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5-(4-Methoxybenzoyl)-4-(4-methoxyphenyl)-1-[1-(4-methoxyphenyl)ethylidenenamino]-pyrimidin-2(1*H*)-one

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.143
Data-to-parameter ratio = 13.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

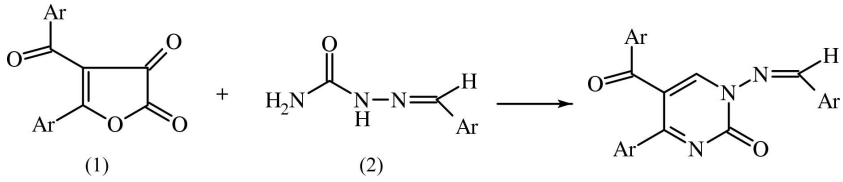
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In the title compound, $C_{27}H_{23}N_3O_5$, the pyrimidine ring is slightly puckered. The mean plane of the pyrimidine ring forms dihedral angles of 28.26 (10), 55.53 (9) and 55.96 (10)° with the three benzene rings in the molecule. There are intramolecular and intermolecular C—H···O interactions.

Comment

Pyrimidines in general have attracted much interest for biological and medicinal reasons. In particular, various analogues of pyrimidines possess effective antibacterial, antifungal, antiviral, insecticidal and miticidal activities (Cheng, 1969; McNair-Scott *et al.*, 1959; Sankyo Co. Ltd/Ube Industries Ltd, 1984; Kollenz, 1972; Maslivets *et al.*, 1988; Kruglenko *et al.*, 1987; Kozlov *et al.*, 1986). Conformational analysis and quantum chemical calculations have also been carried out by means of semi-empirical calculations for a series of functionalized 1*H*-pyrimidines (Yıldırım *et al.*, 1995, 1996; Sarıpınar *et al.*, 1996). In the present study, we have carried out the reaction of the furan-2,3-dione (1), which is obtained from *p,p′*-dimethoxydibenzoylmethane and oxalyl dichloride (Sarıpınar *et al.*, 2000), with the semicarbazone (2) to obtain the 1,4,5-trisubstituted 1*H*-pyrimidine-2-one (3) (see scheme).



(1) (2) (3)

Ar = p−$CH_3OC_6H_4$−

Fig. 1 shows the molecular structure and conformation of (3) with the atomic numbering scheme. Although close to being planar, the pyrimidine ring is slightly puckered. The angle between the planes formed by the ring atoms N2—C3—C4 and C2—N1—C1 is 7.7 (4)°. The corresponding angle in 1-allyl-5-benzoyl-4-phenylpyrimidin-2-one (Öztürk *et al.*, 1997) is 9.0 (7)°. Selected bond lengths, angles and torsion angles are presented in Table 1. In the compound, the *A* (C13–C18), *B* (C6–C11) and *C* (C21–C26) benzene rings form dihedral angles of 28.26 (10), 55.53 (9) and 55.96 (10)° with the pyrimidine ring, respectively. There are weak C—H···O interactions (Table 2), but no π–π or C—H···π interactions.

Experimental

For the preparation of the title compound, 4-(4-methoxybenzoyl)-5-(4-methoxyphenyl)furan-2,3-dione, (1) (0.32 g, 0.95 mmol), and *p*-methoxybenzaldehyde semicarbazone, (2) (0.18 g, 0.95 mmol), were

