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2-{2-[3-(3,5-Dimethoxyphenyl)-1,2,4-oxadiazol-5-yl]phenoxy}-*N*-(2,6-dimethylphenyl)acetamide

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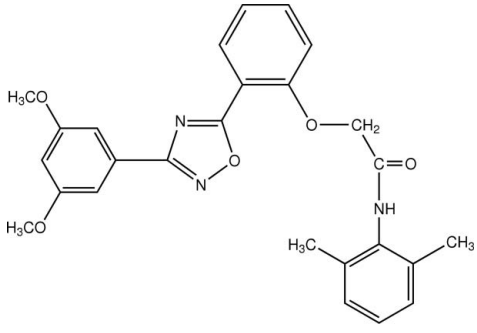
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; R factor = 0.083; wR factor = 0.179; data-to-parameter ratio = 15.5.

In the molecule of the title compound, $C_{26}H_{25}N_3O_5$, the dihedral angles between the oxadiazole ring and the adjacent benzene rings are 3.56 (12) and 5.72 (11)°. Intramolecular N—H···O and C—H···O hydrogen bonds result in the formation of four more five-membered planar rings, which are nearly coplanar with the adjacent rings.

Related literature

For related literature, see: Romero (2001); Terashita *et al.* (2002). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{26}H_{25}N_3O_5$
M_r = 459.49
Triclinic, $P\overline{1}$
a = 7.3200 (15) Å
b = 12.630 (3) Å
c = 13.106 (3) Å
α = 95.37 (3)°
β = 101.06 (3)°
γ = 103.48 (3)°
V = 1144.2 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.30 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.989, T_{max} = 0.991
4846 measured reflections
4473 independent reflections
2028 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.179
S = 1.06
4473 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O4	0.86	2.17	2.582 (5)	109
C6—H6A···N2	0.93	2.52	2.850 (5)	101
C12—H12A···N2	0.93	2.53	2.864 (5)	102
C26—H26A···N3	0.96	2.37	2.846 (7)	110

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2336).

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supplementary materials

Acta Cryst. (2007). E**63**, o4314 [**doi:10.1107/S1600536807049501**]

2-{2-[3-(3,5-Dimethoxyphenyl)-1,2,4-oxadiazol-5-yl]phenoxy}-*N*-(2,6-dimethylphenyl)acetamide

H.-L. Li, H.-B. Wang, J. Yin, S.-S. Kang and H.-S. Zeng

Comment

1,2,4-Oxadiazole derivatives possess biological properties such as intrinsic analgesic (Terashita *et al.*, 2002) and antipicornaviral (Romero, 2001) effects. As part of our studies in this area, we report herein the synthesis and crystal structure of the title compound, (I).

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987).

Rings A (C3—C8), B (N1/N2/O3/C9/C10), C (C11—C16) and D (C19—C24) are, of course, planar and the dihedral angles between them are A/B = 3.54 (3)°, A/C = 5.65 (2)°, B/C = 5.56 (3)° and C/D = 68.17 (2)°.

The intramolecular N—H···O and C—H···O hydrogen bonds (Table 1) cause to the formation of four five-membered planar rings E (N2/H6A/C6/C7/C9), F (N1/N2/O3/C9/C10), G (O4/N3/H3A/C17/C18) and H (N3/C19/C20/C26/H26A) (Fig. 1), in which they are also nearly co-planar with the adjacent rings, as can be deduced from the dihedral angles of A/E = 2.20 (3)°, B/E = 1.52 (2)°, B/F = 3.03 (3)°, C/F = 2.54 (2)° and D/H = 2.48 (3)°. Hydrogen bonds may be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, (I), potassium carbonate (15 mmol) and 5-(2-hydroxyphenyl)-3-(3,5-dimethoxyl)-phenyl-1,2,4-oxadiazole (10 mmol) were added, respectively, to the solution of 2-chloro-*N*-(2,6-dimethylphenyl)- acetamide (10 mmol) in acetone (100 ml). The resulting mixture was refluxed for 12 h. After cooling and filtering, the crude title compound was obtained and purified by recrystalization from ethyl acetate. Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution (yield; 3.62 g, 78.8%, m.p. 419–420 K).

