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3-[(2,4-Diethoxyphenyl)(hydroxy)methylene]-1-isopropylpyrrolidine-2,4-dione

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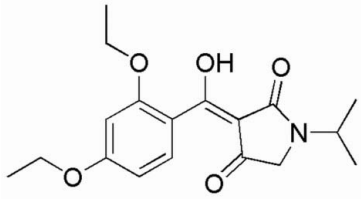
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.155; data-to-parameter ratio = 16.3.

The title compound, $C_{18}H_{23}NO_5$, is a potential potent new herbicide containing the pyrrolidine-2,4-dione ring system. In the crystalline state, the molecular skeleton contains one enol grouping, which is intramolecularly hydrogen bonded to a neighbouring keto O atom. The dihedral angle between the six-membered ring formed by the enol group and the benzene ring is 41.29 (10)°.

Related literature

For related literature, see: Allen *et al.* (1987); Ellis & Spek (2001); Holzapfel *et al.* (1970); MacKellar *et al.* (1971); Matsuo *et al.* (1980); Rinehart *et al.* (1963); van Rooyen *et al.* (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).



Experimental

Crystal data

$C_{18}H_{23}NO_5$
M_r = 333.37
Monoclinic, $P2_1/n$
a = 13.513 (7) Å
b = 8.135 (4) Å
c = 16.312 (8) Å
β = 99.518 (9)°
V = 1768.5 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.28 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.982
9501 measured reflections
3612 independent reflections
2072 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.156
S = 1.00
3612 reflections
222 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O4	0.82	1.74	2.505 (2)	154
C6—H6···O5	0.93	2.56	2.994 (3)	109
C16—H16···O4	0.98	2.52	2.880 (3)	102

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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2023).

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.
MacKellar, F. A., Grostic, M. F., Olson, E. C., Wnuk, R. J., Branfman, A. R. & Rinehart, K. L. (1971). *J. Am. Chem. Soc.* **93**, 4943–4945.
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.
Rooyen, P. H. van (1992). *Acta Cryst.* C**48**, 551–552.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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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supplementary materials

Acta Cryst. (2007). E**63**, o3384 [**doi:10.1107/S1600536807030759**]

3-[(2,4-Diethoxyphenyl)(hydroxy)methylene]-1-isopropylpyrrolidine-2,4-dione

G.-S. Yu, H.-Z. Xu and Y.-Q. Zhu

Comment

Many compounds containing the 3-acylpyrrolidine-2,4-dione system belong to heterocycles with antibiotic activity, such as tenuazonic acid (Stickings, 1959), streptolydigin (Rinehart *et al.*, 1963), tirandamycin (MacKellar *et al.*, 1971), malonomycin (Van Der Baan *et al.*, 1978), *α*-cyclopiazonic acid (Stickings, 1959; van Rooyen *et al.*, 1992) and *β*- 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 *et al.*, 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 C15=O4 distance is 1.264 (2) Å, which is longer than the normal carbonyl bond length (C13=O1) of 1.227 (3) Å. In contrast, the C11=O3 distance [1.320 (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-(*α*-hydroxybenzylidene)pyrrolidine- 2,4-dione, (I) (Zhu, Song, Li *et al.*, 2004), 1-*tert*-butyl-3-(*α*-hydroxy-4-isopropylbenzylidene)pyrrolidine-2,4-dione, (II) (Xu, 2005), and 3-(*α*-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 41.29 (10) °, 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 two weak intramolecular C—H···O hydrogenbonding interactions (Table 2).

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*-hydroxy-2,4-diethoxylbenzylidene) pyrrolidine-2,4-dione from petroleum ether and ethyl acetate (1:3).

Refinement

The hydroxyl H atom (O3)H3 was was found in a difference map and the coordinates were fixed. The other H atoms were placed in calculated positions, with C—H=0.93–0.98 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H)=1.2Ueq(C).

Figures

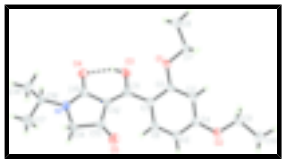


Fig. 1. View of the title compound with 30% probability ellipsoid.