heated at 413 K for 1 h without any solvent. After cooling to room temperature, the residue was treated with dry diethyl ether and the crude product formed was crystallized from ethanol and dried over P_2O_5 (yield: 0.2 g, 45%; m.p. 490 K). IR (KBr, ν, cm^{-1}): 3450 (C═O, carbonyl overtone), 3050 (aromatic C—H), 1665 and 1650 (C═O). ^{1}H NMR ($CDCl_3$): δ 9.68 (*s*, 1H, —N═C—H), 8.30 (*s*, 1H, C6—H), 6.87–6.74 (*m*, 12H, ArH), 3.82, 3.76 and 3.68 (*q*, 9H, —OCH_3). ^{13}C NMR ($CDCl_3$): δ 192.44 (*t*, ArCO), 171.56 (*s*, C-4), 153.57 (*s*, C-2), 150.72 (*s*, C-6), 135.02 (*s*, C-8), 134.45–115.78 (*m*, aromatic C), 118.68 (*s*, C-5), 57.58, 57.46 and 57.40 (*q*, 3CH_3O). Analysis calculated for $C_{27}H_{23}N_3O_5$: C 69.06, H 4.94, N 8.95%; found: C 69.20, H 5.19, N 8.88%.

Crystal data

$C_{27}H_{23}N_3O_5$
M_r = 469.48
Triclinic, $P\overline{1}$
a = 8.1127 (7) Å
b = 10.9405 (9) Å
c = 13.9263 (11) Å
α = 77.147 (7)°
β = 83.542 (7)°
γ = 76.749 (7)°
V = 1170.54 (17) Å^3
Z = 2
D_x = 1.332 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15633 reflections
θ = 2.0–28.8°
μ = 0.09 mm^{-1}
T = 296 K
Plate, colorless
0.46 × 0.27 × 0.07 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: by integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.965, T_{max} = 0.994
12784 measured reflections
4119 independent reflections
2655 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 25.0°
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.143
S = 1.01
4119 reflections
316 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0787P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C2	1.215 (3)	N3—C20	1.278 (3)
N1—C1	1.316 (3)	C1—C4	1.430 (3)
N1—C2	1.362 (3)	C3—C4	1.359 (3)
N2—C3	1.337 (3)	C4—C5	1.498 (3)
N2—C2	1.419 (3)		
C1—C4—C5	127.80 (19)	N3—C20—C21	121.0 (2)
O3—C9—C10	125.7 (3)	C22—C21—C20	122.6 (2)
C14—C13—C1	122.69 (18)		
C3—N2—N3—C20	−135.3 (2)	C4—C5—C6—C7	154.0 (2)
C3—C4—C5—C6	137.2 (2)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20···O1	0.93	2.34	2.737 (3)	105
C11—H11···O4^{i}	0.93	2.60	3.512 (3)	166
C3—H3···O2^{ii}	0.93	2.54	3.330 (3)	143

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

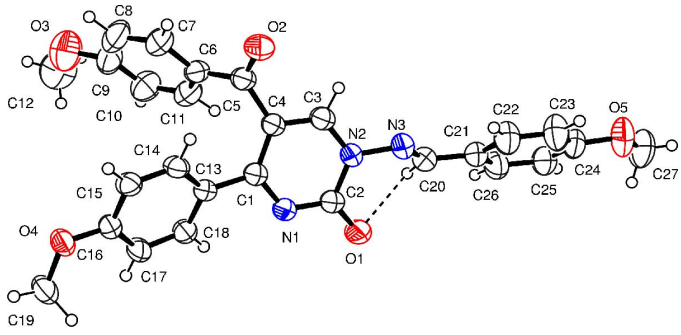


Figure 1
An *ORTEP-3* (Farrugia, 1997) drawing of the structure of (3), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates a C—H···O interaction.

H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.96 Å and with U_{iso}(H) = 1.2U_{eq}(C) (1.5U_{eq} for methyl).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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Crystal data

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Hall symbol: -P 1
$a = 8.1127$ (7) Å
$b = 10.9405$ (9) Å
$c = 13.9263$ (11) Å
$\alpha = 77.147$ (7)°
$\beta = 83.542$ (7)°
$\gamma = 76.749$ (7)°
$V = 1170.54$ (17) Å^3
$Z = 2$
$F(000) = 492$
$D_x = 1.332$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 15633 reflections
$\theta = 2.0$–$28.8°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Plate, colorless
0.46 × 0.27 × 0.07 mm

