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3-[(Hydroxy)(4-isopropoxy-2-methoxyphenyl)methylene]-1-isopropylpyrrolidine-2,4-dione

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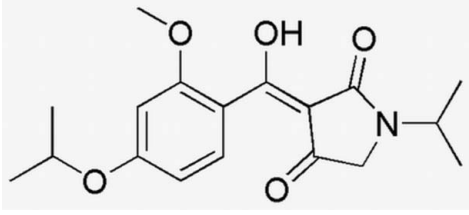
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.131; data-to-parameter ratio = 16.2.

The title compound, $C_{18}H_{23}NO_5$, a potential herbicide, has an enol group that is intramolecularly hydrogen bonded to a keto O atom. The dihedral angle between the six-membered ring formed by the enol group and the aromatic benzene ring is 53.35 (6)°.

Related literature

For structural and herbicidal literature on this class of compounds, see: Ellis & Spek (2001); Holzapfel *et al.* (1970); Rinehart *et al.* (1971, 1963); Matsuo *et al.* (1980); van Rooyen (1992); Stickings (1959); Van Der Baan *et al.* (1978); Xu (2005); Zhu, Hu & Yang (2004); Zhu, Song, Li *et al.* (2004); Zhu, Song, Yao *et al.* (2004). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{23}NO_5$
M_r = 333.37
Monoclinic, $C2/c$
a = 14.694 (2) Å
b = 12.249 (2) Å
c = 20.308 (3) Å
β = 103.864 (3)°
V = 3548.5 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
9820 measured reflections
3622 independent reflections
2199 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.131
S = 1.04
3622 reflections
223 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O4	0.82	1.80	2.555 (2)	152
C16—H16···O4	0.98	2.50	2.891 (2)	104

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2379).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1999). *SMART* (Version 5.618), *SAINT* (Version 6.45) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Ellis, D. D. & Spek, A. L. (2001). *Acta Cryst.* C**57**, 433–434.
Holzapfel, C. W., Hutchison, R. D. & Wilkins, D. C. (1970). *Tetrahedron*, **26**, 5239–5246.
Matsuo, K., Kitaguchi, I., Takata, Y. & Tanaka, K. (1980). *Chem. Pharm. Bull.* **28**, 2494–2502.
Rinehart, K. L., Beck, J. R., Borders, D. B., Kinstle, T. H. & Krauss, D. (1963). *J. Am. Chem. Soc.* **85**, 4038–4039.
Rinehart, K. L., MacKellar, F. A., Grostic, M. F., Olson, E. C., Wnuk, R. J. & Branfman, A. R. (1971). *J. Am. Chem. Soc.* **93**, 4943–4945.
Rooyen, P. H. van (1992). *Acta Cryst.* C**48**, 551–552.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stickings, C. E. (1959). *Biochem. J.* **72**, 332–334.
Van Der Baan, J. L., Barnick, J. W. F. K. & Bickelhaupt, F. (1978). *Tetrahedron*, **34**, 223–231.
Xu, H.-Z. (2005). *Acta Cryst.* E**61**, o292–o294.
Zhu, Y.-Q., Hu, F.-Z. & Yang, H.-Z. (2004). *Huaxue Tongbao*, **67**, 1–7.
Zhu, Y.-Q., Song, H.-B., Li, J.-R., Yao, C.-S., Hu, F.-Z., Zou, X.-M. & Yang, H.-Z. (2004). *Acta Cryst.* E**60**, o196–o198.
Zhu, Y.-Q., Song, H.-B., Yao, C.-S., Gao, Y., Hu, F.-Z., Zou, X.-M. & Yang, H.-Z. (2004). *Acta Cryst.* E**60**, o599–o601.

