Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl *N*-{2-[(4,6-dimethoxypyrimidin-2-yl)(hydroxy)methyl]phenyl}carbamate

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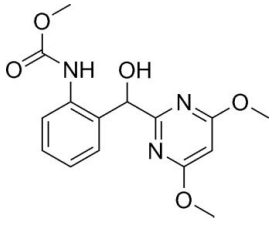
Received 12 November 2007; accepted 18 November 2007

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.064; wR factor = 0.149; data-to-parameter ratio = 14.3.

In the title compound, $C_{15}H_{16}N_3O_5$, the hydroxy group is disordered over two positions, with site-occupation factors of 0.211 (4) and 0.789 (4). The pyrimidine and benzene rings are oriented at a dihedral angle of 72.31 (3)°. Intramolecular C—H···O and N—H···N hydrogen bonds result in the formation of five-, six- and seven-membered rings. In the crystal structure, intermolecular C—H···O and O—H···O hydrogen bonds link the molecules. Further stability is provided by offset π–π stacking interactions; adjacent pyrimidine rings have a centroid-to-centroid distance of 3.81 (1) Å.

Related literature

For general background, see: Duggleby & Pang (2000). For related literature, see: Li & Wang (2007). For bond-length data, see: Allen *et al.* (1987). For definitions of π–π stacking interactions, see: Janiak (2000).



Experimental

Crystal data

$C_{15}H_{16}N_3O_5$
M_r = 318.31
Triclinic, $P\overline{1}$
a = 7.894 (2) Å
b = 9.302 (2) Å
c = 11.697 (3) Å
α = 111.518 (4)°
β = 98.887 (4)°
γ = 100.230 (4)°
V = 763.4 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 292 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
8360 measured reflections
3292 independent reflections
2064 reflections with $I > 2\sigma(I)$
R_{int} = 0.099

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.149
S = 1.01
3292 reflections
230 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O3	0.93	2.46	2.796 (3)	101
C2—H2···O1	0.93	2.43	2.913 (3)	112
N1—H1···N3	0.88 (2)	2.20 (2)	3.020 (3)	154 (2)
C14—H14B···O1^{i}	0.96	2.58	3.471 (3)	154
O3—H3A···O1^{ii}	0.814 (10)	2.039 (14)	2.827 (3)	163 (3)

Symmetry codes: (i) $x-1, y-1, z-1$; (ii) $-x+2, -y, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

The authors are indebted to Professor Guang-Fu Yang. This work was supported by the National 973 Project (grant No. 2003CB114400), the National NSFC (grant Nos. 20572030, 20528201 and 20432010), the Key Project of the Ministry of Education (grant Nos. 103116 and 104205) and the Programme for Excellent Research Groups of Hubei Province (grant No. 2004ABC002).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2382).

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 doi:10.1107/S1600536807060394

supplementary materials

Acta Cryst. (2007). E**63**, o4857 [**doi:10.1107/S1600536807060394**]

Methyl *N*-{2-[(4,6-dimethoxypyrimidin-2-yl)(hydroxy)methyl]phenyl}carbamate

Y.-X. Li and D.-M. Cheng

Comment

Pyrimidine derivatives have broad biological properties: in particular pyrimidinylbenzoate is a highly effective herbicide with acetohydroxy acid synthese (AHAS) as target (Duggleby & Pang, 2000). We report herein the crystal structure of one such pyrimidine derivative, the title compound, (I).

In the molecule of (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). When the crystal structure was solved, the atoms O3 and H3A were found to be disordered.

Rings A (C1—C6) and B (N2/N3/C10–C13) are, of course, planar and the dihedral angle between them is A/B = 72.31 (3)°. The intramolecular C—H···O hydrogen bonds (Table 1) result in the formation of five- and six-membered rings, while intramolecular N—H···N hydrogen bond (Table 1) results in the formation of a seven-membered ring.