Data collection

Stoe IPDS-2 diffractometer
Radiation source: sealed X-ray tube
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
w scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
$T_{min} = 0.965$, $T_{max} = 0.994$
12784 measured reflections
4119 independent reflections
2655 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.143$
$S = 1.01$
4119 reflections
316 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0787P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ 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	−0.5455 (3)	0.3112 (2)	0.93913 (12)	0.0817 (6)
O2	−0.2904 (2)	0.50032 (19)	0.50724 (12)	0.0710 (5)
O3	−0.2300 (3)	1.0589 (2)	0.5215 (2)	0.1080 (8)
O4	0.2983 (2)	0.65841 (17)	0.79851 (11)	0.0597 (5)
O5	−1.1885 (3)	−0.0808 (2)	0.84405 (19)	0.0965 (7)
N1	−0.3494 (2)	0.42094 (19)	0.85484 (13)	0.0509 (5)
N2	−0.5262 (2)	0.34252 (18)	0.77080 (13)	0.0495 (5)
N3	−0.6249 (3)	0.25214 (19)	0.76694 (14)	0.0556 (5)
C1	−0.2875 (3)	0.4783 (2)	0.76965 (15)	0.0448 (5)
C2	−0.4779 (3)	0.3576 (2)	0.86157 (16)	0.0565 (6)
C3	−0.4664 (3)	0.4029 (2)	0.68417 (16)	0.0498 (5)
H3	−0.5031	0.3924	0.6262	0.060*
C4	−0.3534 (3)	0.4792 (2)	0.67844 (15)	0.0450 (5)
C5	−0.3115 (3)	0.5529 (2)	0.57783 (16)	0.0506 (6)
C6	−0.3001 (3)	0.6878 (2)	0.56547 (16)	0.0512 (6)
C7	−0.1985 (4)	0.7406 (3)	0.48683 (19)	0.0701 (7)
H7	−0.1435	0.6913	0.4415	0.084*
C8	−0.1789 (4)	0.8634 (3)	0.4757 (2)	0.0826 (9)
H8	−0.1087	0.8967	0.4238	0.099*
C9	−0.2622 (4)	0.9385 (3)	0.5407 (2)	0.0746 (8)
C10	−0.3675 (4)	0.8899 (3)	0.6175 (2)	0.0725 (7)
H10	−0.4266	0.9411	0.6606	0.087*
C11	−0.3840 (3)	0.7649 (2)	0.62953 (18)	0.0619 (6)
H11	−0.4532	0.7316	0.6820	0.074*
C12	−0.3106 (5)	1.1400 (4)	0.5802 (3)	0.1132 (12)
H12A	−0.2766	1.2207	0.5588	0.170*
H12B	−0.2815	1.1041	0.6471	0.170*
H12C	−0.4310	1.1528	0.5766	0.170*
C13	−0.1378 (3)	0.5313 (2)	0.77558 (14)	0.0428 (5)
C14	−0.0098 (3)	0.5388 (2)	0.69996 (15)	0.0457 (5)
H14	−0.0204	0.5129	0.6421	0.055*
C15	0.1311 (3)	0.5834 (2)	0.70897 (15)	0.0475 (5)
H15	0.2131	0.5899	0.6568	0.057*
C16	0.1515 (3)	0.6189 (2)	0.79550 (15)	0.0475 (5)
C17	0.0267 (3)	0.6125 (2)	0.87214 (16)	0.0517 (6)

