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N-[2-(4,6-Dimethoxypyrimidin-2-ylcarbonyl)phenyl]benzamide

Yuanxiang Li[a]* and Gang Huang[b]

[a]Chemistry and Chemical Engineering Department, Huaihua University, Huaihua 418008, People's Republic of China, and [b]Pharmaceutical Department, Huaihua Medical College, Huaihua 418008, People's Republic of China
Correspondence e-mail: hhhhxylyx@yahoo.com.cn

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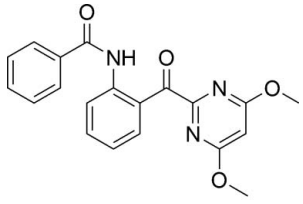
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.132; data-to-parameter ratio = 13.6.

In the molecule of the title compound, $C_{20}H_{17}N_3O_4$, intramolecular C—H···O and N—H···O hydrogen bonds result in the formation of two nearly planar six-membered rings; these are almost coplanar with the adjacent six-membered ring. In the crystal structure, C—H···O hydrogen bonds link the molecules.

Related literature

For general background, see: Duggleby *et al.* (2000). For related literature, see: Li *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{17}N_3O_4$
M_r = 363.37
Triclinic, $P\overline{1}$
a = 7.7723 (10) Å
b = 9.9453 (13) Å
c = 11.8667 (16) Å
α = 95.774 (2)°
β = 91.581 (2)°
γ = 98.657 (2)°
V = 901.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 292 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
5032 measured reflections
3386 independent reflections
2340 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.132
S = 0.98
3386 reflections
249 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O1	0.93	2.21	2.826 (2)	123
N1—H1A···O2	0.920 (18)	1.868 (18)	2.6651 (18)	143.6 (15)
C12—H12···O4^{i}	0.93	2.59	3.374 (2)	142

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

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2369).

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supplementary materials

Acta Cryst. (2007). E**63**, o4667 [**doi:10.1107/S1600536807056553**]

N-[2-(4,6-Dimethoxypyrimidin-2-ylcarbonyl)phenyl]benzamide

Y. Li and G. Huang

Comment

Pyrimidine derivatives have broad biological properties: in particular pyrimidinylbenzoate is a highly effective herbicide with acetohydroxy acid synthese (AHAS) as target (Duggleby *et al.*, 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). Rings A (C1—C6), B (C8—C13) and C (N2/N3/C15—C18) are, of course, planar and the dihedral angles between them are A/B = 16.40 (3)°, A/C = 87.51 (2)° and B/C = 87.15 (3)°. The intramolecular C—H···O and N—H···O hydrogen bonds (Table 1) result in the formation of the nearly planar six-membered rings; D (O1/N1/C7—C9/H9) and E (N1/O2/C8/C13/C14/H1A), which are oriented at a dihedral angle of D/E = 3.05 (2)°. They are also oriented with respect to ring B at dihedral angles of D/B = 2.60 (3)° and E/B = 0.94 (3)°. So, rings B, D and E are nearly co-planar.

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 1) link the molecules, in which they may be effective in the stabilization of the structure.

Experimental

The title compound was synthesized according to the literature method (Li *et al.*, 2006). Crystals appropriate for X-ray analysis were obtained by slow evaporation of the dichloromethane solution at 283 K.

Refinement

H atom (for NH) was located in difference syntheses and refined [N—H = 0.920 (18) Å and U_{iso}(H) = 1.2U_{eq}(N)]. 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) = xU_{eq}(C), where x = 1.2 for aromatic H and x = 1.5 for methyl H atoms.