In the crystal structure, intermolecular C—H···O and O—H···O hydrogen bonds (Table 1, Fig. 2) link the molecules, in which they may be effective in the stabilization of the structure. Further stability is provided by offset π–π stacking interactions (Janiak, 2000). The adjacent B rings have a centroid-centroid distance of 3.81 (1) Å [symmetry code: 1 − *x*, − *y*, − *z*].

Experimental

The title compound was synthesized according to the literature method (Li & Wang, 2007). Crystals appropriate for X-ray analysis were obtained by slow evaporation of the dichloromethane solution at 283 K.

Refinement

When the crystal structure was solved, the atoms O3 and H3A were found to be disordered. During refinement with isotropic thermal parameters, the occupancies of disordered H atoms were refined as H3A = 0.789 (4) and H3B = 0.211 (4). The remaining site occupancy factors were also refined as O3 = 0.789 (4) and O3' = 0.211 (4), during anisotropic refinement. H atoms (for NH and OH groups) were located in difference syntheses and refined [N—H = 0.88 (2) Å, O—H = 0.814 (10) and 0.819 (10) Å and U_{iso}(H) = 1.2U_{eq}(N,*O*)]. The remaining H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å, for aromatic and methyl H atoms and constrained to ride on their parent atoms, with U_{iso}(H) = *x*U_{eq}(C), where *x* = 1.2 for aromatic H and *x* = 1.5 for methyl H atoms.

Figures

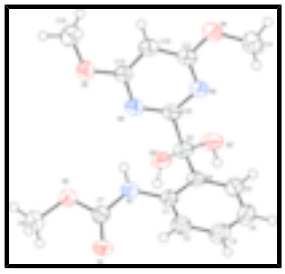

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

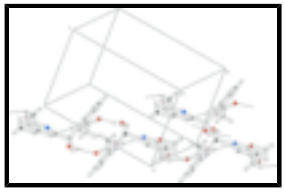

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Methyl *N*-{2-[(4,6-dimethoxypyrimidin-2-yl)(hydroxy)methyl]phenyl}carbamate

Crystal data

$C_{15}H_{16}N_3O_5$	$Z = 2$
$M_r = 318.31$	$F_{000} = 334$
Triclinic, $P\overline{1}$	$D_x = 1.385$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.894$ (2) Å	Cell parameters from 1926 reflections
$b = 9.302$ (2) Å	$\theta = 2.4$–25.0°
$c = 11.697$ (3) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 111.518$ (4)°	$T = 292$ (2) K
$\beta = 98.887$ (4)°	Block, colourless
$\gamma = 100.230$ (4)°	0.20 × 0.10 × 0.10 mm
$V = 763.4$ (3) Å^3	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	2064 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.099$
Monochromator: graphite	$\theta_{max} = 27.0^\circ$
$T = 292(2)$ K	$\theta_{min} = 1.9^\circ$
φ and ω scans	$h = -10 \rightarrow 10$
Absorption correction: none	$k = -11 \rightarrow 11$
8360 measured reflections	$l = -14 \rightarrow 14$
3292 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.149$	$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.003$
3292 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
230 parameters	$\Delta\rho_{min} = -0.26$ 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 $F^2 > 2$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	1.3432 (2)	0.29230 (18)	0.54228 (15)	0.0468 (4)	
O2	1.1760 (2)	0.42049 (18)	0.46153 (15)	0.0530 (5)	
O3	0.6181 (3)	−0.1852 (3)	0.26033 (19)	0.0491 (7)	0.789 (4)
H3A	0.632 (4)	−0.196 (4)	0.3268 (17)	0.059*	0.789 (4)
O3'	0.7255 (12)	0.0317 (10)	0.3606 (7)	0.060 (3)	0.211 (4)
H3B	0.789 (11)	0.060 (12)	0.4314 (19)	0.072*	0.211 (4)
O4	0.6414 (3)	−0.2561 (2)	−0.17285 (15)	0.0648 (6)	
O5	0.8081 (3)	0.2944 (2)	0.09025 (15)	0.0647 (6)	
N1	1.1052 (3)	0.1588 (2)	0.37305 (18)	0.0423 (5)	
H1	1.017 (3)	0.177 (3)	0.329 (2)	0.051*	
N2	0.7001 (2)	−0.1685 (2)	0.04352 (17)	0.0434 (5)	
N3	0.7866 (3)	0.1109 (2)	0.17055 (16)	0.0432 (5)	
C1	1.1024 (3)	−0.0018 (3)	0.35143 (19)	0.0372 (5)	
C2	1.2571 (3)	−0.0466 (3)	0.3780 (2)	0.0469 (6)	
H2	1.3658	0.0289	0.4089	0.056*	
C3	1.2498 (4)	−0.2038 (3)	0.3586 (2)	0.0529 (7)	

