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Doxofylline–acrylic acid (1/1)

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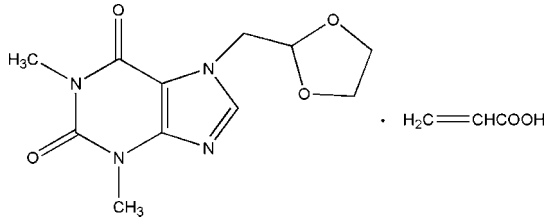
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.069; wR factor = 0.169; data-to-parameter ratio = 12.2.

The title compound, $C_{11}H_{14}N_4O_4{\cdot}C_3H_4O_2$, a 1:1 doxofylline–acrylic acid complex, forms *via* O—H···N and C—H···O hydrogen bonds in the solid state. Dimers of (I) aggregate *via* methyl–acid C—H···O interactions about inversion centres, and the three-dimensional structure arises from π–π stacking interactions of the purine molecules.

Related literature

For related literature, see: Chen, Tu & Jin (2007); Chen, Tu *et al.* (2007); Franzone *et al.* (1981, 1989); Villani *et al.* (1997); Zhao & Li (2001).



Experimental

Crystal data

$C_{11}H_{14}N_4O_4{\cdot}C_3H_4O_2$
M_r = 338.32
Triclinic, $P\overline{1}$
a = 5.5365 (6) Å
b = 10.1199 (12) Å
c = 14.2916 (16) Å
α = 87.182 (2)°
β = 88.023 (2)°
γ = 80.578 (2)°
V = 788.70 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 273 (2) K
0.32 × 0.23 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.969, T_{max} = 0.978
4155 measured reflections
2785 independent reflections
2445 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.169
S = 1.15
2785 reflections
229 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 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
O5—H5···N4	0.82	1.92	2.736 (3)	178
C5—H5A···O6	0.93	2.50	3.131 (4)	125
C6—H6A···O1	0.97	2.58	3.202 (3)	122
C13—H13B···O5^{i}	0.96	2.58	3.365 (4)	140

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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, 2000); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2028).

References

Bruker (2000). *SMART* (Version 5.618), *SADABS* (Version 2.05), *SAINT* (Version 6.02a) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, Z.-H., Tu, B. & Jin, Z.-M. (2007). *Acta Cryst.* E**63**, o2676–o2677.
Chen, H.-X., Tu, B., Shu, Z., Ma, X.-J. & Jin, Z.-M. (2007). *Acta Cryst.* E**63**, o726–o727.
Franzone, J. S., Cirillo, R. & Biffignandi, P. (1989). *Eur. J. Pharmacol.* **165**, 269–277.
Franzone, J. S., Reboani, C. & Fonzo, D. (1981). *Farmaco Ed. Sci.* **36**, 201–219.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Villani, F., De Maria, P., Ronchi, E. & Galimberti, M. (1997). *Int. J. Clin. Pharmacol. Ther.* **35**, 107–111.
Zhao, J. J. & Li, L. (2001). *J. Norman Bethune Univ. Med. Sci.* **27**, 646–676.

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supplementary materials

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Doxofylline-acrylic acid (1/1)

W.-J. Feng, X.-J. Ma, Z. Shu and Z.-M. Jin

Comment

Doxofylline [7-(1,3-dioxolan-2-ylmethyl)-1,3-dimethyl-3,7-dihydro-1*H*-purine-2,6-dione] is a therapeutic agent with anti-asthmatic (Franzone *et al.*, 1989), antiinflammatory activities (Zhao *et al.*, 2001) and a bronchodilating effect on smooth muscle (Franzone *et al.*, 1981; Villani *et al.*, 1997). These studies provide important reference points for futher research into doxofylline. Herein we present the structure of the title compound, (I), a 1:1 complex of doxofylline:acrylic acid.

As shown in Fig. 1, compound (I) is comprised of a doxofylline and acrylic acid molecule. The atoms of acrylic acid molecule are almost coplanar. The angle between the plane of acrylic acid and the plane of the purine ring is 8.2°. The doxofylline molecule in (I) adopts a different conformation from that observed in doxofylline (Chen, Tu, *et al.*, 2007; Chen, Tu & Jin, 2007). In (I), a disordered carbon atom in the dioxolane ring is observed and modelled with site occupancies of 0.759 (17):0.241 (17) for the major and minor sites, respectively.