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3-[(Hydroxy)(4-isopropoxy-2-methoxyphenyl)methylene]-1-isopropyl-pyrrolidine-2,4-dione

Hai-zhen Xu, You-quan Zhu, Yu-hong Xiao and Ran Zhu

S1. Comment

Many compounds containing the 3-acylpyrrolidine-2,4-dione system belong to heterocycles with antibiotic activity, suchas tenuazonic acid (Stickings, 1959), streptolydigin (Rinehart *et al.*, 1963), tirandamycin (Rinehart *et al.*, 1971), malonomycin (Van Der Baan *et al.*, 1978), alpha-cyclopiazonic acid (Stickings, 1959; van Rooyen, 1992) and bata-cyclopiazonic acid (Holzapfel *et al.*, 1970). All these compounds possess a 3-acyltetramic acid grouping as a tricarbonylmethane fragment. Most of the excellent inhibitors of *p*-hydroxyphenylpyruvate dioxygenase also possess similar characteristics, which are crucial for their two kinds of bioactivity (Zhu, Hu & Yang, 2004). In order to develop new herbicides, we synthesized the title compound. The molecular structure of the title compound is shown in Fig. 1. Atom H3, involved in intramolecular hydrogen bonding between atoms O3 and O4, was assigned to O3 rather than to O4. The C13?O4 distance is 1.251 (2) Å, which is longer than the normal carbonyl bond length (C13?O1) of 1.219 (2) Å. In contrast, the C11?O3 distance [1.318 (2) Å] is intermediate between a normal carbonyl C?O double bond and a C—O single-bond length (Allen *et al.*, 1987) (Table 1). A similar situation was reported for 3-(1-hydroxyethylidene)-1-phenylpyrrolidine-2,4-dione (Ellis & Spek, 2001), 1-benzyl-3-(alpha-hydroxybenzylidene)pyrrolidine-2,4-dione, (I) (Zhu, Song, Li *et al.*, 2004), 1-*tert*-butyl-3-(alpha-hydroxy-4-isopropylbenzylidene)pyrrolidine-2,4-dione, (II) (Xu, 2005), and 3-(alpha-hydroxyl-2-methoxylbenzylidene)-1-isopropylpyrrolidine-2,4-dione, (III) (Zhu, Song, Yao *et al.*, 2004). The dihedral angle formed by the enol ring A with the benzene ring is 53.35 (6)°, which is larger than the dihedral angles for (I), (II) (10 and 21°, respectively) and smaller than the dihedral angle for (III) (53°). The crystal structure of the title compound also involves a weak intramolecular C—H···O hydrogenbonding interactions (Table 2).

S2. Experimental

The title compound was obtained according to the procedure reported by Matsuo et al. (1980). Colourless single crystals of the title compound were obtained by recrystallization of 1-isopropyl-3-(*α*<i/>-hydroxy-4-isopropoxyl-2-methoxybenzylidene) pyrrolidine-2,4-dione from petroleum ether and ethyl acetate(1:3).

S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å and O—H = 0.82 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2Ueq(C) or 1.5Ueq(O). Friedel pairs were not merged.

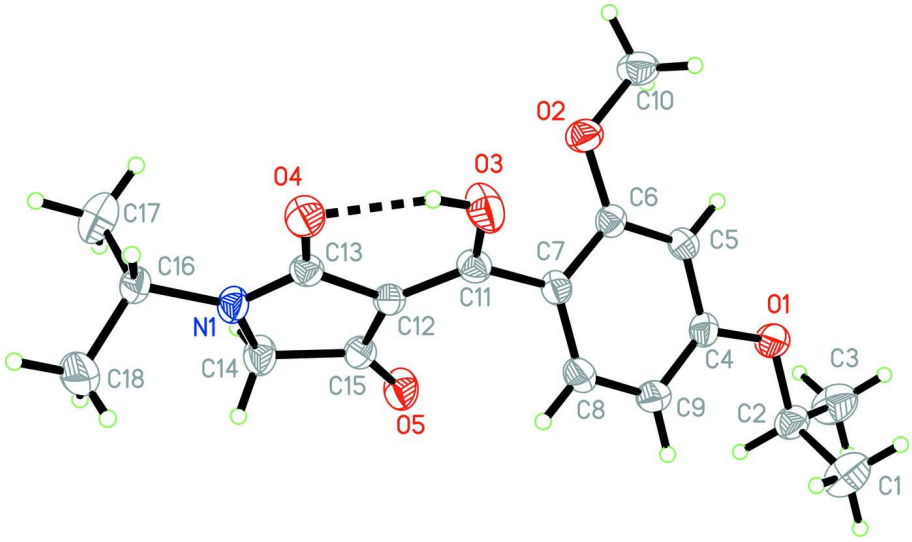

Figure 1

View of the title compound, with displacement ellipsoids drawn at the 30% probability level.