Refinement

The highest peak in the final difference electron-density map is located 1.95 Å from the N2 atom. H atoms were positioned geometrically, with N—H = 0.86 (for NH) and C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*N*), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

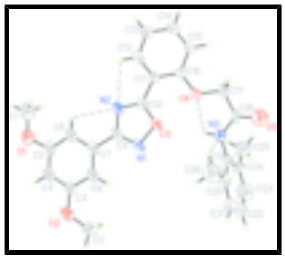


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

2-{2-[3-(3,5-Dimethoxyphenyl)-1,2,4-oxadiazol-5-yl]phenoxy}- *N*-(2,6-dimethylphenyl)acetamide

Crystal data

$C_{26}H_{25}N_3O_5$	$Z = 2$
$M_r = 459.49$	$F_{000} = 484$
Triclinic, $P\overline{1}$	$D_x = 1.334$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.3200$ (15) Å	Cell parameters from 25 reflections
$b = 12.630$ (3) Å	$\theta = 9$–13º
$c = 13.106$ (3) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 95.37$ (3)º	$T = 294$ (2) K
$\beta = 101.06$ (3)º	Block, colorless
$\gamma = 103.48$ (3)º	0.30 × 0.10 × 0.10 mm
$V = 1144.2$ (5) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.047$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.0$º
Monochromator: graphite	$\theta_{min} = 1.6$º
$T = 294$(2) K	$h = -9 \rightarrow 8$
$\omega/2\theta$ scans	$k = -15 \rightarrow 15$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = 0 \rightarrow 16$
$T_{min} = 0.989$, $T_{max} = 0.991$	3 standard reflections
4846 measured reflections	every 120 min
4473 independent reflections	intensity decay: none
2028 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.083$	H-atom parameters constrained
$wR(F^2) = 0.179$	$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.89P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
4473 reflections	$\Delta\rho_{max} = 0.67$ e Å^{-3}
289 parameters	$\Delta\rho_{min} = -0.37$ 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 $F^2 > 2$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	0.3738 (5)	−0.2031 (3)	0.7085 (3)	0.0770 (11)
O2	0.6959 (4)	0.1635 (3)	0.8227 (2)	0.0674 (9)
O3	0.1682 (4)	0.1486 (2)	0.3487 (2)	0.0544 (8)
O4	0.0182 (4)	0.1649 (2)	0.1575 (2)	0.0618 (9)
O5	0.1340 (5)	0.4105 (3)	0.0536 (2)	0.073
N1	0.2816 (5)	0.1636 (3)	0.4531 (2)	0.0578 (11)
N2	0.1300 (5)	−0.0156 (3)	0.3976 (2)	0.0449 (9)
N3	0.2857 (5)	0.3462 (3)	0.1901 (3)	0.0601 (11)
H3A	0.2880	0.2884	0.2197	0.072*
C1	0.2473 (8)	−0.2889 (4)	0.6317 (5)	0.102 (2)
H1B	0.2419	−0.3582	0.6571	0.153*
H1C	0.2935	−0.2899	0.5680	0.153*
H1D	0.1208	−0.2766	0.6182	0.153*
C2	0.7412 (7)	0.2758 (4)	0.8085 (4)	0.0839 (18)
H2B	0.8343	0.3184	0.8688	0.126*
H2C	0.6266	0.3016	0.8001	0.126*
H2D	0.7935	0.2834	0.7470	0.126*
C3	0.5675 (6)	0.0903 (4)	0.7431 (3)	0.0533 (12)
C4	0.5289 (6)	−0.0181 (4)	0.7583 (3)	0.0601 (13)
H4A	0.5905	−0.0374	0.8200	0.072*
C5	0.4015 (6)	−0.0979 (4)	0.6841 (3)	0.0526 (12)
C6	0.3069 (6)	−0.0714 (4)	0.5914 (3)	0.0514 (11)
H6A	0.2181	−0.1256	0.5414	0.062*
C7	0.3476 (6)	0.0364 (4)	0.5754 (3)	0.0448 (10)