The geometrical arrangement in the crystal is characterized by formation of the parallel purine rings (Fig. 2). While the O5—H5···N4 hydrogen bond plays an important role in forming the complex, the hydrogen bonds of C5—H5A···O6 and C6—H6A···O1 (Table 2) play roles in dimer formation (forming dimers of (I)) and ultimately a three-dimensional structure is seen *via* interlocking dioxalane groups and π···π stacking interactions

Experimental

Doxofylline and acrylic acid in 1:1 molar ratio were mixed together in suffient ethanol and heated to afford a clear solution. Crystals of (I) were formed by gradual evaporation of ethanol over a period of one week at 293 K.

Refinement

All H atoms were placed in calculated positions and allowed to ride on their parent atoms at distances of 0.82 (O—H), 0.93 (unsaturated), 0.96 (methyl), 0.97 (methylene) and 0.98 Å (methine), with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C) and U_{eq}(O).

Figures

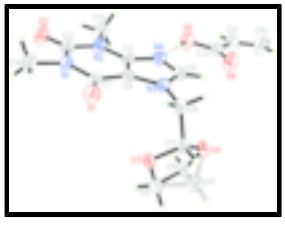


Fig. 1. An *ORTEP* diagram of the 1:1 complex of (I) with atoms displayed with 30% probability displacement ellipsoids.
Fig. 2. The cell unit of (I) with atom labels, showing 30% probability displacement ellipsoids. Hydrogen bonds is illustrated as dashed lines.
Fig. 3. A packing diagram viewed down along the *a* axis. Hydrogen bonds are illustrated as dashed lines.

Doxofylline–acrylic acid (1/1)

Crystal data

$C_{11}H_{14}N_4O_4·C_3H_4O_2$	V = 788.70 (15) Å^3
M_r = 338.32	Z = 2
Triclinic, $P\overline{1}$	F_{000} = 356
Hall symbol: -P 1	D_x = 1.425 Mg m^{-3}
a = 5.5365 (6) Å	Melting point: 428 K
b = 10.1199 (12) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
c = 14.2916 (16) Å	μ = 0.11 mm^{-1}
α = 87.182 (2)º	T = 273 (2) K
β = 88.023 (2)º	Block, colourless
γ = 80.578 (2)º	0.32 × 0.23 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer	2785 independent reflections
Radiation source: fine-focus sealed tube	2445 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.014
T = 273(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	h = −4→6
T_{min} = 0.969, T_{max} = 0.978	k = −12→12
4155 measured reflections	l = −16→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.069	H-atom parameters constrained
$wR(F^2)$ = 0.169	$w = 1/[\sigma^2(F_o^2) + (0.0731P)^2 + 0.3726P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.15	$(\Delta/\sigma)_{max} < 0.001$
2785 reflections	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
229 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)
O1	−0.1246 (4)	1.0444 (2)	0.77706 (15)	0.0621 (6)	
O2	−0.1415 (5)	0.8294 (3)	0.50445 (15)	0.0777 (7)	
O3	0.0059 (3)	0.82622 (19)	0.96331 (14)	0.0521 (5)	
O4	0.3894 (3)	0.7265 (2)	0.99833 (15)	0.0604 (6)	
O5	0.8511 (4)	0.4874 (3)	0.66161 (16)	0.0743 (7)	
H5	0.7459	0.5509	0.6752	0.111*	
O6	1.0023 (4)	0.5298 (3)	0.79567 (17)	0.0796 (7)	
N1	−0.1292 (4)	0.9348 (2)	0.64116 (16)	0.0507 (6)	
N2	0.1766 (5)	0.7543 (2)	0.59918 (15)	0.0526 (6)	
N3	0.3591 (4)	0.8519 (2)	0.81369 (15)	0.0450 (5)	
N4	0.5041 (4)	0.6996 (2)	0.71012 (16)	0.0518 (6)	
C1	−0.0279 (5)	0.9562 (3)	0.72678 (19)	0.0451 (6)	
C2	−0.0371 (6)	0.8378 (3)	0.5766 (2)	0.0564 (8)	
C3	0.2886 (5)	0.7699 (3)	0.68106 (18)	0.0447 (6)	
C4	0.1916 (5)	0.8642 (3)	0.74297 (18)	0.0427 (6)	
C5	0.5383 (5)	0.7531 (3)	0.7905 (2)	0.0513 (7)	
H5A	0.6741	0.7245	0.8272	0.062*	
C6	0.3419 (5)	0.9260 (3)	0.89930 (19)	0.0497 (7)	
H6A	0.2372	1.0118	0.8889	0.060*	
H6B	0.5034	0.9433	0.9139	0.060*	
C7	0.2412 (5)	0.8517 (3)	0.98124 (19)	0.0485 (7)	
H7	0.2343	0.9049	1.0370	0.058*	
C8	−0.0116 (6)	0.7026 (3)	1.0123 (3)	0.0731 (10)	
H8A	−0.1271	0.6565	0.9827	0.088*	
H8B	−0.0649	0.7172	1.0768	0.088*	
C9	0.2359 (7)	0.6245 (5)	1.0077 (7)	0.065 (2)	0.759 (17)
H9A	0.2707	0.5688	1.0644	0.078*	0.759 (17)
H9B	0.2571	0.5681	0.9542	0.078*	0.759 (17)
C9'	0.2275 (17)	0.664 (2)	1.0606 (12)	0.067 (5)	0.241 (17)
H9'1	0.2199	0.7000	1.1226	0.080*	0.241 (17)
H9'2	0.2765	0.5678	1.0656	0.080*	0.241 (17)
C10	1.3987 (7)	0.3237 (4)	0.7628 (3)	0.0873 (12)	
H10A	1.4119	0.3776	0.8127	0.105*	