3-[(Hydroxy)(4-isopropoxy-2-methoxyphenyl)methylene]-1- isopropylpyrrolidine-2,4-dione

Crystal data

$C_{18}H_{23}NO_5$
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Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 14.694$ (2) Å
$b = 12.249$ (2) Å
$c = 20.308$ (3) Å
$\beta = 103.864$ (3)°
$V = 3548.5$ (10) Å^3
$Z = 8$
$F(000) = 1424$
$D_x = 1.248$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\theta = 2.6$–$23.1°$
$\mu = 0.09$ mm^{-1}
$T = 294$ K
Prism, colourless
0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
9820 measured reflections
3622 independent reflections
2199 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.1°$
$h = -18 \rightarrow 8$
$k = -15 \rightarrow 15$
$l = -24 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.131$
$S = 1.04$
3622 reflections
223 parameters
12 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
$w = 1/[\sigma^2(F_o^2) + (0.066P)^2 + 0.41P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.08411 (12)	0.33480 (12)	0.57101 (7)	0.0604 (4)
O2	0.17331 (10)	0.25752 (11)	0.36755 (7)	0.0532 (4)
O3	0.10441 (13)	0.05253 (13)	0.31692 (7)	0.0695 (5)
H3	0.1164	0.0047	0.2921	0.104*
O4	0.18049 (11)	−0.11472 (12)	0.27727 (7)	0.0566 (4)
O5	0.28614 (11)	−0.06071 (13)	0.51329 (7)	0.0625 (5)
N1	0.28941 (12)	−0.19911 (14)	0.36200 (8)	0.0452 (4)
C1	−0.0325 (2)	0.2778 (3)	0.63023 (14)	0.0851 (9)
H1A	−0.0707	0.3396	0.6124	0.128*
H1B	−0.0417	0.2597	0.6742	0.128*
H1C	−0.0499	0.2167	0.6003	0.128*
C2	0.06866 (16)	0.30512 (19)	0.63625 (11)	0.0552 (6)
H2	0.1076	0.2419	0.6542	0.066*
C3	0.1002 (2)	0.4022 (2)	0.68087 (13)	0.0837 (9)
H3A	0.1648	0.4172	0.6826	0.126*
H3B	0.0931	0.3871	0.7258	0.126*
H3C	0.0628	0.4645	0.6628	0.126*
C4	0.09829 (14)	0.25628 (16)	0.52731 (10)	0.0441 (5)
C5	0.12539 (13)	0.29580 (16)	0.47092 (10)	0.0427 (5)
H5	0.1314	0.3706	0.4655	0.051*
C6	0.14353 (13)	0.22495 (16)	0.42277 (9)	0.0400 (5)
C7	0.13459 (14)	0.11166 (15)	0.43064 (10)	0.0416 (5)
C8	0.10772 (15)	0.07488 (17)	0.48725 (11)	0.0509 (5)
H8	0.1023	0.0001	0.4931	0.061*
C9	0.08852 (16)	0.14464 (17)	0.53562 (11)	0.0531 (6)
H9	0.0695	0.1175	0.5729	0.064*
C10	0.18157 (18)	0.37182 (18)	0.35704 (11)	0.0608 (6)
H10A	0.1205	0.4048	0.3477	0.091*
H10B	0.2091	0.3835	0.3193	0.091*
H10C	0.2206	0.4041	0.3970	0.091*
C11	0.15126 (14)	0.03387 (16)	0.37983 (10)	0.0442 (5)
C12	0.20977 (14)	−0.05513 (15)	0.39318 (9)	0.0391 (5)
C13	0.22342 (14)	−0.12462 (15)	0.33812 (10)	0.0409 (5)
C14	0.32846 (17)	−0.18606 (18)	0.43457 (10)	0.0555 (6)
H14A	0.3948	−0.1692	0.4439	0.067*