C8	0.4766 (6)	0.1189 (4)	0.6499 (3)	0.0493 (11)
H8A	0.5019	0.1918	0.6380	0.059*
C9	0.2518 (6)	0.0642 (3)	0.4753 (3)	0.0462 (11)
C10	0.0835 (6)	0.0413 (3)	0.3235 (3)	0.0436 (10)
C11	−0.0464 (5)	−0.0039 (3)	0.2205 (3)	0.0385 (10)
C12	−0.1374 (6)	−0.1151 (3)	0.2040 (3)	0.0543 (12)
H12A	−0.1090	−0.1578	0.2560	0.065*
C13	−0.2688 (7)	−0.1638 (4)	0.1123 (3)	0.0579 (13)
H13A	−0.3291	−0.2386	0.1018	0.070*
C14	−0.3091 (7)	−0.0993 (4)	0.0366 (3)	0.0615 (13)
H14A	−0.4016	−0.1307	−0.0246	0.074*
C15	−0.2177 (6)	0.0085 (3)	0.0487 (3)	0.0516 (12)
H15A	−0.2460	0.0502	−0.0042	0.062*
C16	−0.0824 (6)	0.0568 (3)	0.1396 (3)	0.0426 (10)
C17	−0.0099 (6)	0.2329 (3)	0.0789 (3)	0.0551 (12)
H17A	−0.1362	0.2469	0.0720	0.066*
H17B	−0.0031	0.1962	0.0118	0.066*
C18	0.1413 (7)	0.3383 (4)	0.1084 (3)	0.0623 (14)
C19	0.4371 (7)	0.4428 (3)	0.2324 (4)	0.0619 (14)
C20	0.4323 (9)	0.5036 (4)	0.3245 (4)	0.0835 (18)
C21	0.5882 (11)	0.5932 (4)	0.3679 (5)	0.107 (3)
H21A	0.5907	0.6348	0.4308	0.129*
C22	0.7353 (10)	0.6200 (4)	0.3197 (5)	0.103 (3)
H22A	0.8349	0.6820	0.3495	0.124*
C23	0.7467 (9)	0.5593 (5)	0.2266 (5)	0.096
H23A	0.8520	0.5785	0.1959	0.115*
C24	0.5918 (8)	0.4688 (4)	0.1826 (4)	0.0690 (15)
C25	0.5993 (8)	0.4040 (4)	0.0840 (5)	0.0942 (19)
H25A	0.7151	0.4367	0.0623	0.141*
H25B	0.4895	0.4034	0.0302	0.141*
H25C	0.5981	0.3299	0.0955	0.141*
C26	0.2561 (8)	0.4750 (5)	0.3734 (5)	0.097
H26A	0.1659	0.4099	0.3333	0.146*
H26B	0.1961	0.5349	0.3733	0.146*
H26C	0.2959	0.4622	0.4444	0.146*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.085 (3)	0.067 (2)	0.069 (2)	0.014 (2)	−0.0115 (19)	0.0325 (19)
O2	0.055 (2)	0.082 (2)	0.0471 (18)	0.0023 (18)	−0.0171 (16)	0.0205 (17)
O3	0.067 (2)	0.0465 (18)	0.0357 (15)	0.0081 (15)	−0.0181 (14)	0.0108 (13)
O4	0.072 (2)	0.0492 (18)	0.0425 (17)	−0.0050 (16)	−0.0215 (15)	0.0210 (14)
O5	0.073	0.073	0.073	0.019	0.016	0.011
N1	0.069 (3)	0.061 (2)	0.0306 (19)	0.013 (2)	−0.0184 (18)	0.0103 (17)
N2	0.042 (2)	0.054 (2)	0.0353 (18)	0.0088 (17)	−0.0011 (16)	0.0151 (16)
N3	0.061 (2)	0.043 (2)	0.059 (2)	−0.0001 (19)	−0.018 (2)	0.0212 (18)
C1	0.101 (5)	0.079 (4)	0.112 (5)	0.015 (4)	−0.014 (4)	0.042 (4)