H10B	1.5211	0.2515	0.7509	0.105*
C11	1.2085 (6)	0.3495 (3)	0.7096 (2)	0.0695 (9)
H11	1.1959	0.2954	0.6599	0.083*
C12	1.0133 (5)	0.4639 (3)	0.7279 (2)	0.0539 (7)
C13	0.2871 (7)	0.6508 (3)	0.5350 (2)	0.0693 (9)
H13A	0.4423	0.6706	0.5115	0.104*
H13B	0.1805	0.6493	0.4836	0.104*
H13C	0.3105	0.5649	0.5679	0.104*
C14	−0.3516 (6)	1.0260 (4)	0.6145 (2)	0.0715 (9)
H14A	−0.3993	1.0880	0.6631	0.107*
H14B	−0.4807	0.9754	0.6059	0.107*
H14C	−0.3206	1.0746	0.5572	0.107*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0637 (13)	0.0575 (12)	0.0594 (13)	0.0109 (10)	−0.0033 (10)	−0.0151 (10)
O2	0.0814 (16)	0.0993 (18)	0.0498 (13)	0.0009 (14)	−0.0222 (12)	−0.0146 (12)
O3	0.0338 (10)	0.0583 (12)	0.0626 (13)	−0.0032 (8)	−0.0045 (9)	−0.0001 (10)
O4	0.0349 (10)	0.0802 (15)	0.0636 (13)	−0.0032 (10)	−0.0104 (9)	0.0089 (11)
O5	0.0660 (15)	0.0874 (18)	0.0625 (14)	0.0172 (12)	−0.0082 (12)	−0.0293 (12)
O6	0.0764 (16)	0.0865 (17)	0.0690 (15)	0.0183 (13)	−0.0147 (12)	−0.0305 (13)
N1	0.0496 (14)	0.0566 (14)	0.0439 (13)	−0.0013 (11)	−0.0066 (11)	−0.0020 (11)
N2	0.0608 (15)	0.0570 (14)	0.0385 (13)	−0.0017 (12)	−0.0028 (11)	−0.0113 (11)
N3	0.0425 (12)	0.0520 (13)	0.0405 (12)	−0.0055 (10)	0.0006 (10)	−0.0093 (10)
N4	0.0501 (14)	0.0581 (14)	0.0434 (13)	0.0038 (11)	0.0018 (10)	−0.0085 (11)
C1	0.0459 (15)	0.0450 (15)	0.0434 (15)	−0.0053 (12)	0.0043 (12)	−0.0025 (12)
C2	0.0603 (19)	0.0653 (19)	0.0436 (17)	−0.0085 (15)	−0.0065 (14)	−0.0045 (14)
C3	0.0471 (15)	0.0488 (15)	0.0373 (14)	−0.0042 (12)	0.0004 (11)	−0.0047 (11)
C4	0.0437 (14)	0.0464 (15)	0.0384 (14)	−0.0083 (12)	0.0007 (11)	−0.0046 (11)
C5	0.0437 (15)	0.0624 (18)	0.0449 (16)	0.0017 (13)	−0.0013 (12)	−0.0060 (13)
C6	0.0495 (16)	0.0547 (16)	0.0479 (16)	−0.0133 (13)	−0.0001 (13)	−0.0172 (13)
C7	0.0420 (15)	0.0624 (17)	0.0432 (15)	−0.0100 (13)	−0.0039 (12)	−0.0161 (13)
C8	0.0477 (18)	0.073 (2)	0.099 (3)	−0.0149 (16)	−0.0117 (18)	0.020 (2)
C9	0.047 (2)	0.060 (3)	0.088 (5)	−0.007 (2)	−0.012 (2)	0.006 (3)
C9'	0.073 (10)	0.064 (10)	0.059 (11)	−0.001 (7)	0.000 (8)	−0.009 (8)
C10	0.074 (2)	0.090 (3)	0.088 (3)	0.022 (2)	−0.007 (2)	−0.023 (2)
C11	0.070 (2)	0.066 (2)	0.067 (2)	0.0065 (17)	0.0001 (18)	−0.0171 (17)
C12	0.0528 (17)	0.0547 (17)	0.0524 (17)	−0.0025 (14)	0.0050 (14)	−0.0095 (14)
C13	0.090 (2)	0.069 (2)	0.0462 (18)	0.0015 (18)	0.0000 (16)	−0.0195 (15)
C14	0.063 (2)	0.081 (2)	0.063 (2)	0.0099 (17)	−0.0122 (16)	0.0023 (17)

