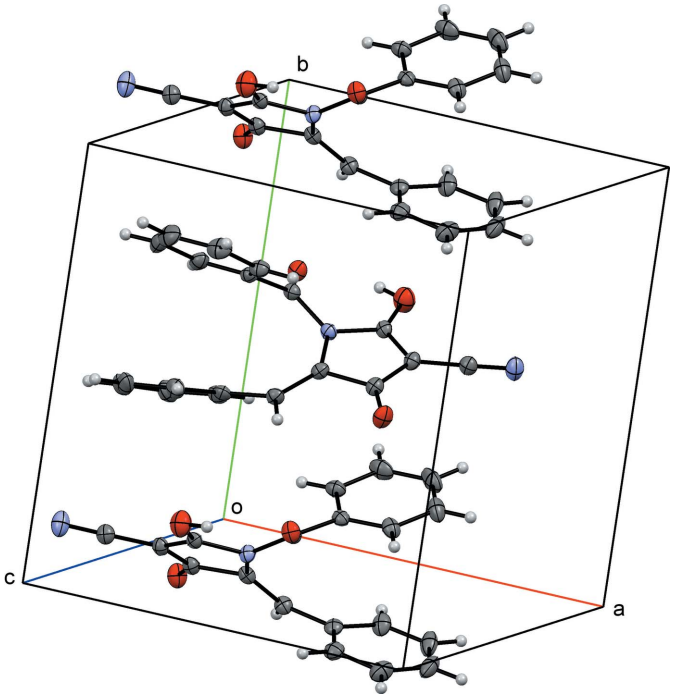

Figure 2
Arrangement of molecules along the *b*-axis direction.

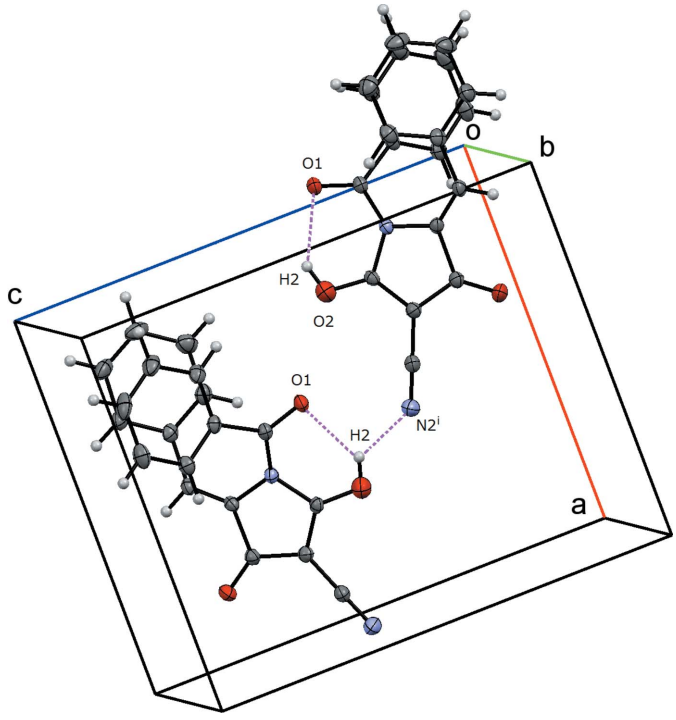

Figure 3
Hydrogen bonds (dashed lines) in the title structure.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{12}N_2O_3$
M_r	316.31
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	296
a, b, c (Å)	10.432 (2), 11.297 (2), 12.688 (2)
V (Å^3)	1495.3 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.58 × 0.27 × 0.17
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2001)
T_{min}, T_{max}	0.55, 0.97
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8161, 3341, 3139
R_{int}	0.085
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.071, 0.173, 1.08
No. of reflections	3341
No. of parameters	218
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.46

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2019). **4**, x190220 [https://doi.org/10.1107/S2414314619002207]

(*Z*)-1-Benzoyl-5-benzylidene-2-hydroxy-4-oxo-4,5-dihydro-1*H*-pyrrole-3-carbonitrile