Figures

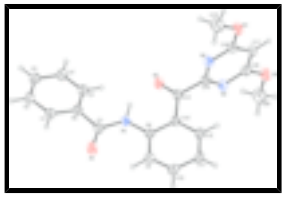

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

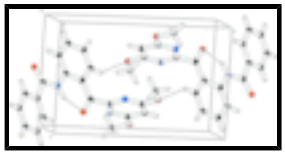

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

N-[2-(4,6-Dimethoxypyrimidin-2-ylcarbonyl)phenyl]benzamide

Crystal data

$C_{20}H_{17}N_3O_4$	$Z = 2$
$M_r = 363.37$	$F_{000} = 380$
Triclinic, $P\overline{1}$	$D_x = 1.339$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.7723$ (10) Å	Cell parameters from 1758 reflections
$b = 9.9453$ (13) Å	$\theta = 2.6$–26.4º
$c = 11.8667$ (16) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 95.774$ (2)º	$T = 292$ (2) K
$\beta = 91.581$ (2)º	Block, colorless
$\gamma = 98.657$ (2)º	0.30 × 0.20 × 0.10 mm
$V = 901.4$ (2) Å^3	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	2340 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.048$
Monochromator: graphite	$\theta_{max} = 25.8$º
$T = 292(2)$ K	$\theta_{min} = 2.1$º
φ and ω scans	$h = -9\rightarrow9$
Absorption correction: none	$k = -10\rightarrow12$
5032 measured reflections	$l = -14\rightarrow14$
3386 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
$R[F^2 > 2\sigma(F^2)] = 0.049$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.132$	$w = 1/[\sigma^2(F_o^2) + (0.0701P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} < 0.001$
3386 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
249 parameters	$\Delta\rho_{min} = -0.23$ 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	0.61486 (19)	0.38351 (18)	1.17647 (12)	0.0971 (6)
O2	0.21277 (16)	0.18961 (15)	0.85457 (10)	0.0768 (4)
O4	0.3427 (2)	0.17339 (15)	0.42123 (10)	0.0792 (4)
O3	0.08396 (19)	−0.23710 (14)	0.53910 (11)	0.0800 (4)
N1	0.44601 (19)	0.28284 (14)	1.02392 (11)	0.0507 (4)
H1A	0.343 (2)	0.2783 (17)	0.9827 (14)	0.061*
N2	0.33883 (19)	0.14925 (15)	0.61258 (11)	0.0587 (4)
N3	0.2033 (2)	−0.06098 (16)	0.67381 (12)	0.0594 (4)
C1	0.3827 (2)	0.56041 (18)	1.23623 (14)	0.0571 (5)
H1	0.4963	0.5807	1.2667	0.069*
C2	0.2605 (3)	0.63962 (19)	1.27421 (15)	0.0650 (5)
H2	0.2919	0.7125	1.3301	0.078*
C3	0.0936 (3)	0.6111 (2)	1.22983 (16)	0.0687 (5)
H3	0.0112	0.6646	1.2551	0.082*
C4	0.0476 (3)	0.5030 (2)	1.14772 (16)	0.0695 (6)
H4	−0.0662	0.4832	1.1176	0.083*
C5	0.1699 (2)	0.42366 (19)	1.10982 (15)	0.0618 (5)
H5	0.1378	0.3507	1.0542	0.074*
C6	0.3393 (2)	0.45170 (16)	1.15385 (13)	0.0486 (4)
C7	0.4798 (2)	0.37067 (18)	1.11999 (14)	0.0541 (4)
C8	0.5518 (2)	0.19496 (16)	0.97185 (13)	0.0474 (4)
C9	0.7138 (2)	0.18155 (19)	1.01697 (15)	0.0597 (5)
H9	0.7550	0.2307	1.0857	0.072*
C10	0.8143 (2)	0.0960 (2)	0.96084 (17)	0.0668 (5)
H10	0.9235	0.0896	0.9919	0.080*
C11	0.7570 (2)	0.0197 (2)	0.85983 (16)	0.0648 (5)
H11	0.8260	−0.0382	0.8232	0.078*
C12	0.5967 (2)	0.03076 (18)	0.81442 (14)	0.0561 (5)
H12	0.5568	−0.0210	0.7465	0.067*
C13	0.4912 (2)	0.11829 (16)	0.86788 (13)	0.0472 (4)
C14	0.3246 (2)	0.12940 (18)	0.81204 (14)	0.0536 (4)