Geometric parameters (Å, °)

O1—C1	1.216 (3)	C6—C7	1.501 (4)
O2—C2	1.213 (4)	C6—H6A	0.9700
O3—C7	1.403 (3)	C6—H6B	0.9700
O3—C8	1.418 (4)	C7—H7	0.9800
O4—C7	1.407 (3)	C8—C9	1.467 (5)

O4—C9'	1.437 (9)	C8—C9'	1.499 (9)
O4—C9	1.440 (5)	C8—H8A	0.9700
O5—C12	1.315 (4)	C8—H8B	0.9700
O5—H5	0.8200	C9—H9A	0.9700
O6—C12	1.197 (4)	C9—H9B	0.9700
N1—C2	1.403 (4)	C9'—H9'1	0.9700
N1—C1	1.404 (3)	C9'—H9'2	0.9700
N1—C14	1.462 (4)	C10—C11	1.304 (5)
N2—C3	1.371 (3)	C10—H10A	0.9300
N2—C2	1.375 (4)	C10—H10B	0.9300
N2—C13	1.469 (4)	C11—C12	1.476 (4)
N3—C5	1.334 (4)	C11—H11	0.9300
N3—C4	1.383 (3)	C13—H13A	0.9600
N3—C6	1.458 (3)	C13—H13B	0.9600
N4—C5	1.327 (4)	C13—H13C	0.9600
N4—C3	1.353 (4)	C14—H14A	0.9600
C1—C4	1.424 (4)	C14—H14B	0.9600
C3—C4	1.365 (4)	C14—H14C	0.9600
C5—H5A	0.9300		
C7—O3—C8	105.0 (2)	O3—C8—C9'	104.9 (6)
C7—O4—C9'	99.5 (7)	O3—C8—H8A	110.7
C7—O4—C9	108.9 (2)	C9—C8—H8A	110.7
C12—O5—H5	109.5	C9'—C8—H8A	136.8
C2—N1—C1	127.3 (2)	O3—C8—H8B	110.7
C2—N1—C14	116.0 (2)	C9—C8—H8B	110.7
C1—N1—C14	116.7 (2)	C9'—C8—H8B	79.6
C3—N2—C2	119.6 (2)	H8A—C8—H8B	108.8
C3—N2—C13	120.2 (3)	O4—C9—C8	102.9 (3)
C2—N2—C13	120.2 (2)	O4—C9—H9A	111.2
C5—N3—C4	106.2 (2)	C8—C9—H9A	111.2
C5—N3—C6	125.9 (2)	O4—C9—H9B	111.2
C4—N3—C6	127.8 (2)	C8—C9—H9B	111.2
C5—N4—C3	103.6 (2)	H9A—C9—H9B	109.1
O1—C1—N1	121.4 (3)	O4—C9'—C8	101.4 (6)
O1—C1—C4	127.5 (3)	O4—C9'—H9'1	111.5
N1—C1—C4	111.2 (2)	C8—C9'—H9'1	111.5
O2—C2—N2	122.2 (3)	O4—C9'—H9'2	111.5
O2—C2—N1	121.2 (3)	C8—C9'—H9'2	111.5
N2—C2—N1	116.7 (2)	H9'1—C9'—H9'2	109.3
N4—C3—C4	111.8 (2)	C11—C10—H10A	120.0
N4—C3—N2	126.0 (2)	C11—C10—H10B	120.0
C4—C3—N2	122.2 (2)	H10A—C10—H10B	120.0
C3—C4—N3	104.9 (2)	C10—C11—C12	120.4 (3)
C3—C4—C1	123.1 (2)	C10—C11—H11	119.8
N3—C4—C1	131.8 (2)	C12—C11—H11	119.8
N4—C5—N3	113.5 (3)	O6—C12—O5	122.8 (3)
N4—C5—H5A	123.3	O6—C12—C11	124.1 (3)
N3—C5—H5A	123.3	O5—C12—C11	113.1 (3)
N3—C6—C7	112.4 (2)	N2—C13—H13A	109.5