C2	0.071 (4)	0.082 (4)	0.067 (3)	−0.017 (3)	−0.021 (3)	0.021 (3)
C3	0.043 (3)	0.068 (3)	0.044 (2)	0.015 (2)	−0.006 (2)	0.016 (2)
C4	0.054 (3)	0.081 (4)	0.042 (2)	0.021 (3)	−0.010 (2)	0.029 (2)
C5	0.049 (3)	0.068 (3)	0.046 (3)	0.022 (2)	0.006 (2)	0.028 (2)
C6	0.043 (3)	0.064 (3)	0.043 (2)	0.011 (2)	−0.004 (2)	0.020 (2)
C7	0.041 (2)	0.064 (3)	0.032 (2)	0.019 (2)	0.0002 (19)	0.015 (2)
C8	0.047 (3)	0.060 (3)	0.039 (2)	0.013 (2)	−0.001 (2)	0.019 (2)
C9	0.049 (3)	0.055 (3)	0.032 (2)	0.015 (2)	−0.005 (2)	0.016 (2)
C10	0.045 (3)	0.043 (2)	0.038 (2)	0.010 (2)	−0.0029 (19)	0.0126 (19)
C11	0.034 (2)	0.041 (2)	0.035 (2)	0.0071 (19)	−0.0035 (18)	0.0101 (17)
C12	0.060 (3)	0.054 (3)	0.043 (2)	0.011 (2)	−0.002 (2)	0.017 (2)
C13	0.070 (3)	0.047 (3)	0.043 (3)	−0.004 (2)	0.002 (2)	0.011 (2)
C14	0.061 (3)	0.065 (3)	0.041 (2)	−0.002 (3)	−0.012 (2)	0.010 (2)
C15	0.052 (3)	0.052 (3)	0.038 (2)	−0.001 (2)	−0.010 (2)	0.013 (2)
C16	0.045 (3)	0.038 (2)	0.036 (2)	0.002 (2)	−0.0033 (19)	0.0117 (18)
C17	0.050 (3)	0.050 (3)	0.057 (3)	0.004 (2)	−0.008 (2)	0.030 (2)
C18	0.062 (3)	0.054 (3)	0.062 (3)	0.006 (2)	−0.013 (2)	0.040 (2)
C19	0.062 (3)	0.036 (3)	0.066 (3)	−0.002 (2)	−0.023 (3)	0.017 (2)
C20	0.108 (5)	0.050 (3)	0.069 (4)	0.014 (3)	−0.030 (3)	0.010 (3)
C21	0.177 (7)	0.047 (3)	0.062 (4)	0.010 (4)	−0.036 (4)	0.007 (3)
C22	0.117 (6)	0.050 (4)	0.106 (5)	−0.009 (3)	−0.037 (4)	0.041 (4)
C23	0.096	0.096	0.096	0.025	0.021	0.014
C24	0.064 (3)	0.034 (3)	0.084 (4)	−0.007 (2)	−0.023 (3)	0.013 (3)
C25	0.080 (4)	0.075 (4)	0.120 (5)	0.008 (3)	0.011 (4)	0.024 (4)
C26	0.097	0.097	0.097	0.025	0.021	0.014

Geometric parameters (Å, °)