H17	0.0390	0.6370	0.9303	0.062*
C18	−0.1160 (3)	0.5696 (2)	0.86121 (15)	0.0499 (6)
H18	−0.1999	0.5663	0.9125	0.060*
C19	0.3380 (3)	0.6786 (3)	0.89034 (19)	0.0677 (7)
H19A	0.4439	0.7060	0.8819	0.102*
H19B	0.3469	0.6000	0.9386	0.102*
H19C	0.2498	0.7433	0.9122	0.102*
C20	−0.7608 (3)	0.2585 (2)	0.82336 (17)	0.0531 (6)
H20	−0.7903	0.3219	0.8607	0.064*
C21	−0.8695 (3)	0.1685 (2)	0.83012 (17)	0.0506 (5)
C22	−0.8279 (4)	0.0664 (3)	0.7813 (2)	0.0691 (7)
H22	−0.7251	0.0526	0.7442	0.083*
C23	−0.9376 (4)	−0.0135 (3)	0.7876 (2)	0.0780 (8)
H23	−0.9094	−0.0806	0.7538	0.094*
C24	−1.0897 (3)	0.0041 (2)	0.8435 (2)	0.0651 (7)
C25	−1.1306 (3)	0.1018 (3)	0.8944 (2)	0.0650 (7)
H25	−1.2311	0.1129	0.9339	0.078*
C26	−1.0206 (3)	0.1838 (3)	0.88632 (19)	0.0603 (6)
H26	−1.0497	0.2512	0.9198	0.072*
C27	−1.3447 (5)	−0.0696 (4)	0.9016 (3)	0.1079 (12)
H27A	−1.4008	−0.1354	0.8951	0.162*
H27B	−1.4154	0.0131	0.8791	0.162*
H27C	−1.3238	−0.0789	0.9696	0.162*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0922 (14)	0.1245 (17)	0.0419 (9)	−0.0703 (13)	−0.0084 (9)	0.0060 (10)
O2	0.0947 (14)	0.0894 (13)	0.0393 (9)	−0.0383 (11)	0.0013 (9)	−0.0182 (9)
O3	0.1193 (19)	0.0773 (15)	0.130 (2)	−0.0326 (14)	−0.0009 (16)	−0.0171 (15)
O4	0.0563 (10)	0.0902 (12)	0.0455 (9)	−0.0392 (9)	0.0003 (7)	−0.0175 (9)
O5	0.0975 (16)	0.0800 (14)	0.1268 (19)	−0.0541 (13)	−0.0016 (14)	−0.0183 (13)
N1	0.0511 (11)	0.0656 (12)	0.0398 (10)	−0.0251 (10)	−0.0077 (8)	−0.0028 (9)
N2	0.0514 (11)	0.0588 (11)	0.0437 (10)	−0.0248 (9)	−0.0085 (8)	−0.0053 (9)
N3	0.0611 (12)	0.0616 (12)	0.0512 (11)	−0.0287 (10)	−0.0068 (10)	−0.0084 (9)
C1	0.0460 (12)	0.0500 (12)	0.0396 (11)	−0.0129 (10)	−0.0051 (9)	−0.0076 (10)
C2	0.0609 (15)	0.0711 (16)	0.0417 (13)	−0.0302 (13)	−0.0093 (11)	−0.0008 (12)
C3	0.0508 (13)	0.0615 (14)	0.0405 (12)	−0.0177 (11)	−0.0055 (10)	−0.0099 (11)
C4	0.0447 (12)	0.0544 (13)	0.0384 (11)	−0.0157 (10)	−0.0055 (9)	−0.0074 (10)
C5	0.0465 (12)	0.0689 (15)	0.0396 (12)	−0.0209 (11)	−0.0049 (10)	−0.0073 (11)
C6	0.0494 (13)	0.0645 (15)	0.0387 (11)	−0.0184 (11)	−0.0063 (10)	0.0001 (11)
C7	0.0806 (19)	0.0816 (19)	0.0507 (14)	−0.0350 (16)	0.0087 (13)	−0.0069 (13)
C8	0.096 (2)	0.083 (2)	0.0681 (18)	−0.0442 (18)	0.0164 (16)	0.0010 (16)
C9	0.079 (2)	0.0618 (17)	0.082 (2)	−0.0287 (15)	−0.0124 (16)	0.0049 (15)
C10	0.0767 (18)	0.0635 (17)	0.0718 (17)	−0.0109 (14)	0.0017 (14)	−0.0098 (14)
C11	0.0606 (15)	0.0642 (16)	0.0544 (14)	−0.0135 (13)	0.0017 (12)	−0.0008 (12)
C12	0.112 (3)	0.089 (2)	0.130 (3)	−0.010 (2)	−0.005 (3)	−0.020 (2)
C13	0.0445 (12)	0.0490 (12)	0.0363 (11)	−0.0141 (10)	−0.0063 (9)	−0.0054 (9)