H3	1.3536	−0.2329	0.3783	0.064*
C4	1.0900 (4)	−0.3174 (3)	0.3104 (2)	0.0506 (6)
H4	1.0853	−0.4227	0.2983	0.061*
C5	0.9383 (3)	−0.2735 (3)	0.2805 (2)	0.0432 (6)
H5	0.8312	−0.3513	0.2449	0.052*
C6	0.9393 (3)	−0.1169 (3)	0.30152 (19)	0.0361 (5)
C7	1.2198 (3)	0.2899 (3)	0.4654 (2)	0.0385 (5)
C8	1.2710 (4)	0.5698 (3)	0.5647 (2)	0.0595 (7)
H8A	1.2637	0.5621	0.6436	0.089*
H8B	1.2198	0.6535	0.5583	0.089*
H8C	1.3931	0.5933	0.5613	0.089*
C9	0.7669 (3)	−0.0706 (3)	0.2735 (2)	0.0415 (6)
C10	0.7478 (3)	−0.0409 (3)	0.1541 (2)	0.0373 (5)
C11	0.6872 (3)	−0.1352 (3)	−0.0576 (2)	0.0456 (6)
C12	0.7191 (3)	0.0175 (3)	−0.0535 (2)	0.0483 (6)
H12	0.7068	0.0371	−0.1264	0.058*
C13	0.7701 (3)	0.1383 (3)	0.0652 (2)	0.0452 (6)
C14	0.6185 (5)	−0.4148 (3)	−0.1773 (3)	0.0813 (10)
H14A	0.7297	−0.4267	−0.1404	0.122*
H14B	0.5775	−0.4911	−0.2637	0.122*
H14C	0.5329	−0.4327	−0.1307	0.122*
C15	0.7919 (5)	0.3374 (3)	−0.0168 (3)	0.0796 (10)
H15A	0.8728	0.2971	−0.0661	0.119*
H15B	0.8192	0.4516	0.0126	0.119*
H15C	0.6727	0.2920	−0.0682	0.119*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0433 (10)	0.0482 (10)	0.0397 (9)	0.0037 (7)	−0.0066 (7)	0.0180 (8)
O2	0.0629 (12)	0.0366 (9)	0.0471 (10)	0.0079 (8)	−0.0085 (8)	0.0141 (8)
O3	0.0354 (12)	0.0678 (16)	0.0463 (14)	−0.0004 (10)	0.0016 (10)	0.0351 (12)
O3'	0.089 (7)	0.051 (5)	0.036 (5)	0.029 (5)	−0.004 (4)	0.015 (4)
O4	0.0996 (15)	0.0478 (11)	0.0307 (9)	0.0177 (10)	−0.0025 (9)	0.0056 (8)
O5	0.1001 (15)	0.0386 (10)	0.0433 (10)	−0.0004 (9)	−0.0001 (10)	0.0181 (8)
N1	0.0411 (12)	0.0386 (11)	0.0397 (11)	0.0060 (9)	−0.0060 (9)	0.0155 (9)
N2	0.0503 (13)	0.0415 (11)	0.0326 (11)	0.0097 (9)	0.0018 (9)	0.0129 (9)
N3	0.0515 (13)	0.0412 (11)	0.0310 (10)	0.0049 (9)	0.0019 (9)	0.0143 (9)
C1	0.0432 (14)	0.0392 (13)	0.0293 (12)	0.0118 (10)	0.0070 (10)	0.0141 (10)
C2	0.0413 (15)	0.0486 (15)	0.0461 (15)	0.0127 (11)	0.0053 (11)	0.0155 (12)
C3	0.0512 (17)	0.0581 (17)	0.0549 (16)	0.0255 (14)	0.0103 (13)	0.0245 (14)
C4	0.0620 (18)	0.0427 (14)	0.0515 (15)	0.0210 (13)	0.0127 (13)	0.0210 (12)
C5	0.0474 (15)	0.0411 (14)	0.0399 (13)	0.0080 (11)	0.0107 (11)	0.0165 (11)
C6	0.0406 (13)	0.0434 (13)	0.0238 (11)	0.0091 (10)	0.0063 (9)	0.0144 (10)
C7	0.0403 (14)	0.0407 (13)	0.0359 (13)	0.0053 (11)	0.0091 (11)	0.0195 (11)
C8	0.0704 (19)	0.0387 (14)	0.0553 (17)	0.0056 (13)	−0.0012 (14)	0.0139 (13)
C9	0.0387 (14)	0.0519 (15)	0.0379 (13)	0.0093 (11)	0.0074 (11)	0.0246 (12)
C10	0.0310 (12)	0.0455 (14)	0.0330 (12)	0.0073 (10)	0.0017 (9)	0.0167 (11)