3-[(2,4-Diethoxyphenyl)(hydroxy)methylene]-1-isopropylpyrrolidine-2,4-dione

Crystal data

$C_{18}H_{23}NO_5$	F_{000} = 712
M_r = 333.37	D_x = 1.252 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2383 reflections
a = 13.513 (7) Å	θ = 2.8–23.7º
b = 8.135 (4) Å	μ = 0.09 mm^{-1}
c = 16.312 (8) Å	T = 294 (2) K
β = 99.518 (9)º	Prism, colorless
V = 1768.5 (15) Å^3	0.28 × 0.24 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3612 independent reflections
Radiation source: fine-focus sealed tube	2072 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.052
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −9→16
T_{min} = 0.975, T_{max} = 0.982	k = −10→8
9501 measured reflections	l = −18→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.052	H-atom parameters constrained
$wR(F^2)$ = 0.156	$w = 1/[\sigma^2(F_o^2) + (0.0745P)^2 + 0.2597P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.001
3612 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}

222 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.71221 (12)	−0.20692 (19)	0.38809 (10)	0.0520 (5)
O2	0.96831 (12)	−0.2405 (2)	0.21363 (10)	0.0562 (5)
O3	0.78362 (14)	−0.06279 (19)	0.53402 (10)	0.0586 (5)
H3	0.7691	−0.0117	0.5737	0.088*
O4	0.76454 (13)	0.16486 (19)	0.63361 (10)	0.0558 (5)
O5	0.88238 (16)	0.3662 (2)	0.39616 (10)	0.0679 (6)
N1	0.81988 (15)	0.4165 (2)	0.59623 (11)	0.0468 (5)
C1	0.85415 (16)	−0.0350 (3)	0.41169 (12)	0.0375 (5)
C2	0.80068 (16)	−0.1612 (3)	0.36515 (13)	0.0390 (5)
C3	0.83646 (17)	−0.2313 (3)	0.29811 (13)	0.0432 (6)
H3A	0.7996	−0.3126	0.2666	0.052*
C4	0.92752 (17)	−0.1795 (3)	0.27832 (13)	0.0415 (5)
C5	0.98245 (17)	−0.0563 (3)	0.32420 (13)	0.0435 (6)
H5	1.0437	−0.0221	0.3112	0.052*
C6	0.94493 (16)	0.0141 (3)	0.38891 (13)	0.0414 (5)
H6	0.9813	0.0978	0.4189	0.050*
C7	0.65284 (19)	−0.3318 (3)	0.34169 (16)	0.0567 (7)
H7A	0.6918	−0.4315	0.3400	0.068*
H7B	0.6299	−0.2952	0.2851	0.068*
C8	0.5653 (2)	−0.3624 (4)	0.38525 (19)	0.0799 (10)
H8A	0.5891	−0.4007	0.4407	0.120*
H8B	0.5223	−0.4440	0.3554	0.120*
H8C	0.5284	−0.2622	0.3876	0.120*
C9	0.9102 (2)	−0.3523 (3)	0.15804 (17)	0.0652 (8)
H9A	0.8444	−0.3063	0.1381	0.078*
H9B	0.9018	−0.4551	0.1862	0.078*
C10	0.9652 (3)	−0.3810 (4)	0.08683 (19)	0.0993 (12)
H10A	0.9695	−0.2798	0.0574	0.149*
H10B	0.9297	−0.4611	0.0499	0.149*
H10C	1.0315	−0.4206	0.1075	0.149*