N3—C6—H6A	109.1	N2—C13—H13B	109.5
C7—C6—H6A	109.1	H13A—C13—H13B	109.5
N3—C6—H6B	109.1	N2—C13—H13C	109.5
C7—C6—H6B	109.1	H13A—C13—H13C	109.5
H6A—C6—H6B	107.9	H13B—C13—H13C	109.5
O3—C7—O4	106.9 (2)	N1—C14—H14A	109.5
O3—C7—C6	110.9 (2)	N1—C14—H14B	109.5
O4—C7—C6	110.6 (2)	H14A—C14—H14B	109.5
O3—C7—H7	109.5	N1—C14—H14C	109.5
O4—C7—H7	109.5	H14A—C14—H14C	109.5
C6—C7—H7	109.5	H14B—C14—H14C	109.5
O3—C8—C9	105.4 (3)		

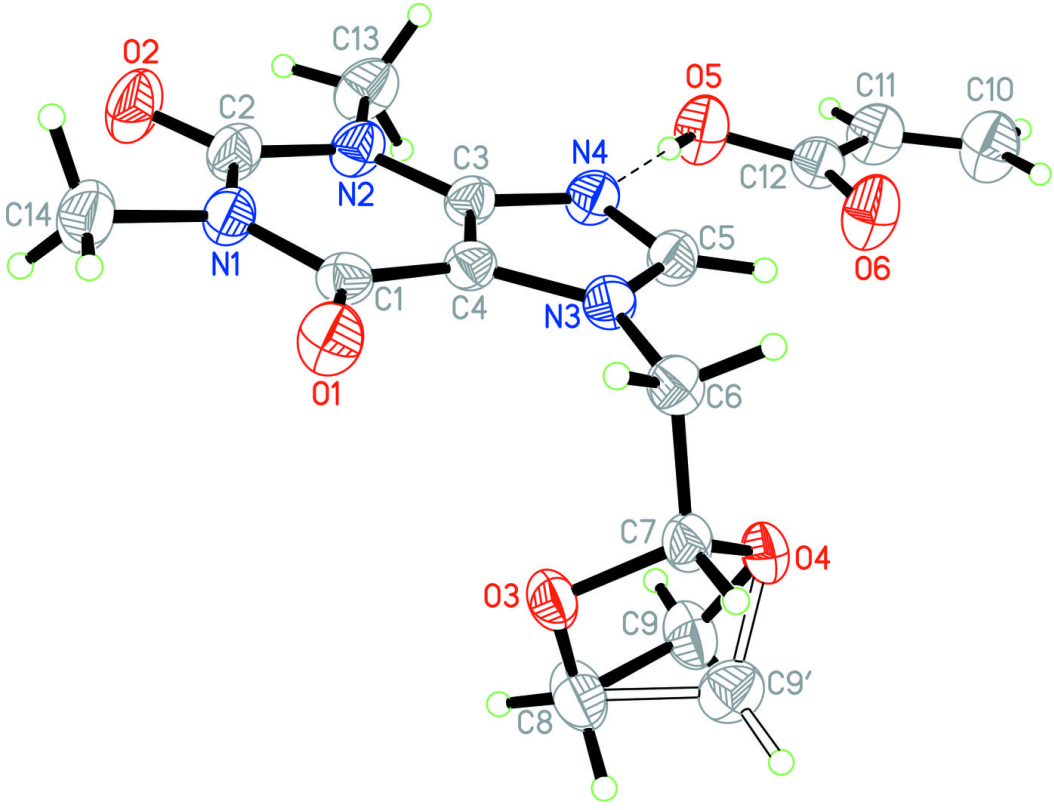
C2—N1—C1—O1	179.7 (3)	O1—C1—C4—C3	−178.6 (3)
C14—N1—C1—O1	1.7 (4)	N1—C1—C4—C3	1.0 (4)
C2—N1—C1—C4	0.0 (4)	O1—C1—C4—N3	−3.8 (5)
C14—N1—C1—C4	−178.0 (3)	N1—C1—C4—N3	175.9 (3)
C3—N2—C2—O2	179.0 (3)	C3—N4—C5—N3	0.0 (3)
C13—N2—C2—O2	0.3 (5)	C4—N3—C5—N4	0.4 (3)
C3—N2—C2—N1	−0.7 (4)	C6—N3—C5—N4	177.6 (2)
C13—N2—C2—N1	−179.4 (3)	C5—N3—C6—C7	−81.2 (3)
C1—N1—C2—O2	−179.8 (3)	C4—N3—C6—C7	95.5 (3)
C14—N1—C2—O2	−1.9 (4)	C8—O3—C7—O4	27.3 (3)
C1—N1—C2—N2	−0.1 (4)	C8—O3—C7—C6	147.9 (3)