H14B	0.3199	−0.2520	0.4589	0.067*
C15	0.27400 (14)	−0.09173 (16)	0.45477 (10)	0.0449 (5)
C16	0.32451 (15)	−0.27819 (16)	0.31986 (10)	0.0477 (5)
H16	0.2810	−0.2783	0.2750	0.057*
C17	0.41877 (18)	−0.2440 (2)	0.31078 (13)	0.0768 (8)
H17A	0.4149	−0.1711	0.2930	0.115*
H17B	0.4381	−0.2930	0.2798	0.115*
H17C	0.4636	−0.2461	0.3538	0.115*
C18	0.3244 (3)	−0.3906 (2)	0.34875 (15)	0.1083 (12)
H18A	0.3691	−0.3942	0.3917	0.162*
H18B	0.3408	−0.4427	0.3182	0.162*
H18C	0.2630	−0.4071	0.3548	0.162*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0880 (12)	0.0482 (9)	0.0541 (9)	0.0052 (8)	0.0351 (8)	−0.0034 (7)
O2	0.0704 (10)	0.0466 (9)	0.0480 (8)	−0.0046 (7)	0.0246 (8)	−0.0024 (7)
O3	0.0945 (13)	0.0603 (11)	0.0440 (9)	0.0274 (9)	−0.0025 (9)	−0.0056 (7)
O4	0.0720 (11)	0.0573 (10)	0.0373 (8)	0.0081 (8)	0.0068 (7)	−0.0042 (7)
O5	0.0824 (12)	0.0634 (10)	0.0395 (9)	0.0174 (8)	0.0101 (8)	−0.0075 (7)
N1	0.0523 (10)	0.0456 (10)	0.0383 (9)	0.0075 (8)	0.0118 (8)	−0.0051 (7)
C1	0.0769 (19)	0.102 (2)	0.0840 (19)	−0.0169 (16)	0.0350 (15)	−0.0154 (17)
C2	0.0629 (15)	0.0592 (14)	0.0482 (13)	−0.0004 (11)	0.0226 (11)	−0.0032 (11)
C3	0.104 (2)	0.087 (2)	0.0674 (17)	−0.0210 (17)	0.0350 (16)	−0.0227 (15)
C4	0.0459 (12)	0.0423 (12)	0.0453 (11)	0.0049 (9)	0.0131 (9)	−0.0042 (10)
C5	0.0466 (12)	0.0352 (11)	0.0465 (12)	0.0000 (9)	0.0120 (9)	−0.0009 (9)
C6	0.0353 (10)	0.0439 (11)	0.0399 (11)	0.0016 (9)	0.0072 (8)	−0.0001 (9)
C7	0.0433 (11)	0.0403 (11)	0.0399 (11)	0.0061 (9)	0.0071 (9)	−0.0007 (9)
C8	0.0634 (14)	0.0361 (11)	0.0548 (13)	0.0048 (10)	0.0175 (11)	0.0019 (10)
C9	0.0662 (15)	0.0485 (13)	0.0504 (13)	0.0024 (11)	0.0254 (11)	0.0041 (10)
C10	0.0796 (17)	0.0506 (14)	0.0574 (14)	−0.0129 (12)	0.0266 (13)	0.0002 (11)
C11	0.0503 (12)	0.0426 (12)	0.0384 (11)	0.0009 (10)	0.0082 (9)	0.0016 (9)
C12	0.0456 (11)	0.0357 (10)	0.0373 (11)	−0.0017 (9)	0.0123 (9)	−0.0014 (8)
C13	0.0449 (12)	0.0377 (11)	0.0413 (12)	−0.0047 (9)	0.0129 (9)	−0.0008 (9)
C14	0.0636 (15)	0.0585 (14)	0.0424 (12)	0.0162 (11)	0.0087 (10)	−0.0029 (10)
C15	0.0532 (13)	0.0428 (11)	0.0401 (12)	0.0016 (9)	0.0137 (10)	−0.0014 (9)
C16	0.0599 (14)	0.0442 (12)	0.0418 (11)	0.0064 (10)	0.0178 (10)	−0.0059 (9)
C17	0.0618 (16)	0.100 (2)	0.0716 (16)	0.0071 (14)	0.0221 (13)	−0.0198 (14)
C18	0.200 (3)	0.0501 (16)	0.099 (2)	0.0141 (18)	0.084 (2)	−0.0003 (14)