C14	0.0475 (12)	0.0562 (13)	0.0350 (11)	−0.0113 (10)	−0.0063 (9)	−0.0105 (10)
C15	0.0424 (12)	0.0613 (14)	0.0380 (11)	−0.0126 (10)	−0.0008 (9)	−0.0077 (10)
C16	0.0471 (12)	0.0574 (13)	0.0421 (12)	−0.0203 (11)	−0.0044 (10)	−0.0079 (10)
C17	0.0598 (14)	0.0678 (15)	0.0370 (11)	−0.0269 (12)	−0.0010 (10)	−0.0174 (11)
C18	0.0504 (13)	0.0648 (15)	0.0381 (11)	−0.0217 (12)	0.0031 (10)	−0.0110 (11)
C19	0.0701 (17)	0.094 (2)	0.0551 (15)	−0.0410 (15)	−0.0085 (12)	−0.0213 (14)
C20	0.0552 (14)	0.0547 (14)	0.0516 (13)	−0.0173 (11)	−0.0101 (11)	−0.0066 (11)
C21	0.0526 (13)	0.0512 (13)	0.0497 (13)	−0.0173 (11)	−0.0066 (10)	−0.0058 (10)
C22	0.0655 (17)	0.0686 (17)	0.0800 (18)	−0.0265 (14)	0.0087 (14)	−0.0231 (15)
C23	0.085 (2)	0.0660 (17)	0.095 (2)	−0.0311 (16)	0.0091 (17)	−0.0318 (16)
C24	0.0685 (17)	0.0575 (15)	0.0738 (17)	−0.0323 (14)	−0.0087 (14)	−0.0008 (13)
C25	0.0595 (15)	0.0703 (17)	0.0686 (16)	−0.0266 (13)	−0.0021 (13)	−0.0090 (14)
C26	0.0588 (15)	0.0661 (16)	0.0613 (15)	−0.0225 (13)	0.0001 (12)	−0.0161 (13)
C27	0.092 (3)	0.122 (3)	0.119 (3)	−0.073 (2)	0.001 (2)	0.004 (2)

Geometric parameters (Å, º)

O1—C2	1.215 (3)	C12—H12B	0.9600
O2—C5	1.223 (3)	C12—H12C	0.9600
O3—C12	1.349 (4)	C13—C18	1.391 (3)
O3—C9	1.363 (3)	C13—C14	1.396 (3)
O4—C16	1.365 (3)	C14—C15	1.369 (3)
O4—C19	1.428 (3)	C14—H14	0.9300
O5—C24	1.357 (3)	C15—C16	1.383 (3)
O5—C27	1.417 (4)	C15—H15	0.9300
N1—C1	1.316 (3)	C16—C17	1.388 (3)
N1—C2	1.362 (3)	C17—C18	1.380 (3)
N2—C3	1.337 (3)	C17—H17	0.9300
N2—C2	1.419 (3)	C18—H18	0.9300
N2—N3	1.420 (2)	C19—H19A	0.9600
N3—C20	1.278 (3)	C19—H19B	0.9600
C1—C4	1.430 (3)	C19—H19C	0.9600
C1—C13	1.478 (3)	C20—C21	1.447 (3)
C3—C4	1.359 (3)	C20—H20	0.9300
C3—H3	0.9300	C21—C26	1.376 (3)
C4—C5	1.498 (3)	C21—C22	1.391 (3)
C5—C6	1.470 (3)	C22—C23	1.368 (4)
C6—C11	1.381 (3)	C22—H22	0.9300
C6—C7	1.395 (3)	C23—C24	1.381 (4)
C7—C8	1.363 (4)	C23—H23	0.9300
C7—H7	0.9300	C24—C25	1.370 (4)
C8—C9	1.374 (4)	C25—C26	1.382 (3)
C8—H8	0.9300	C25—H25	0.9300
C9—C10	1.380 (4)	C26—H26	0.9300
C10—C11	1.376 (4)	C27—H27A	0.9600
C10—H10	0.9300	C27—H27B	0.9600
C11—H11	0.9300	C27—H27C	0.9600
C12—H12A	0.9600		