C11	0.82072 (16)	0.0394 (3)	0.48406 (13)	0.0397 (5)
C12	0.82908 (16)	0.2029 (3)	0.50607 (12)	0.0383 (5)
C13	0.85927 (18)	0.3479 (3)	0.46522 (14)	0.0468 (6)
C14	0.8572 (2)	0.4900 (3)	0.52583 (14)	0.0521 (6)
H14A	0.9238	0.5352	0.5428	0.062*
H14B	0.8128	0.5766	0.5010	0.062*
C15	0.80136 (16)	0.2574 (3)	0.58414 (13)	0.0416 (6)
C16	0.79723 (19)	0.5096 (3)	0.66811 (14)	0.0510 (6)
H16	0.7915	0.4313	0.7127	0.061*
C17	0.8813 (2)	0.6273 (4)	0.69922 (18)	0.0773 (9)
H17A	0.9433	0.5677	0.7116	0.116*
H17B	0.8677	0.6809	0.7486	0.116*
H17C	0.8863	0.7081	0.6572	0.116*
C18	0.6977 (2)	0.5972 (4)	0.64567 (19)	0.0783 (9)
H18A	0.7012	0.6732	0.6012	0.118*
H18B	0.6829	0.6558	0.6933	0.118*
H18C	0.6457	0.5181	0.6282	0.118*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0456 (9)	0.0513 (10)	0.0616 (10)	−0.0146 (8)	0.0164 (8)	−0.0173 (8)
O2	0.0573 (10)	0.0580 (11)	0.0573 (10)	−0.0122 (9)	0.0220 (9)	−0.0213 (8)
O3	0.0876 (13)	0.0431 (10)	0.0493 (10)	−0.0178 (10)	0.0238 (10)	−0.0030 (8)
O4	0.0748 (12)	0.0498 (10)	0.0489 (9)	−0.0123 (9)	0.0276 (9)	0.0002 (8)
O5	0.1104 (16)	0.0489 (11)	0.0530 (11)	0.0001 (10)	0.0384 (11)	0.0057 (8)
N1	0.0619 (13)	0.0400 (11)	0.0428 (11)	−0.0033 (10)	0.0213 (10)	−0.0041 (9)
C1	0.0396 (12)	0.0346 (12)	0.0370 (12)	−0.0010 (10)	0.0027 (10)	−0.0004 (9)
C2	0.0370 (12)	0.0358 (12)	0.0439 (12)	−0.0028 (10)	0.0056 (10)	−0.0020 (10)
C3	0.0450 (13)	0.0390 (13)	0.0447 (13)	−0.0064 (11)	0.0048 (10)	−0.0084 (10)
C4	0.0464 (13)	0.0398 (13)	0.0385 (12)	0.0009 (11)	0.0075 (10)	−0.0036 (10)
C5	0.0395 (12)	0.0457 (14)	0.0448 (13)	−0.0032 (11)	0.0057 (10)	−0.0027 (11)
C6	0.0434 (13)	0.0379 (12)	0.0408 (12)	−0.0053 (10)	0.0012 (10)	−0.0038 (10)
C7	0.0503 (14)	0.0570 (16)	0.0634 (16)	−0.0183 (13)	0.0112 (13)	−0.0172 (13)
C8	0.0602 (18)	0.091 (2)	0.094 (2)	−0.0343 (17)	0.0280 (17)	−0.0295 (18)
C9	0.0723 (18)	0.0656 (18)	0.0611 (16)	−0.0120 (15)	0.0208 (14)	−0.0276 (14)
C10	0.116 (3)	0.108 (3)	0.086 (2)	−0.037 (2)	0.052 (2)	−0.053 (2)
C11	0.0410 (12)	0.0398 (13)	0.0376 (12)	−0.0057 (10)	0.0047 (10)	0.0028 (10)
C12	0.0418 (12)	0.0383 (12)	0.0350 (11)	−0.0009 (10)	0.0068 (10)	−0.0004 (9)
C13	0.0560 (15)	0.0431 (13)	0.0438 (13)	0.0018 (12)	0.0155 (11)	0.0014 (11)
C14	0.0705 (17)	0.0396 (14)	0.0508 (14)	−0.0038 (12)	0.0237 (13)	−0.0017 (11)
C15	0.0445 (13)	0.0407 (14)	0.0402 (12)	−0.0008 (11)	0.0082 (10)	0.0005 (10)
C16	0.0675 (17)	0.0460 (14)	0.0444 (13)	−0.0033 (13)	0.0236 (13)	−0.0085 (11)
C17	0.0680 (19)	0.095 (2)	0.0686 (18)	−0.0088 (17)	0.0092 (15)	−0.0351 (17)
C18	0.0592 (17)	0.095 (2)	0.087 (2)	0.0036 (17)	0.0316 (16)	−0.0250 (18)

Geometric parameters (Å, °)