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Crystal data

$C_{19}H_{12}N_2O_3$
M_r = 316.31
Orthorhombic, $P2_12_12_1$
a = 10.432 (2) Å
b = 11.297 (2) Å
c = 12.688 (2) Å
V = 1495.3 (5) Å^3
Z = 4
$F(000)$ = 656
D_x = 1.405 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5372 reflections
θ = 2.4–27.5°
μ = 0.10 mm^{-1}
T = 296 K
Prism, yellow
0.58 × 0.27 × 0.17 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2001)
T_{min} = 0.55, T_{max} = 0.97
8161 measured reflections
3341 independent reflections
3139 reflections with $I > 2\sigma(I)$
R_{int} = 0.085
θ_{max} = 27.6°, θ_{min} = 2.4°
h = −13→8
k = −14→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.173
S = 1.08
3341 reflections
218 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
$w = 1/[\sigma^2(F_o^2) + (0.0946P)^2 + 0.6486P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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. All H atoms were located on difference Fourier maps. The C-bound H atoms were constrained using a riding model [C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl H atom] The N-bound H atoms were constrained using a riding model [O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq}(O) for amine H atoms]

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.3806 (2)	0.7264 (2)	0.58946 (17)	0.0230 (5)
O3	0.7778 (2)	0.5105 (3)	0.84556 (18)	0.0268 (6)
O2	0.6352 (3)	0.7026 (3)	0.5317 (2)	0.0357 (7)
H2	0.5601	0.7133	0.5151	0.054*
N1	0.5311 (3)	0.6322 (3)	0.6886 (2)	0.0179 (6)
N2	0.9763 (3)	0.6243 (3)	0.6021 (2)	0.0299 (7)
C7	0.4168 (3)	0.6986 (3)	0.6766 (2)	0.0177 (7)
C11	0.7122 (3)	0.5563 (3)	0.7764 (2)	0.0191 (7)
C12	0.5681 (3)	0.5634 (3)	0.7786 (2)	0.0176 (6)
C9	0.7491 (3)	0.6073 (3)	0.6772 (3)	0.0194 (7)
C6	0.3488 (3)	0.7375 (3)	0.7744 (2)	0.0184 (6)
C8	0.6403 (3)	0.6502 (3)	0.6251 (2)	0.0173 (6)
C14	0.3553 (3)	0.4793 (3)	0.8357 (3)	0.0209 (7)
C13	0.4949 (3)	0.5000 (3)	0.8427 (2)	0.0192 (7)
H13	0.5366	0.4641	0.8991	0.023*
C10	0.8740 (3)	0.6158 (3)	0.6366 (2)	0.0208 (7)
C1	0.4160 (4)	0.7778 (3)	0.8625 (3)	0.0223 (7)
H1	0.5051	0.7748	0.8639	0.027*
C5	0.2156 (3)	0.7417 (3)	0.7713 (3)	0.0238 (7)
H5	0.1715	0.7168	0.7116	0.029*
C15	0.2784 (4)	0.4872 (4)	0.9260 (3)	0.0263 (8)
H15	0.3152	0.5032	0.9912	0.032*
C19	0.2982 (4)	0.4502 (3)	0.7397 (3)	0.0251 (7)
H19	0.3486	0.4436	0.6796	0.03*
C4	0.1494 (4)	0.7839 (4)	0.8589 (3)	0.0305 (9)
H4	0.0602	0.7845	0.8587	0.037*
C18	0.1670 (4)	0.4310 (4)	0.7329 (3)	0.0320 (9)
H18	0.1304	0.4099	0.6688	0.038*
C16	0.1462 (4)	0.4711 (4)	0.9175 (3)	0.0321 (9)
H16	0.0952	0.4791	0.9771	0.039*
C2	0.3483 (4)	0.8226 (4)	0.9484 (3)	0.0317 (9)
H2A	0.3923	0.8509	1.0069	0.038*
C17	0.0900 (4)	0.4435 (4)	0.8225 (3)	0.0340 (9)
H17	0.0017	0.4333	0.8179	0.041*
C3	0.2154 (5)	0.8251 (4)	0.9467 (3)	0.0351 (9)