C11	0.0525 (16)	0.0475 (15)	0.0311 (13)	0.0109 (12)	0.0017 (11)	0.0138 (11)
C12	0.0598 (17)	0.0520 (16)	0.0321 (13)	0.0107 (12)	0.0044 (11)	0.0202 (12)
C13	0.0533 (15)	0.0413 (14)	0.0349 (14)	0.0021 (11)	0.0000 (11)	0.0174 (11)
C14	0.125 (3)	0.0447 (17)	0.0528 (18)	0.0280 (17)	−0.0066 (18)	0.0044 (14)
C15	0.118 (3)	0.0553 (18)	0.0591 (19)	−0.0033 (17)	−0.0007 (17)	0.0368 (16)

Geometric parameters (Å, °)

C1—C2	1.386 (3)	C9—C10	1.511 (3)
C1—C6	1.402 (3)	C10—N3	1.324 (3)
C1—N1	1.416 (3)	C10—N2	1.337 (3)
C2—C3	1.384 (3)	C11—N2	1.322 (3)
C2—H2	0.9300	C11—O4	1.344 (3)
C3—C4	1.376 (3)	C11—C12	1.379 (3)
C3—H3	0.9300	C12—C13	1.368 (3)
C4—C5	1.368 (3)	C12—H12	0.9300
C4—H4	0.9300	C13—O5	1.338 (3)
C5—C6	1.384 (3)	C13—N3	1.339 (3)
C5—H5	0.9300	C14—O4	1.435 (3)
C6—C9	1.523 (3)	C14—H14A	0.9600
C7—O1	1.211 (2)	C14—H14B	0.9600
C7—O2	1.335 (3)	C14—H14C	0.9600
C7—N1	1.346 (3)	C15—O5	1.443 (3)
C8—O2	1.438 (3)	C15—H15A	0.9600
C8—H8A	0.9600	C15—H15B	0.9600
C8—H8B	0.9600	C15—H15C	0.9600
C8—H8C	0.9600	N1—H1	0.88 (2)
C9—O3'	1.246 (6)	O3—H3A	0.814 (10)
C9—O3	1.385 (3)	O3'—H3B	0.819 (10)
C2—C1—C6	119.8 (2)	N3—C10—C9	115.8 (2)
C2—C1—N1	121.3 (2)	N2—C10—C9	117.5 (2)
C6—C1—N1	118.9 (2)	N2—C11—O4	118.9 (2)
C3—C2—C1	120.0 (2)	N2—C11—C12	124.3 (2)
C3—C2—H2	120.0	O4—C11—C12	116.8 (2)
C1—C2—H2	120.0	C13—C12—C11	115.5 (2)
C4—C3—C2	120.5 (2)	C13—C12—H12	122.3
C4—C3—H3	119.7	C11—C12—H12	122.3
C2—C3—H3	119.7	O5—C13—N3	112.35 (19)
C5—C4—C3	119.2 (2)	O5—C13—C12	125.1 (2)
C5—C4—H4	120.4	N3—C13—C12	122.6 (2)
C3—C4—H4	120.4	O4—C14—H14A	109.5
C4—C5—C6	122.0 (2)	O4—C14—H14B	109.5
C4—C5—H5	119.0	H14A—C14—H14B	109.5
C6—C5—H5	119.0	O4—C14—H14C	109.5
C5—C6—C1	118.3 (2)	H14A—C14—H14C	109.5
C5—C6—C9	120.7 (2)	H14B—C14—H14C	109.5
C1—C6—C9	120.9 (2)	O5—C15—H15A	109.5
O1—C7—O2	124.1 (2)	O5—C15—H15B	109.5
O1—C7—N1	126.3 (2)	H15A—C15—H15B	109.5