O1—C5	1.374 (5)	C10—C11	1.471 (5)
O1—C1	1.419 (6)	C11—C12	1.384 (5)
O2—C3	1.365 (5)	C11—C16	1.386 (5)
O2—C2	1.418 (5)	C12—C13	1.374 (5)
O3—C10	1.332 (4)	C12—H12A	0.9300
O3—N1	1.428 (4)	C13—C14	1.374 (5)
O4—C16	1.366 (4)	C13—H13A	0.9300
O4—C17	1.417 (4)	C14—C15	1.350 (5)
O5—C18	1.217 (4)	C14—H14A	0.9300
N1—C9	1.294 (5)	C15—C16	1.379 (5)
N2—C10	1.302 (4)	C15—H15A	0.9300
N2—C9	1.374 (5)	C17—C18	1.484 (5)
N3—C18	1.331 (5)	C17—H17A	0.9700
N3—C19	1.425 (5)	C17—H17B	0.9700
N3—H3A	0.8600	C19—C20	1.379 (7)
C1—H1B	0.9600	C19—C24	1.402 (7)
C1—H1C	0.9600	C20—C21	1.391 (7)
C1—H1D	0.9600	C20—C26	1.533 (8)
C2—H2B	0.9600	C21—C22	1.343 (9)
C2—H2C	0.9600	C21—H21A	0.9300
C2—H2D	0.9600	C22—C23	1.406 (8)

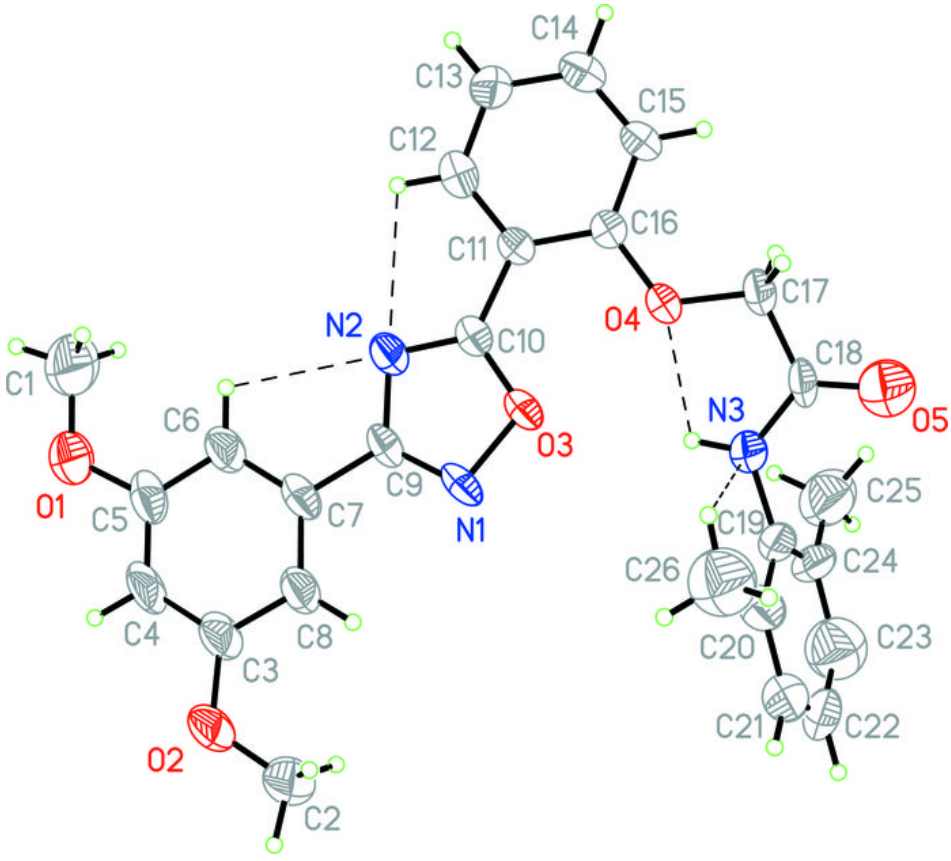
C3—C4	1.374 (6)	C22—H22A	0.9300
C3—C8	1.395 (5)	C23—C24	1.395 (7)
C4—C5	1.364 (6)	C23—H23A	0.9300
C4—H4A	0.9300	C24—C25	1.481 (7)
C5—C6	1.389 (5)	C25—H25A	0.9600
C6—C7	1.370 (5)	C25—H25B	0.9600
C6—H6A	0.9300	C25—H25C	0.9600
C7—C8	1.388 (5)	C26—H26A	0.9600
C7—C9	1.478 (5)	C26—H26B	0.9600
C8—H8A	0.9300	C26—H26C	0.9600
C5—O1—C1	117.2 (3)	C14—C13—C12	118.5 (4)
C3—O2—C2	117.4 (3)	C14—C13—H13A	120.8
C10—O3—N1	106.5 (3)	C12—C13—H13A	120.8
C16—O4—C17	119.8 (3)	C15—C14—C13	121.6 (4)
C9—N1—O3	102.4 (3)	C15—C14—H14A	119.2
C10—N2—C9	102.3 (3)	C13—C14—H14A	119.2