C12—O3—C9	118.1 (3)	C14—C13—C1	122.69 (18)
C16—O4—C19	118.25 (17)	C15—C14—C13	121.53 (19)
C24—O5—C27	118.5 (3)	C15—C14—H14	119.2
C1—N1—C2	122.31 (19)	C13—C14—H14	119.2
C3—N2—C2	121.47 (18)	C14—C15—C16	120.1 (2)
C3—N2—N3	116.41 (18)	C14—C15—H15	120.0
C2—N2—N3	121.76 (18)	C16—C15—H15	120.0
C20—N3—N2	115.2 (2)	O4—C16—C15	115.74 (19)
N1—C1—C4	121.7 (2)	O4—C16—C17	124.44 (19)
N1—C1—C13	114.86 (19)	C15—C16—C17	119.82 (19)
C4—C1—C13	123.25 (19)	C18—C17—C16	119.39 (19)
O1—C2—N1	124.0 (2)	C18—C17—H17	120.3
O1—C2—N2	120.2 (2)	C16—C17—H17	120.3
N1—C2—N2	115.83 (19)	C17—C18—C13	121.8 (2)
N2—C3—C4	121.9 (2)	C17—C18—H18	119.1
N2—C3—H3	119.1	C13—C18—H18	119.1
C4—C3—H3	119.1	O4—C19—H19A	109.5
C3—C4—C1	115.7 (2)	O4—C19—H19B	109.5
C3—C4—C5	116.51 (19)	H19A—C19—H19B	109.5
C1—C4—C5	127.80 (19)	O4—C19—H19C	109.5
O2—C5—C6	121.2 (2)	H19A—C19—H19C	109.5
O2—C5—C4	119.3 (2)	H19B—C19—H19C	109.5
C6—C5—C4	119.44 (19)	N3—C20—C21	121.0 (2)
C11—C6—C7	118.1 (2)	N3—C20—H20	119.5
C11—C6—C5	122.8 (2)	C21—C20—H20	119.5
C7—C6—C5	119.1 (2)	C26—C21—C22	118.1 (2)
C8—C7—C6	120.7 (3)	C26—C21—C20	119.3 (2)
C8—C7—H7	119.7	C22—C21—C20	122.6 (2)
C6—C7—H7	119.7	C23—C22—C21	120.3 (3)
C7—C8—C9	120.4 (3)	C23—C22—H22	119.9
C7—C8—H8	119.8	C21—C22—H22	119.9
C9—C8—H8	119.8	C22—C23—C24	120.8 (3)
O3—C9—C8	114.3 (3)	C22—C23—H23	119.6
O3—C9—C10	125.7 (3)	C24—C23—H23	119.6
C8—C9—C10	120.0 (3)	O5—C24—C25	124.6 (3)
C11—C10—C9	119.3 (3)	O5—C24—C23	115.6 (2)
C11—C10—H10	120.4	C25—C24—C23	119.7 (2)
C9—C10—H10	120.4	C24—C25—C26	119.2 (2)
C10—C11—C6	121.5 (2)	C24—C25—H25	120.4
C10—C11—H11	119.3	C26—C25—H25	120.4
C6—C11—H11	119.3	C21—C26—C25	121.9 (2)
O3—C12—H12A	109.5	C21—C26—H26	119.1
O3—C12—H12B	109.5	C25—C26—H26	119.1
H12A—C12—H12B	109.5	O5—C27—H27A	109.5
O3—C12—H12C	109.5	O5—C27—H27B	109.5
H12A—C12—H12C	109.5	H27A—C27—H27B	109.5
H12B—C12—H12C	109.5	O5—C27—H27C	109.5