C15	0.2867 (2)	0.06568 (19)	0.69021 (14)	0.0532 (4)
C16	0.2977 (2)	0.09688 (19)	0.50574 (14)	0.0587 (5)
C17	0.2109 (2)	−0.03313 (19)	0.47669 (14)	0.0603 (5)
H17	0.1835	−0.0681	0.4016	0.072*
C18	0.1669 (2)	−0.10860 (19)	0.56526 (15)	0.0592 (5)
C19	0.4327 (4)	0.3102 (2)	0.4506 (2)	0.1002 (8)
H19A	0.3609	0.3618	0.4967	0.150*
H19B	0.4578	0.3531	0.3827	0.150*
H19C	0.5397	0.3070	0.4920	0.150*
C20	0.0442 (4)	−0.3184 (2)	0.6325 (2)	0.0977 (8)
H20A	0.1505	−0.3274	0.6723	0.146*
H20B	−0.0152	−0.4075	0.6036	0.146*
H20C	−0.0289	−0.2743	0.6834	0.146*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0690 (9)	0.1285 (14)	0.0882 (10)	0.0411 (9)	−0.0227 (8)	−0.0468 (10)
O2	0.0624 (8)	0.1085 (12)	0.0605 (8)	0.0368 (8)	−0.0032 (6)	−0.0203 (7)
O4	0.1189 (12)	0.0693 (9)	0.0483 (7)	0.0105 (8)	0.0106 (7)	0.0050 (6)
O3	0.1021 (11)	0.0630 (9)	0.0675 (8)	−0.0029 (8)	−0.0023 (8)	−0.0035 (7)
N1	0.0500 (8)	0.0582 (9)	0.0447 (8)	0.0176 (7)	−0.0005 (6)	−0.0035 (7)
N2	0.0677 (10)	0.0595 (9)	0.0484 (8)	0.0126 (8)	0.0045 (7)	−0.0016 (7)
N3	0.0642 (9)	0.0607 (10)	0.0520 (9)	0.0102 (8)	0.0001 (7)	−0.0001 (7)
C1	0.0637 (11)	0.0525 (11)	0.0546 (10)	0.0106 (9)	0.0024 (8)	0.0007 (8)
C2	0.0840 (14)	0.0514 (11)	0.0607 (11)	0.0191 (10)	0.0084 (10)	−0.0040 (9)
C3	0.0798 (14)	0.0671 (13)	0.0664 (12)	0.0331 (11)	0.0154 (11)	0.0068 (10)
C4	0.0605 (11)	0.0857 (15)	0.0644 (11)	0.0243 (11)	0.0044 (9)	−0.0014 (11)
C5	0.0579 (11)	0.0681 (12)	0.0580 (11)	0.0148 (9)	0.0024 (9)	−0.0077 (9)
C6	0.0541 (10)	0.0484 (10)	0.0438 (9)	0.0092 (8)	0.0053 (7)	0.0041 (7)
C7	0.0516 (10)	0.0620 (11)	0.0479 (9)	0.0127 (9)	−0.0003 (8)	−0.0037 (8)
C8	0.0501 (10)	0.0482 (10)	0.0468 (9)	0.0146 (8)	0.0076 (7)	0.0071 (7)
C9	0.0594 (11)	0.0635 (12)	0.0587 (10)	0.0206 (9)	−0.0005 (8)	0.0019 (9)
C10	0.0593 (11)	0.0704 (13)	0.0749 (13)	0.0267 (10)	−0.0008 (9)	0.0032 (11)
C11	0.0665 (12)	0.0612 (12)	0.0743 (13)	0.0319 (10)	0.0155 (10)	0.0068 (10)
C12	0.0647 (11)	0.0536 (11)	0.0522 (10)	0.0168 (9)	0.0115 (8)	0.0026 (8)
C13	0.0524 (10)	0.0470 (10)	0.0437 (9)	0.0117 (8)	0.0094 (7)	0.0042 (7)
C14	0.0549 (10)	0.0582 (11)	0.0479 (9)	0.0134 (9)	0.0070 (8)	−0.0018 (8)
C15	0.0526 (10)	0.0616 (12)	0.0465 (9)	0.0175 (9)	0.0031 (8)	−0.0025 (8)
C16	0.0697 (12)	0.0592 (12)	0.0495 (10)	0.0197 (10)	0.0050 (8)	0.0014 (9)
C17	0.0755 (13)	0.0638 (12)	0.0421 (9)	0.0201 (10)	0.0022 (8)	−0.0062 (8)
C18	0.0622 (11)	0.0570 (11)	0.0570 (11)	0.0134 (9)	−0.0013 (9)	−0.0059 (9)
C19	0.139 (2)	0.0753 (16)	0.0820 (15)	−0.0038 (15)	0.0033 (15)	0.0188 (13)
C20	0.120 (2)	0.0714 (15)	0.0945 (17)	−0.0124 (14)	0.0013 (14)	0.0169 (13)

Geometric parameters (Å, °)