H3	0.1704	0.8543	1.0043	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0245 (12)	0.0301 (13)	0.0143 (11)	0.0031 (11)	−0.0006 (9)	0.0009 (10)
O3	0.0228 (12)	0.0379 (15)	0.0197 (11)	0.0048 (12)	−0.0034 (9)	0.0032 (11)
O2	0.0334 (15)	0.0454 (18)	0.0284 (14)	0.0018 (15)	0.0022 (12)	0.0046 (13)
N1	0.0189 (14)	0.0198 (13)	0.0150 (13)	0.0002 (12)	0.0016 (9)	0.0027 (11)
N2	0.0217 (15)	0.0419 (19)	0.0261 (15)	0.0021 (15)	0.0026 (12)	0.0079 (15)
C7	0.0208 (16)	0.0175 (14)	0.0147 (14)	−0.0004 (13)	0.0002 (11)	−0.0002 (12)
C11	0.0195 (15)	0.0215 (15)	0.0162 (15)	0.0009 (13)	−0.0010 (12)	−0.0024 (12)
C12	0.0190 (15)	0.0194 (15)	0.0144 (14)	0.0037 (13)	−0.0016 (11)	−0.0011 (12)
C9	0.0185 (16)	0.0221 (16)	0.0178 (15)	0.0008 (13)	0.0001 (11)	−0.0026 (13)
C6	0.0230 (15)	0.0156 (14)	0.0165 (15)	0.0017 (13)	0.0023 (11)	0.0021 (11)
C8	0.0194 (15)	0.0188 (14)	0.0138 (14)	−0.0011 (12)	0.0019 (12)	−0.0025 (11)
C14	0.0234 (17)	0.0173 (15)	0.0219 (15)	0.0004 (13)	0.0014 (12)	0.0063 (12)
C13	0.0223 (16)	0.0206 (16)	0.0148 (14)	0.0025 (13)	0.0001 (11)	0.0034 (13)
C10	0.0219 (16)	0.0245 (17)	0.0161 (14)	0.0010 (14)	−0.0006 (12)	0.0013 (12)
C1	0.0279 (18)	0.0195 (15)	0.0195 (16)	0.0005 (14)	−0.0005 (12)	−0.0021 (13)
C5	0.0249 (17)	0.0248 (16)	0.0215 (17)	0.0068 (15)	0.0017 (12)	0.0051 (13)
C15	0.0261 (18)	0.0316 (19)	0.0211 (16)	0.0025 (16)	0.0030 (13)	0.0091 (14)
C19	0.0297 (18)	0.0216 (16)	0.0240 (17)	−0.0021 (15)	0.0028 (13)	0.0036 (14)
C4	0.0267 (18)	0.036 (2)	0.0292 (18)	0.0116 (16)	0.0082 (14)	0.0073 (16)
C18	0.0297 (19)	0.0320 (19)	0.034 (2)	−0.0049 (17)	−0.0045 (15)	0.0045 (16)
C16	0.0242 (19)	0.037 (2)	0.035 (2)	0.0035 (17)	0.0097 (14)	0.0155 (17)
C2	0.047 (2)	0.0283 (18)	0.0201 (17)	0.0029 (19)	0.0030 (16)	−0.0051 (14)
C17	0.0204 (18)	0.032 (2)	0.050 (2)	−0.0048 (17)	0.0012 (15)	0.0140 (19)
C3	0.046 (2)	0.034 (2)	0.0249 (18)	0.012 (2)	0.0153 (16)	−0.0001 (16)

Geometric parameters (Å, º)

O1—C7	1.211 (4)	C13—H13	0.93
O3—C11	1.228 (4)	C1—C2	1.394 (5)
O2—C8	1.326 (4)	C1—H1	0.93
O2—H2	0.82	C5—C4	1.393 (5)
N1—C8	1.410 (4)	C5—H5	0.93
N1—C7	1.416 (4)	C15—C16	1.395 (6)
N1—C12	1.434 (4)	C15—H15	0.93
N2—C10	1.157 (5)	C19—C18	1.388 (6)
C7—C6	1.495 (4)	C19—H19	0.93
C11—C9	1.436 (4)	C4—C3	1.390 (6)
C11—C12	1.506 (4)	C4—H4	0.93
C12—C13	1.326 (5)	C18—C17	1.400 (6)
C9—C8	1.401 (5)	C18—H18	0.93
C9—C10	1.405 (5)	C16—C17	1.376 (6)
C6—C5	1.391 (5)	C16—H16	0.93
C6—C1	1.396 (5)	C2—C3	1.387 (6)