O2—C7—N1	109.6 (2)	O5—C15—H15C	109.5
O2—C8—H8A	109.5	H15A—C15—H15C	109.5
O2—C8—H8B	109.5	H15B—C15—H15C	109.5
H8A—C8—H8B	109.5	C7—N1—C1	126.21 (19)
O2—C8—H8C	109.5	C7—N1—H1	115.0 (15)
H8A—C8—H8C	109.5	C1—N1—H1	118.3 (16)
H8B—C8—H8C	109.5	C11—N2—C10	114.8 (2)
O3'—C9—O3	90.7 (5)	C10—N3—C13	116.22 (19)
O3'—C9—C10	112.9 (4)	C7—O2—C8	116.31 (18)
O3—C9—C10	108.42 (19)	C9—O3—H3A	105 (2)
O3'—C9—C6	119.2 (4)	C9—O3'—H3B	115.2 (15)
O3—C9—C6	113.1 (2)	C11—O4—C14	116.9 (2)
C10—C9—C6	110.68 (18)	C13—O5—C15	116.94 (19)
N3—C10—N2	126.6 (2)		
C6—C1—C2—C3	−1.8 (3)	N2—C11—C12—C13	1.2 (4)
N1—C1—C2—C3	178.5 (2)	O4—C11—C12—C13	−178.3 (2)
C1—C2—C3—C4	1.4 (4)	C11—C12—C13—O5	179.7 (2)
C2—C3—C4—C5	0.7 (4)	C11—C12—C13—N3	−0.6 (4)
C3—C4—C5—C6	−2.4 (4)	O1—C7—N1—C1	2.8 (4)
C4—C5—C6—C1	2.0 (3)	O2—C7—N1—C1	−176.3 (2)
C4—C5—C6—C9	−176.8 (2)	C2—C1—N1—C7	−32.3 (3)
C2—C1—C6—C5	0.1 (3)	C6—C1—N1—C7	148.0 (2)
N1—C1—C6—C5	179.84 (19)	O4—C11—N2—C10	179.4 (2)
C2—C1—C6—C9	178.94 (19)	C12—C11—N2—C10	−0.1 (4)
N1—C1—C6—C9	−1.4 (3)	N3—C10—N2—C11	−1.9 (3)
C5—C6—C9—O3'	121.1 (5)	C9—C10—N2—C11	−179.4 (2)
C1—C6—C9—O3'	−57.7 (6)	N2—C10—N3—C13	2.5 (3)
C5—C6—C9—O3	16.4 (3)	C9—C10—N3—C13	180.0 (2)
C1—C6—C9—O3	−162.4 (2)	O5—C13—N3—C10	178.7 (2)
C5—C6—C9—C10	−105.4 (2)	C12—C13—N3—C10	−1.1 (4)
C1—C6—C9—C10	75.8 (3)	O1—C7—O2—C8	−7.3 (3)
O3'—C9—C10—N3	35.3 (6)	N1—C7—O2—C8	171.83 (19)
O3—C9—C10—N3	134.2 (2)	N2—C11—O4—C14	−3.2 (4)
C6—C9—C10—N3	−101.3 (2)	C12—C11—O4—C14	176.4 (2)
O3'—C9—C10—N2	−146.9 (5)	N3—C13—O5—C15	−179.1 (2)
O3—C9—C10—N2	−48.0 (3)	C12—C13—O5—C15	0.7 (4)
C6—C9—C10—N2	76.5 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O3	0.93	2.46	2.796 (3)	101
C2—H2···O1	0.93	2.43	2.913 (3)	112
N1—H1···N3	0.88 (2)	2.20 (2)	3.020 (3)	154 (2)
C14—H14B···O1^{i}	0.96	2.58	3.471 (3)	154
O3—H3A···O1^{ii}	0.814 (10)	2.039 (14)	2.827 (3)	163 (3)