C1—C6	1.378 (2)	C12—C13	1.402 (2)
C1—C2	1.379 (2)	C12—H12	0.9300

C1—H1	0.9300	C13—C14	1.462 (2)
C2—C3	1.365 (3)	C14—O2	1.2202 (19)
C2—H2	0.9300	C14—C15	1.521 (2)
C3—C4	1.374 (3)	C15—N3	1.320 (2)
C3—H3	0.9300	C15—N2	1.333 (2)
C4—C5	1.381 (2)	C16—N2	1.333 (2)
C4—H4	0.9300	C16—O4	1.341 (2)
C5—C6	1.381 (2)	C16—C17	1.371 (2)
C5—H5	0.9300	C17—C18	1.374 (2)
C6—C7	1.492 (2)	C17—H17	0.9300
C7—O1	1.213 (2)	C18—N3	1.334 (2)
C7—N1	1.359 (2)	C18—O3	1.344 (2)
C8—C9	1.385 (2)	C19—O4	1.438 (3)
C8—N1	1.399 (2)	C19—H19A	0.9600
C8—C13	1.413 (2)	C19—H19B	0.9600
C9—C10	1.375 (2)	C19—H19C	0.9600
C9—H9	0.9300	C20—O3	1.450 (2)
C10—C11	1.377 (3)	C20—H20A	0.9600
C10—H10	0.9300	C20—H20B	0.9600
C11—C12	1.368 (2)	C20—H20C	0.9600
C11—H11	0.9300	N1—H1A	0.920 (18)
C6—C1—C2	121.09 (18)	C12—C13—C14	118.55 (15)
C6—C1—H1	119.5	C8—C13—C14	122.58 (14)
C2—C1—H1	119.5	O2—C14—C13	125.05 (15)
C3—C2—C1	120.00 (18)	O2—C14—C15	116.24 (15)
C3—C2—H2	120.0	C13—C14—C15	118.68 (14)
C1—C2—H2	120.0	N3—C15—N2	128.16 (15)
C2—C3—C4	119.81 (18)	N3—C15—C14	117.58 (15)
C2—C3—H3	120.1	N2—C15—C14	114.22 (16)
C4—C3—H3	120.1	N2—C16—O4	119.32 (17)
C3—C4—C5	120.17 (19)	N2—C16—C17	123.23 (17)
C3—C4—H4	119.9	O4—C16—C17	117.45 (16)
C5—C4—H4	119.9	C16—C17—C18	115.92 (16)
C4—C5—C6	120.57 (18)	C16—C17—H17	122.0
C4—C5—H5	119.7	C18—C17—H17	122.0
C6—C5—H5	119.7	N3—C18—O3	119.44 (17)
C1—C6—C5	118.36 (16)	N3—C18—C17	123.41 (18)
C1—C6—C7	117.05 (15)	O3—C18—C17	117.15 (16)
C5—C6—C7	124.58 (15)	O4—C19—H19A	109.5
O1—C7—N1	122.95 (16)	O4—C19—H19B	109.5
O1—C7—C6	120.97 (16)	H19A—C19—H19B	109.5
N1—C7—C6	116.07 (15)	O4—C19—H19C	109.5
C9—C8—N1	122.86 (16)	H19A—C19—H19C	109.5
C9—C8—C13	118.79 (15)	H19B—C19—H19C	109.5
N1—C8—C13	118.34 (14)	O3—C20—H20A	109.5
C10—C9—C8	120.46 (17)	O3—C20—H20B	109.5
C10—C9—H9	119.8	H20A—C20—H20B	109.5
C8—C9—H9	119.8	O3—C20—H20C	109.5
C9—C10—C11	121.61 (17)	H20A—C20—H20C	109.5