O1—C2	1.362 (3)	C8—H8A	0.96

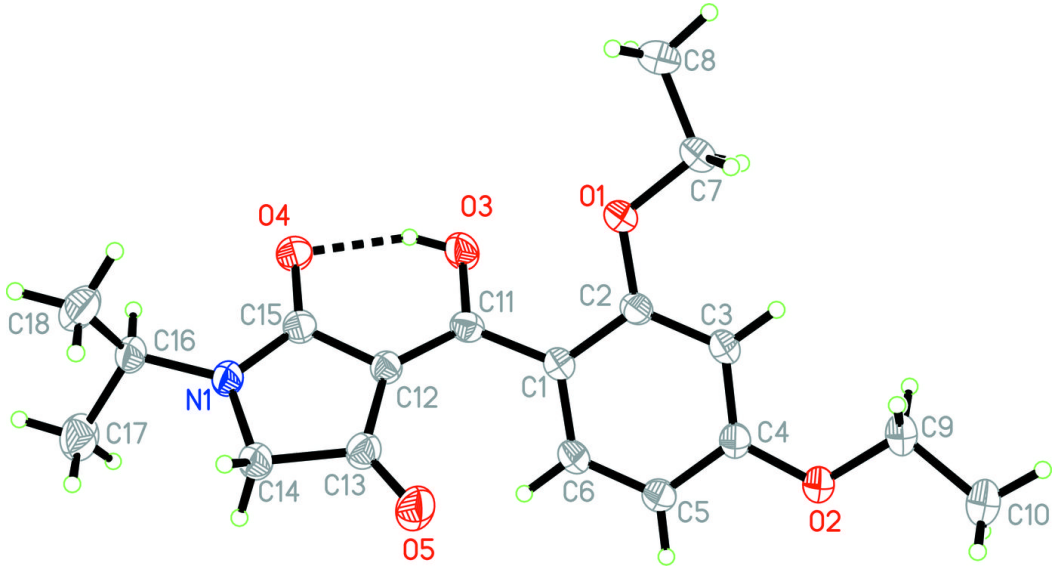
O1—C7	1.431 (3)	C8—H8B	0.96
O2—C4	1.362 (3)	C8—H8C	0.96
O2—C9	1.425 (3)	C9—C10	1.497 (4)
O3—C11	1.320 (2)	C9—H9A	0.97
O3—H3	0.82	C9—H9B	0.97
O4—C15	1.264 (2)	C10—H10A	0.96
O5—C13	1.227 (3)	C10—H10B	0.96
N1—C15	1.327 (3)	C10—H10C	0.96
N1—C14	1.456 (3)	C11—C12	1.378 (3)
N1—C16	1.470 (3)	C12—C13	1.446 (3)
C1—C6	1.397 (3)	C12—C15	1.455 (3)
C1—C2	1.404 (3)	C13—C14	1.524 (3)
C1—C11	1.463 (3)	C14—H14A	0.97
C2—C3	1.389 (3)	C14—H14B	0.97
C3—C4	1.388 (3)	C16—C17	1.508 (4)
C3—H3A	0.93	C16—C18	1.513 (4)
C4—C5	1.390 (3)	C16—H16	0.98
C5—C6	1.370 (3)	C17—H17A	0.96
C5—H5	0.93	C17—H17B	0.96
C6—H6	0.93	C17—H17C	0.96
C7—C8	1.498 (3)	C18—H18A	0.96
C7—H7A	0.97	C18—H18B	0.96
C7—H7B	0.97	C18—H18C	0.96
C2—O1—C7	119.30 (17)	C9—C10—H10A	109.5
C4—O2—C9	118.34 (18)	C9—C10—H10B	109.5
C11—O3—H3	109.5	H10A—C10—H10B	109.5
C15—N1—C14	111.37 (17)	C9—C10—H10C	109.5
C15—N1—C16	124.19 (18)	H10A—C10—H10C	109.5
C14—N1—C16	124.24 (19)	H10B—C10—H10C	109.5
C6—C1—C2	117.45 (19)	O3—C11—C12	118.06 (19)
C6—C1—C11	119.89 (19)	O3—C11—C1	115.94 (19)
C2—C1—C11	122.59 (19)	C12—C11—C1	125.92 (19)
O1—C2—C3	122.64 (19)	C11—C12—C13	133.2 (2)
O1—C2—C1	116.61 (18)	C11—C12—C15	120.02 (19)
C3—C2—C1	120.7 (2)	C13—C12—C15	106.74 (19)
C4—C3—C2	119.7 (2)	O5—C13—C12	131.0 (2)
C4—C3—H3A	120.1	O5—C13—C14	122.6 (2)
C2—C3—H3A	120.1	C12—C13—C14	106.41 (18)
O2—C4—C3	123.9 (2)	N1—C14—C13	104.27 (18)
O2—C4—C5	115.5 (2)	N1—C14—H14A	110.9
C3—C4—C5	120.6 (2)	C13—C14—H14A	110.9
C6—C5—C4	118.9 (2)	N1—C14—H14B	110.9
C6—C5—H5	120.5	C13—C14—H14B	110.9
C4—C5—H5	120.5	H14A—C14—H14B	108.9
C5—C6—C1	122.6 (2)	O4—C15—N1	124.8 (2)
C5—C6—H6	118.7	O4—C15—C12	124.3 (2)
C1—C6—H6	118.7	N1—C15—C12	110.95 (19)
O1—C7—C8	106.6 (2)	N1—C16—C17	110.5 (2)
O1—C7—H7A	110.4	N1—C16—C18	110.1 (2)