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

Fig. 1

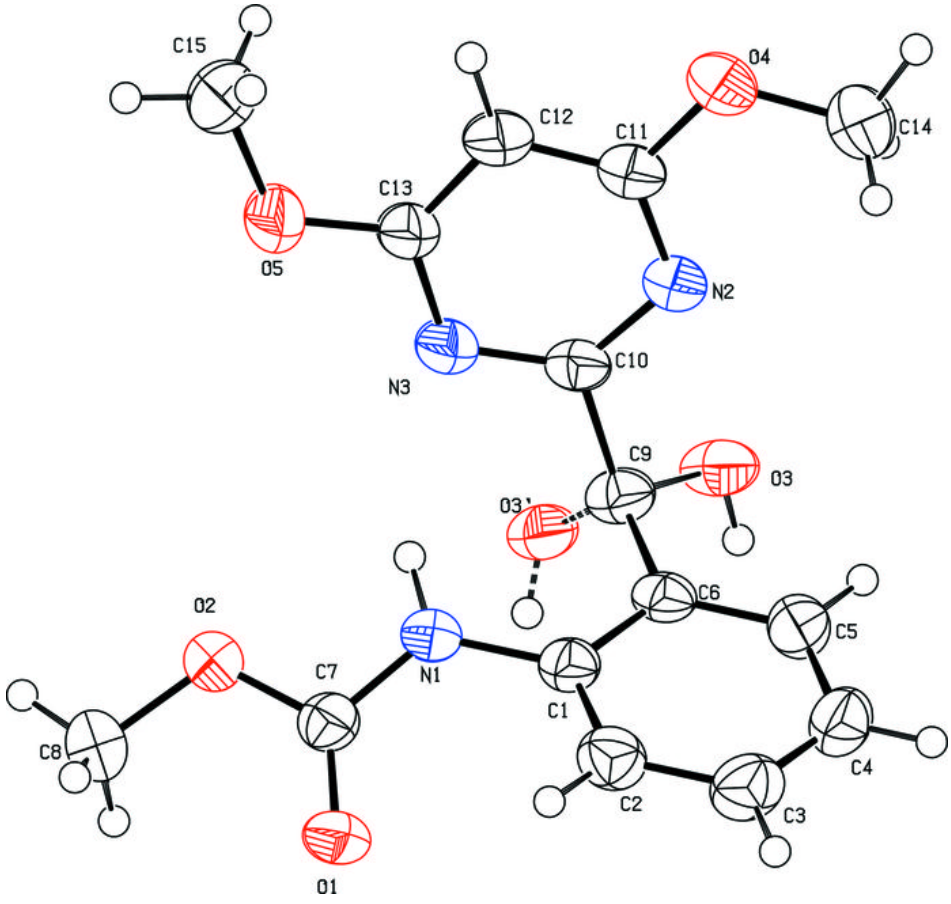
C15
O4
C12
C11
C14
C13
O5
N2
N3
C10
C9
O3
O3'
C6
O2
C5
C7
N1
C1
C8
C4
C2
C3
O1

Fig. 2