C9—C10—H10	119.2	H20B—C20—H20C	109.5
C11—C10—H10	119.2	C7—N1—C8	128.87 (15)
C12—C11—C10	118.78 (17)	C7—N1—H1A	119.9 (11)
C12—C11—H11	120.6	C8—N1—H1A	111.2 (11)
C10—C11—H11	120.6	C16—N2—C15	114.66 (16)
C11—C12—C13	121.51 (17)	C15—N3—C18	114.62 (15)
C11—C12—H12	119.2	C16—O4—C19	117.99 (15)
C13—C12—H12	119.2	C18—O3—C20	117.02 (15)
C12—C13—C8	118.85 (15)		
C6—C1—C2—C3	−0.2 (3)	C8—C13—C14—C15	167.82 (15)
C1—C2—C3—C4	0.3 (3)	O2—C14—C15—N3	−89.3 (2)
C2—C3—C4—C5	−0.2 (3)	C13—C14—C15—N3	92.49 (19)
C3—C4—C5—C6	0.1 (3)	O2—C14—C15—N2	88.6 (2)
C2—C1—C6—C5	0.0 (3)	C13—C14—C15—N2	−89.62 (19)
C2—C1—C6—C7	−178.89 (15)	N2—C16—C17—C18	0.2 (3)
C4—C5—C6—C1	0.0 (3)	O4—C16—C17—C18	180.00 (15)
C4—C5—C6—C7	178.87 (16)	C16—C17—C18—N3	0.5 (3)
C1—C6—C7—O1	13.4 (3)	C16—C17—C18—O3	−179.04 (16)
C5—C6—C7—O1	−165.47 (18)	O1—C7—N1—C8	−0.6 (3)
C1—C6—C7—N1	−166.98 (15)	C6—C7—N1—C8	179.81 (14)
C5—C6—C7—N1	14.2 (2)	C9—C8—N1—C7	2.6 (3)
N1—C8—C9—C10	−178.44 (16)	C13—C8—N1—C7	−176.46 (16)
C13—C8—C9—C10	0.6 (3)	O4—C16—N2—C15	179.28 (15)
C8—C9—C10—C11	−1.1 (3)	C17—C16—N2—C15	−0.9 (3)
C9—C10—C11—C12	0.5 (3)	N3—C15—N2—C16	1.1 (3)
C10—C11—C12—C13	0.5 (3)	C14—C15—N2—C16	−176.49 (15)
C11—C12—C13—C8	−0.9 (2)	N2—C15—N3—C18	−0.6 (3)
C11—C12—C13—C14	177.38 (16)	C14—C15—N3—C18	176.99 (15)
C9—C8—C13—C12	0.4 (2)	O3—C18—N3—C15	179.21 (15)
N1—C8—C13—C12	179.46 (14)	C17—C18—N3—C15	−0.3 (3)
C9—C8—C13—C14	−177.85 (15)	N2—C16—O4—C19	−0.5 (3)
N1—C8—C13—C14	1.2 (2)	C17—C16—O4—C19	179.61 (18)
C12—C13—C14—O2	171.58 (16)	N3—C18—O3—C20	−2.1 (3)
C8—C13—C14—O2	−10.2 (3)	C17—C18—O3—C20	177.45 (18)
C12—C13—C14—C15	−10.4 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O1	0.93	2.21	2.826 (2)	123
N1—H1A···O2	0.920 (18)	1.868 (18)	2.6651 (18)	143.6 (15)
C12—H12···O4^{i}	0.93	2.59	3.374 (2)	142

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

Fig. 1

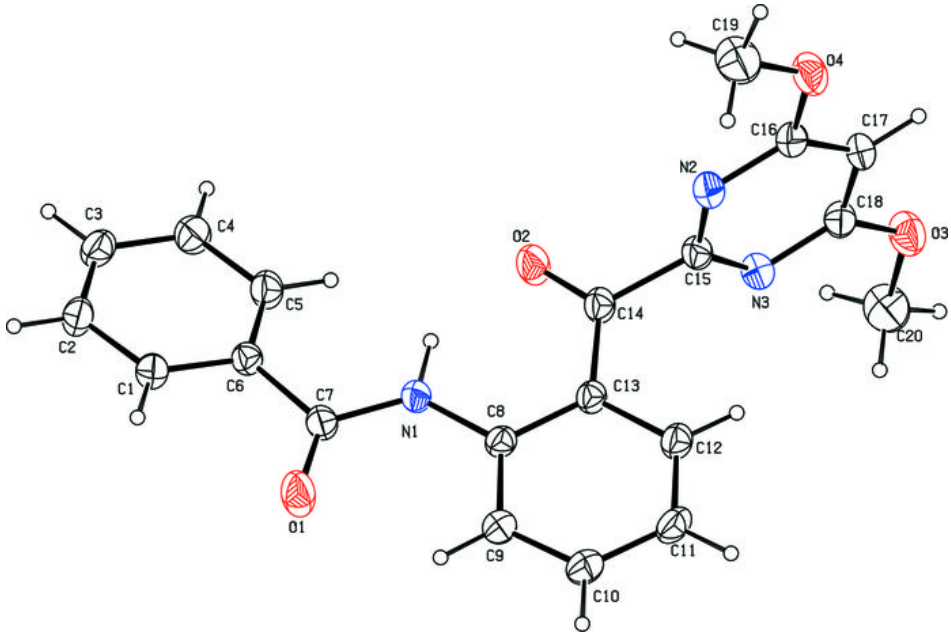
C19
O4
C16
C17
N2
C18
O3
O2
C15
N3
C14
C20
C3
C4
C5
C2
C1
C6
C7
N1
C8
C13
C12
O1
C9
C11
C10

Fig. 2