C18—N3—C19	125.1 (3)	C14—C15—C16	119.9 (4)
C18—N3—H3A	117.4	C14—C15—H15A	120.0
C19—N3—H3A	117.4	C16—C15—H15A	120.0
O1—C1—H1B	109.5	O4—C16—C15	123.6 (3)
O1—C1—H1C	109.5	O4—C16—C11	116.2 (3)
H1B—C1—H1C	109.5	C15—C16—C11	120.1 (4)
O1—C1—H1D	109.5	O4—C17—C18	109.1 (3)
H1B—C1—H1D	109.5	O4—C17—H17A	109.9
H1C—C1—H1D	109.5	C18—C17—H17A	109.9
O2—C2—H2B	109.5	O4—C17—H17B	109.9
O2—C2—H2C	109.5	C18—C17—H17B	109.9
H2B—C2—H2C	109.5	H17A—C17—H17B	108.3
O2—C2—H2D	109.5	O5—C18—N3	123.2 (4)
H2B—C2—H2D	109.5	O5—C18—C17	118.9 (4)
H2C—C2—H2D	109.5	N3—C18—C17	117.8 (3)
O2—C3—C4	116.1 (4)	C20—C19—C24	122.2 (5)
O2—C3—C8	124.5 (4)	C20—C19—N3	118.8 (5)
C4—C3—C8	119.5 (4)	C24—C19—N3	118.8 (5)
C5—C4—C3	120.9 (4)	C19—C20—C21	117.7 (6)
C5—C4—H4A	119.6	C19—C20—C26	120.3 (5)
C3—C4—H4A	119.6	C21—C20—C26	121.9 (6)
C4—C5—O1	115.6 (4)	C22—C21—C20	120.5 (6)
C4—C5—C6	120.8 (4)	C22—C21—H21A	119.8
O1—C5—C6	123.6 (4)	C20—C21—H21A	119.8
C7—C6—C5	118.3 (4)	C21—C22—C23	123.5 (6)
C7—C6—H6A	120.8	C21—C22—H22A	118.3
C5—C6—H6A	120.8	C23—C22—H22A	118.3
C6—C7—C8	121.8 (4)	C24—C23—C22	116.6 (6)
C6—C7—C9	118.4 (4)	C24—C23—H23A	121.7
C8—C7—C9	119.8 (4)	C22—C23—H23A	121.7
C7—C8—C3	118.7 (4)	C23—C24—C19	119.5 (5)
C7—C8—H8A	120.6	C23—C24—C25	117.7 (6)
C3—C8—H8A	120.6	C19—C24—C25	122.8 (4)