C18—C13—C14	117.39 (19)	H27A—C27—H27C	109.5
C18—C13—C1	119.84 (19)	H27B—C27—H27C	109.5
C3—N2—N3—C20	−135.3 (2)	C9—C10—C11—C6	−1.2 (4)
C2—N2—N3—C20	51.5 (3)	C7—C6—C11—C10	−0.6 (4)
C2—N1—C1—C4	0.9 (4)	C5—C6—C11—C10	178.3 (2)
C2—N1—C1—C13	−174.3 (2)	N1—C1—C13—C18	−27.9 (3)
C1—N1—C2—O1	−174.8 (3)	C4—C1—C13—C18	156.9 (2)
C1—N1—C2—N2	8.0 (3)	N1—C1—C13—C14	148.6 (2)
C3—N2—C2—O1	173.3 (2)	C4—C1—C13—C14	−26.6 (3)
N3—N2—C2—O1	−13.8 (4)	C18—C13—C14—C15	−0.7 (3)
C3—N2—C2—N1	−9.4 (3)	C1—C13—C14—C15	−177.3 (2)
N3—N2—C2—N1	163.5 (2)	C13—C14—C15—C16	1.9 (3)
C2—N2—C3—C4	1.6 (3)	C19—O4—C16—C15	−171.2 (2)
N3—N2—C3—C4	−171.6 (2)	C19—O4—C16—C17	8.7 (4)
N2—C3—C4—C1	7.3 (3)	C14—C15—C16—O4	178.1 (2)
N2—C3—C4—C5	−173.3 (2)	C14—C15—C16—C17	−1.8 (4)
N1—C1—C4—C3	−8.8 (3)	O4—C16—C17—C18	−179.3 (2)
C13—C1—C4—C3	166.1 (2)	C15—C16—C17—C18	0.6 (4)
N1—C1—C4—C5	171.9 (2)	C16—C17—C18—C13	0.6 (4)
C13—C1—C4—C5	−13.3 (4)	C14—C13—C18—C17	−0.6 (3)
C3—C4—C5—O2	−41.5 (3)	C1—C13—C18—C17	176.1 (2)
C1—C4—C5—O2	137.8 (2)	N2—N3—C20—C21	−177.2 (2)
C3—C4—C5—C6	137.2 (2)	N3—C20—C21—C26	−175.5 (2)
C1—C4—C5—C6	−43.5 (3)	N3—C20—C21—C22	4.1 (4)
O2—C5—C6—C11	153.8 (2)	C26—C21—C22—C23	1.7 (4)
C4—C5—C6—C11	−24.9 (3)	C20—C21—C22—C23	−177.9 (3)
O2—C5—C6—C7	−27.3 (3)	C21—C22—C23—C24	−1.0 (5)
C4—C5—C6—C7	154.0 (2)	C27—O5—C24—C25	−0.6 (4)
C11—C6—C7—C8	2.0 (4)	C27—O5—C24—C23	178.8 (3)
C5—C6—C7—C8	−177.0 (3)	C22—C23—C24—O5	179.8 (3)
C6—C7—C8—C9	−1.5 (5)	C22—C23—C24—C25	−0.8 (5)
C12—O3—C9—C8	178.1 (3)	O5—C24—C25—C26	−178.7 (3)
C12—O3—C9—C10	−2.0 (5)	C23—C24—C25—C26	2.0 (4)
C7—C8—C9—O3	179.4 (3)	C22—C21—C26—C25	−0.5 (4)
C7—C8—C9—C10	−0.5 (5)	C20—C21—C26—C25	179.1 (2)
O3—C9—C10—C11	−178.1 (3)	C24—C25—C26—C21	−1.3 (4)
C8—C9—C10—C11	1.8 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···O1	0.93	2.34	2.737 (3)	105
C11—H11···O4^{i}	0.93	2.60	3.512 (3)	166
C3—H3···O2^{ii}	0.93	2.54	3.330 (3)	143
C15—H15···O2^{iii}	0.93	2.64	3.374 (3)	136

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