Geometric parameters (Å, º)

O1—C4	1.358 (2)	C6—C7	1.407 (3)
O1—C2	1.443 (3)	C7—C8	1.378 (3)
O2—C6	1.358 (2)	C7—C11	1.468 (3)
O2—C10	1.426 (2)	C8—C9	1.381 (3)
O3—C11	1.318 (2)	C8—H8	0.9300

O3—H3	0.8200	C9—H9	0.9300
O4—C13	1.251 (2)	C10—H10A	0.9600
O5—C15	1.219 (2)	C10—H10B	0.9600
N1—C13	1.335 (3)	C10—H10C	0.9600
N1—C14	1.457 (3)	C11—C12	1.375 (3)
N1—C16	1.466 (2)	C12—C15	1.446 (3)
C1—C2	1.500 (4)	C12—C13	1.457 (3)
C1—H1A	0.9600	C14—C15	1.517 (3)
C1—H1B	0.9600	C14—H14A	0.9700
C1—H1C	0.9600	C14—H14B	0.9700
C2—C3	1.500 (3)	C16—C18	1.497 (3)
C2—H2	0.9800	C16—C17	1.500 (3)
C3—H3A	0.9600	C16—H16	0.9800
C3—H3B	0.9600	C17—H17A	0.9600
C3—H3C	0.9600	C17—H17B	0.9600
C4—C5	1.387 (3)	C17—H17C	0.9600
C4—C9	1.389 (3)	C18—H18A	0.9600
C5—C6	1.380 (3)	C18—H18B	0.9600
C5—H5	0.9300	C18—H18C	0.9600

C4—O1—C2	120.27 (16)	O2—C10—H10A	109.5
C6—O2—C10	117.91 (15)	O2—C10—H10B	109.5
C11—O3—H3	109.5	H10A—C10—H10B	109.5
C13—N1—C14	111.61 (16)	O2—C10—H10C	109.5
C13—N1—C16	124.48 (16)	H10A—C10—H10C	109.5
C14—N1—C16	123.71 (16)	H10B—C10—H10C	109.5
C2—C1—H1A	109.5	O3—C11—C12	119.05 (17)
C2—C1—H1B	109.5	O3—C11—C7	115.64 (17)
H1A—C1—H1B	109.5	C12—C11—C7	125.31 (18)
C2—C1—H1C	109.5	C11—C12—C15	131.63 (18)
H1A—C1—H1C	109.5	C11—C12—C13	120.43 (17)
H1B—C1—H1C	109.5	C15—C12—C13	107.55 (17)
O1—C2—C3	105.14 (19)	O4—C13—N1	125.12 (18)
O1—C2—C1	110.6 (2)	O4—C13—C12	124.87 (18)
C3—C2—C1	112.5 (2)	N1—C13—C12	110.00 (17)
O1—C2—H2	109.5	N1—C14—C15	104.58 (16)
C3—C2—H2	109.5	N1—C14—H14A	110.8
C1—C2—H2	109.5	C15—C14—H14A	110.8
C2—C3—H3A	109.5	N1—C14—H14B	110.8
C2—C3—H3B	109.5	C15—C14—H14B	110.8
H3A—C3—H3B	109.5	H14A—C14—H14B	108.9
C2—C3—H3C	109.5	O5—C15—C12	131.24 (19)
H3A—C3—H3C	109.5	O5—C15—C14	122.51 (18)
H3B—C3—H3C	109.5	C12—C15—C14	106.23 (16)
O1—C4—C5	114.32 (18)	N1—C16—C18	110.20 (17)
O1—C4—C9	125.52 (19)	N1—C16—C17	110.60 (18)
C5—C4—C9	120.15 (18)	C18—C16—C17	113.1 (2)
C6—C5—C4	120.53 (18)	N1—C16—H16	107.6