C14—N1—C2—N2	177.8 (3)	C9'—O4—C7—O3	−45.4 (9)
C5—N4—C3—C4	−0.5 (3)	C9—O4—C7—O3	−10.3 (5)
C5—N4—C3—N2	178.2 (3)	C9'—O4—C7—C6	−166.3 (9)
C2—N2—C3—N4	−176.8 (3)	C9—O4—C7—C6	−131.2 (5)
C13—N2—C3—N4	1.9 (4)	N3—C6—C7—O3	−59.6 (3)
C2—N2—C3—C4	1.8 (4)	N3—C6—C7—O4	58.9 (3)
C13—N2—C3—C4	−179.6 (3)	C7—O3—C8—C9	−33.7 (5)
N4—C3—C4—N3	0.7 (3)	C7—O3—C8—C9'	1.7 (10)
N2—C3—C4—N3	−178.0 (2)	C7—O4—C9—C8	−10.1 (7)
N4—C3—C4—C1	176.7 (2)	O3—C8—C9—O4	26.7 (6)
N2—C3—C4—C1	−2.0 (4)	C7—O4—C9'—C8	43.9 (14)
C5—N3—C4—C3	−0.6 (3)	O3—C8—C9'—O4	−28.8 (15)
C6—N3—C4—C3	−177.8 (2)	C10—C11—C12—O6	−8.0 (6)
C5—N3—C4—C1	−176.2 (3)	C10—C11—C12—O5	171.6 (4)
C6—N3—C4—C1	6.6 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···N4	0.82	1.92	2.736 (3)	178
C5—H5A···O6	0.93	2.50	3.131 (4)	125
C6—H6A···O1	0.97	2.58	3.202 (3)	122
C13—H13B···O5^{i}	0.96	2.58	3.365 (4)	140

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


O2
C13
C2
O5
C11
C10
N2
C3
N4
C12
C14
N1
C5
O6
C1
C4
N3
O1
C6
C7
O4
O3
C9
C9′
C8