C14—C19	1.395 (5)	C2—H2A	0.93
C14—C15	1.401 (5)	C17—H17	0.93
C14—C13	1.478 (5)	C3—H3	0.93

C8—O2—H2	109.5	C2—C1—H1	120.3
C8—N1—C7	122.9 (3)	C6—C1—H1	120.3
C8—N1—C12	108.4 (3)	C6—C5—C4	119.0 (3)
C7—N1—C12	126.8 (3)	C6—C5—H5	120.5
O1—C7—N1	119.9 (3)	C4—C5—H5	120.5
O1—C7—C6	122.2 (3)	C16—C15—C14	119.6 (4)
N1—C7—C6	117.8 (3)	C16—C15—H15	120.2
O3—C11—C9	130.2 (3)	C14—C15—H15	120.2
O3—C11—C12	124.5 (3)	C18—C19—C14	120.8 (3)
C9—C11—C12	105.2 (3)	C18—C19—H19	119.6
C13—C12—N1	128.8 (3)	C14—C19—H19	119.6
C13—C12—C11	123.9 (3)	C3—C4—C5	120.6 (4)
N1—C12—C11	106.4 (3)	C3—C4—H4	119.7
C8—C9—C10	123.7 (3)	C5—C4—H4	119.7
C8—C9—C11	109.6 (3)	C19—C18—C17	120.0 (4)
C10—C9—C11	126.7 (3)	C19—C18—H18	120.0
C5—C6—C1	120.9 (3)	C17—C18—H18	120.0
C5—C6—C7	117.4 (3)	C17—C16—C15	121.3 (4)
C1—C6—C7	121.5 (3)	C17—C16—H16	119.4
O2—C8—C9	127.5 (3)	C15—C16—H16	119.4
O2—C8—N1	122.9 (3)	C3—C2—C1	120.1 (4)
C9—C8—N1	109.6 (3)	C3—C2—H2A	119.9
C19—C14—C15	119.0 (3)	C1—C2—H2A	119.9
C19—C14—C13	120.7 (3)	C16—C17—C18	119.3 (3)
C15—C14—C13	120.3 (3)	C16—C17—H17	120.4
C12—C13—C14	128.0 (3)	C18—C17—H17	120.4
C12—C13—H13	116.0	C2—C3—C4	120.1 (4)
C14—C13—H13	116.0	C2—C3—H3	120.0
N2—C10—C9	178.9 (4)	C4—C3—H3	120.0
C2—C1—C6	119.4 (3)		

C8—N1—C7—O1	37.5 (5)	C7—N1—C8—O2	−20.6 (5)
C12—N1—C7—O1	−160.3 (3)	C12—N1—C8—O2	174.4 (3)
C8—N1—C7—C6	−139.2 (3)	C7—N1—C8—C9	158.1 (3)
C12—N1—C7—C6	23.0 (5)	C12—N1—C8—C9	−6.9 (4)
C8—N1—C12—C13	−160.3 (3)	N1—C12—C13—C14	2.9 (6)
C7—N1—C12—C13	35.5 (5)	C11—C12—C13—C14	−164.8 (3)
C8—N1—C12—C11	9.1 (3)	C19—C14—C13—C12	45.2 (6)
C7—N1—C12—C11	−155.2 (3)	C15—C14—C13—C12	−135.6 (4)
O3—C11—C12—C13	−15.1 (5)	C5—C6—C1—C2	0.2 (5)
C9—C11—C12—C13	162.1 (3)	C7—C6—C1—C2	174.5 (3)
O3—C11—C12—N1	174.9 (3)	C1—C6—C5—C4	−1.8 (5)
C9—C11—C12—N1	−7.9 (3)	C7—C6—C5—C4	−176.4 (3)
O3—C11—C9—C8	−179.2 (3)	C19—C14—C15—C16	−2.7 (5)

C12—C11—C9—C8	3.9 (4)	C13—C14—C15—C16	178.0 (4)
O3—C11—C9—C10	0.1 (6)	C15—C14—C19—C18	0.9 (6)
C12—C11—C9—C10	−176.9 (3)	C13—C14—C19—C18	−179.8 (3)
O1—C7—C6—C5	37.8 (5)	C6—C5—C4—C3	2.3 (6)
N1—C7—C6—C5	−145.5 (3)	C14—C19—C18—C17	1.5 (6)
O1—C7—C6—C1	−136.7 (4)	C14—C15—C16—C17	2.2 (6)
N1—C7—C6—C1	39.9 (4)	C6—C1—C2—C3	1.1 (6)
C10—C9—C8—O2	1.1 (6)	C15—C16—C17—C18	0.2 (6)
C11—C9—C8—O2	−179.7 (3)	C19—C18—C17—C16	−2.1 (6)
C10—C9—C8—N1	−177.6 (3)	C1—C2—C3—C4	−0.6 (6)
C11—C9—C8—N1	1.7 (4)	C5—C4—C3—C2	−1.1 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.82	2.10	2.769 (4)	138
O2—H2···N2^{i}	0.82	2.52	3.074 (5)	126

Symmetry code: (i) $x-1/2, -y+3/2, -z+1$.