C6—C5—H5	119.7	C18—C16—H16	107.6
C4—C5—H5	119.7	C17—C16—H16	107.6
O2—C6—C5	123.75 (18)	C16—C17—H17A	109.5
O2—C6—C7	116.18 (17)	C16—C17—H17B	109.5
C5—C6—C7	120.04 (18)	H17A—C17—H17B	109.5
C8—C7—C6	118.08 (18)	C16—C17—H17C	109.5
C8—C7—C11	120.26 (18)	H17A—C17—H17C	109.5
C6—C7—C11	121.64 (18)	H17B—C17—H17C	109.5
C7—C8—C9	122.64 (19)	C16—C18—H18A	109.5
C7—C8—H8	118.7	C16—C18—H18B	109.5
C9—C8—H8	118.7	H18A—C18—H18B	109.5
C8—C9—C4	118.54 (19)	C16—C18—H18C	109.5
C8—C9—H9	120.7	H18A—C18—H18C	109.5
C4—C9—H9	120.7	H18B—C18—H18C	109.5

C4—O1—C2—C3	154.3 (2)	C7—C11—C12—C15	−5.9 (4)
C4—O1—C2—C1	−84.0 (2)	O3—C11—C12—C13	3.1 (3)
C2—O1—C4—C5	−171.26 (18)	C7—C11—C12—C13	−177.76 (17)
C2—O1—C4—C9	8.2 (3)	C14—N1—C13—O4	177.57 (19)
O1—C4—C5—C6	179.05 (17)	C16—N1—C13—O4	2.7 (3)
C9—C4—C5—C6	−0.4 (3)	C14—N1—C13—C12	−1.4 (2)
C10—O2—C6—C5	−3.4 (3)	C16—N1—C13—C12	−176.37 (17)
C10—O2—C6—C7	178.82 (18)	C11—C12—C13—O4	−4.9 (3)
C4—C5—C6—O2	−177.72 (17)	C15—C12—C13—O4	−178.60 (18)
C4—C5—C6—C7	0.0 (3)	C11—C12—C13—N1	174.08 (18)
O2—C6—C7—C8	177.77 (18)	C15—C12—C13—N1	0.4 (2)
C5—C6—C7—C8	−0.1 (3)	C13—N1—C14—C15	1.8 (2)
O2—C6—C7—C11	−3.5 (3)	C16—N1—C14—C15	176.78 (18)
C5—C6—C7—C11	178.64 (18)	C11—C12—C15—O5	9.5 (4)
C6—C7—C8—C9	0.7 (3)	C13—C12—C15—O5	−177.8 (2)
C11—C7—C8—C9	−178.1 (2)	C11—C12—C15—C14	−172.0 (2)
C7—C8—C9—C4	−1.1 (3)	C13—C12—C15—C14	0.7 (2)
O1—C4—C9—C8	−178.5 (2)	N1—C14—C15—O5	177.22 (19)
C5—C4—C9—C8	1.0 (3)	N1—C14—C15—C12	−1.5 (2)
C8—C7—C11—O3	126.2 (2)	C13—N1—C16—C18	−130.9 (3)
C6—C7—C11—O3	−52.5 (3)	C14—N1—C16—C18	54.8 (3)
C8—C7—C11—C12	−53.0 (3)	C13—N1—C16—C17	103.3 (2)
C6—C7—C11—C12	128.3 (2)	C14—N1—C16—C17	−71.0 (3)
O3—C11—C12—C15	175.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O4	0.82	1.80	2.555 (2)	152
C16—H16···O4	0.98	2.50	2.891 (2)	104