N1—C9—N2	115.6 (3)	C24—C25—H25A	109.5
N1—C9—C7	122.8 (4)	C24—C25—H25B	109.5
N2—C9—C7	121.6 (4)	H25A—C25—H25B	109.5
N2—C10—O3	113.2 (3)	C24—C25—H25C	109.5
N2—C10—C11	125.5 (4)	H25A—C25—H25C	109.5
O3—C10—C11	121.3 (3)	H25B—C25—H25C	109.5
C12—C11—C16	118.4 (3)	C20—C26—H26A	109.5
C12—C11—C10	117.1 (3)	C20—C26—H26B	109.5
C16—C11—C10	124.6 (4)	H26A—C26—H26B	109.5
C13—C12—C11	121.3 (4)	C20—C26—H26C	109.5
C13—C12—H12A	119.3	H26A—C26—H26C	109.5
C11—C12—H12A	119.3	H26B—C26—H26C	109.5
C10—O3—N1—C9	0.8 (4)	C10—C11—C12—C13	176.6 (4)
C2—O2—C3—C4	178.9 (4)	C11—C12—C13—C14	−0.2 (7)
C2—O2—C3—C8	−1.0 (7)	C12—C13—C14—C15	2.6 (8)
O2—C3—C4—C5	179.4 (4)	C13—C14—C15—C16	−1.0 (8)
C8—C3—C4—C5	−0.7 (7)	C17—O4—C16—C15	−2.0 (6)
C3—C4—C5—O1	−179.6 (4)	C17—O4—C16—C11	180.0 (4)
C3—C4—C5—C6	−0.2 (7)	C14—C15—C16—O4	179.1 (4)
C1—O1—C5—C4	−177.9 (5)	C14—C15—C16—C11	−2.9 (7)
C1—O1—C5—C6	2.7 (7)	C12—C11—C16—O4	−176.7 (4)
C4—C5—C6—C7	1.3 (7)	C10—C11—C16—O4	3.0 (6)
O1—C5—C6—C7	−179.4 (4)	C12—C11—C16—C15	5.2 (6)
C5—C6—C7—C8	−1.3 (6)	C10—C11—C16—C15	−175.1 (4)
C5—C6—C7—C9	178.0 (4)	C16—O4—C17—C18	−168.9 (4)
C6—C7—C8—C3	0.4 (6)	C19—N3—C18—O5	8.0 (8)
C9—C7—C8—C3	−178.9 (4)	C19—N3—C18—C17	−176.6 (5)
O2—C3—C8—C7	−179.5 (4)	O4—C17—C18—O5	−175.4 (4)
C4—C3—C8—C7	0.6 (7)	O4—C17—C18—N3	9.0 (6)
O3—N1—C9—N2	−0.4 (5)	C18—N3—C19—C20	103.5 (6)
O3—N1—C9—C7	177.2 (4)	C18—N3—C19—C24	−80.6 (6)
C10—N2—C9—N1	−0.2 (5)	C24—C19—C20—C21	−0.1 (7)
C10—N2—C9—C7	−177.8 (4)	N3—C19—C20—C21	175.6 (4)
C6—C7—C9—N1	−179.8 (4)	C24—C19—C20—C26	177.4 (4)
C8—C7—C9—N1	−0.4 (6)	N3—C19—C20—C26	−6.9 (7)
C6—C7—C9—N2	−2.4 (6)	C19—C20—C21—C22	1.4 (8)
C8—C7—C9—N2	177.0 (4)	C26—C20—C21—C22	−176.0 (5)
C9—N2—C10—O3	0.8 (5)	C20—C21—C22—C23	−2.4 (9)
C9—N2—C10—C11	−180.0 (4)	C21—C22—C23—C24	1.9 (9)
N1—O3—C10—N2	−1.1 (5)	C22—C23—C24—C19	−0.4 (7)
N1—O3—C10—C11	179.7 (4)	C22—C23—C24—C25	179.5 (5)
N2—C10—C11—C12	5.0 (6)	C20—C19—C24—C23	−0.4 (7)
O3—C10—C11—C12	−175.9 (4)	N3—C19—C24—C23	−176.1 (4)
N2—C10—C11—C16	−174.7 (4)	C20—C19—C24—C25	179.7 (4)
O3—C10—C11—C16	4.4 (6)	N3—C19—C24—C25	4.0 (7)
C16—C11—C12—C13	−3.6 (6)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O4	0.86	2.17	2.582 (5)	109
C6—H6A···N2	0.93	2.52	2.850 (5)	101
C12—H12A···N2	0.93	2.53	2.864 (5)	102
C26—H26A···N3	0.96	2.37	2.846 (7)	110

Fig. 1


C14
C13
C15
C12
C16
C11
C17
O4
N2
C10
C18
C1
C6
O3
O5
N3
O1
C5
C7
C9
N1
C25
C19
C26
C24
C4
C8
C20
C23
C3
C21
C22
O2
C2