C8—C7—H7A	110.4	C17—C16—C18	111.9 (2)
O1—C7—H7B	110.4	N1—C16—H16	108.1
C8—C7—H7B	110.4	C17—C16—H16	108.1
H7A—C7—H7B	108.6	C18—C16—H16	108.1
C7—C8—H8A	109.5	C16—C17—H17A	109.5
C7—C8—H8B	109.5	C16—C17—H17B	109.5
H8A—C8—H8B	109.5	H17A—C17—H17B	109.5
C7—C8—H8C	109.5	C16—C17—H17C	109.5
H8A—C8—H8C	109.5	H17A—C17—H17C	109.5
H8B—C8—H8C	109.5	H17B—C17—H17C	109.5
O2—C9—C10	107.6 (2)	C16—C18—H18A	109.5
O2—C9—H9A	110.2	C16—C18—H18B	109.5
C10—C9—H9A	110.2	H18A—C18—H18B	109.5
O2—C9—H9B	110.2	C16—C18—H18C	109.5
C10—C9—H9B	110.2	H18A—C18—H18C	109.5
H9A—C9—H9B	108.5	H18B—C18—H18C	109.5
C7—O1—C2—C3	−0.2 (3)	C1—C11—C12—C13	8.0 (4)
C7—O1—C2—C1	178.3 (2)	O3—C11—C12—C15	2.6 (3)
C6—C1—C2—O1	−179.79 (19)	C1—C11—C12—C15	−174.09 (19)
C11—C1—C2—O1	3.1 (3)	C11—C12—C13—O5	3.6 (5)
C6—C1—C2—C3	−1.3 (3)	C15—C12—C13—O5	−174.5 (3)
C11—C1—C2—C3	−178.3 (2)	C11—C12—C13—C14	−177.0 (2)
O1—C2—C3—C4	−179.7 (2)	C15—C12—C13—C14	4.8 (2)
C1—C2—C3—C4	1.9 (3)	C15—N1—C14—C13	0.1 (3)
C9—O2—C4—C3	6.3 (3)	C16—N1—C14—C13	−174.9 (2)
C9—O2—C4—C5	−172.4 (2)	O5—C13—C14—N1	176.3 (2)
C2—C3—C4—O2	−179.7 (2)	C12—C13—C14—N1	−3.1 (3)
C2—C3—C4—C5	−1.0 (3)	C14—N1—C15—O4	−176.9 (2)
O2—C4—C5—C6	178.33 (19)	C16—N1—C15—O4	−1.9 (4)
C3—C4—C5—C6	−0.4 (3)	C14—N1—C15—C12	3.0 (3)
C4—C5—C6—C1	1.1 (3)	C16—N1—C15—C12	178.0 (2)
C2—C1—C6—C5	−0.2 (3)	C11—C12—C15—O4	−3.5 (3)
C11—C1—C6—C5	176.9 (2)	C13—C12—C15—O4	174.9 (2)
C2—O1—C7—C8	176.1 (2)	C11—C12—C15—N1	176.5 (2)
C4—O2—C9—C10	172.0 (2)	C13—C12—C15—N1	−5.1 (2)
C6—C1—C11—O3	−136.5 (2)	C15—N1—C16—C17	139.1 (2)
C2—C1—C11—O3	40.5 (3)	C14—N1—C16—C17	−46.6 (3)
C6—C1—C11—C12	40.2 (3)	C15—N1—C16—C18	−96.8 (3)
C2—C1—C11—C12	−142.8 (2)	C14—N1—C16—C18	77.5 (3)
O3—C11—C12—C13	−175.4 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O4	0.82	1.74	2.505 (2)	154
C6—H6···O5	0.93	2.56	2.994 (3)	109
C16—H16···O4	0.98	2.52	2.880 (3)	102

Fig. 1


C8
C7
O1
O4
O3
C11
C2
C3
C18
C15
C16
N1
C12
C1
C17
C4
C9
C14
C13
C6
C5
O2
C10
O5