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

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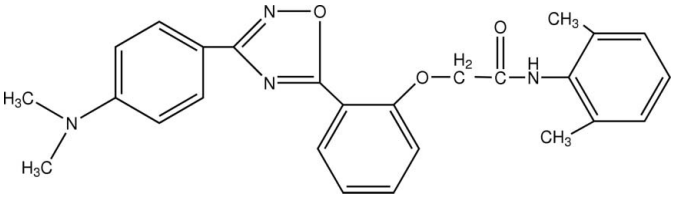
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.077; wR factor = 0.178; data-to-parameter ratio = 15.1.

In the title compound, $C_{26}H_{26}N_4O_3$, a bifurcated intramolecular N—H···(O,N) hydrogen bond helps to establish the molecular conformation. The dihedral angles between the oxadiazole ring and the adjacent benzene rings are 14.10 (19) and 17.90 (18)° for the central benzene ring and the (dimethylamino)phenyl ring, respectively.

Related literature

For background, see: Romero (2001); Terashita *et al.* (2002).



Experimental

Crystal data

$C_{26}H_{26}N_4O_3$
M_r = 442.51
Triclinic, $P\overline{1}$
a = 8.9900 (18) Å
b = 9.0330 (18) Å
c = 15.445 (3) Å
α = 83.01 (3)°
β = 79.76 (3)°
γ = 66.54 (3)°
V = 1130.4 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.974, T_{max} = 0.991
4419 measured reflections
4419 independent reflections
2692 reflections with $I > 2\sigma(I)$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.179
S = 1.03
4419 reflections
293 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O2	0.86	2.10	2.513 (4)	109
N4—H4A···N3	0.86	2.32	3.170 (4)	171

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: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2606).

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supplementary materials

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

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

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 out studies in this area, we report here the synthesis and crystal structure of the title compound, (I), (Fig. 1).

The dihedral angles between the N2/O1/C10/N3/C9 ring and its adjacent bezene rings are 14.10 (19) and 17.90 (18)° for the C11 and C3 rings, respectively.

An intramolecular, bifurcated N—H···(N,*O*) hydrogen bond (Table 1) helps to establish the molecular conformation of (I).

Experimental

2-Chloro-*N*-(2,6-dimethylphenyl)acetamide (10 mmol) was dissolved in acetone (100 ml) and potassium carbonate (15 mmol) was added. Then, 5-(2-hydroxyphenyl)-3-(4-*N*,*N*-dimethyl)-phenyl- 1,2,4-oxadiazole (10 mmol) was added to the reaction. 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. Colourless blocks of (I) were obtained by slow evaporation of an ethanol solution.

Refinement

All the H atoms were placed geometrically (N—H = 0.86 Å, C—H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl carrier).

Figures

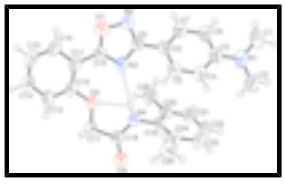


Fig. 1. A view of the molecular structure of (I) showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). Dashed lines indicate the hydrogen bonds.

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

Crystal data

$C_{26}H_{26}N_4O_3$	$Z = 2$
$M_r = 442.51$	$F_{000} = 468$

Triclinic, $P\bar{1}$	D_x = 1.300 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.9900 (18) Å	Cell parameters from 25 reflections
b = 9.0330 (18) Å	θ = 9–13º
c = 15.445 (3) Å	μ = 0.09 mm^{-1}
α = 83.01 (3)º	T = 293 (2) K
β = 79.76 (3)º	Block, colorless
γ = 66.54 (3)º	0.30 × 0.20 × 0.10 mm
V = 1130.4 (4) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.0000
Radiation source: fine-focus sealed tube	θ_{max} = 26.0º
Monochromator: graphite	θ_{min} = 1.3º
T = 293(2) K	h = −10→11
$\omega/2\theta$ scans	k = −10→11
Absorption correction: ψ scan (North *et al.*, 1968)	l = 0→19
T_{min} = 0.974, T_{max} = 0.991	3 standard reflections
4419 measured reflections	every 200 reflections
4419 independent reflections	intensity decay: none
2692 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
$R[F^2 > 2\sigma(F^2)]$ = 0.077	H-atom parameters constrained
$wR(F^2)$ = 0.179	$w = 1/[\sigma^2(F_o^2) + (0.018P)^2 + 2P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
4419 reflections	$\Delta\rho_{max}$ = 0.50 e Å^{-3}
293 parameters	$\Delta\rho_{min}$ = −0.43 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	1.1192 (3)	0.2794 (3)	0.45197 (18)	0.067
O2	1.3415 (3)	0.4254 (4)	0.2256 (2)	0.0914 (11)
O3	1.2793 (3)	0.6748 (3)	0.03292 (18)	0.0696 (8)
N1	0.3072 (4)	0.8914 (5)	0.3050 (3)	0.0988 (14)
N2	0.9452 (4)	0.3580 (5)	0.4585 (2)	0.0774 (11)
N3	1.0722 (4)	0.4657 (4)	0.3431 (2)	0.0581 (8)
N4	1.1088 (3)	0.6202 (4)	0.1492 (2)	0.0552 (8)
H4A	1.1046	0.5840	0.2033	0.066*
C1	0.1610 (5)	0.8702 (7)	0.3466 (4)	0.115 (2)
H1A	0.1627	0.7702	0.3303	0.172*
H1B	0.0673	0.9582	0.3280	0.172*
H1C	0.1549	0.8678	0.4094	0.172*
C2	0.2944 (6)	1.0093 (6)	0.2336 (3)	0.0933 (16)
H2B	0.3948	1.0267	0.2196	0.140*
H2C	0.2057	1.1090	0.2500	0.140*
H2D	0.2740	0.9719	0.1831	0.140*
C3	0.4591 (5)	0.7886 (5)	0.3270 (3)	0.0651 (10)
C4	0.5996 (5)	0.8191 (5)	0.2957 (3)	0.0720 (12)
H4B	0.5927	0.9107	0.2592	0.086*
C5	0.7495 (5)	0.7138 (5)	0.3185 (3)	0.0643 (10)
H5A	0.8421	0.7366	0.2973	0.077*
C6	0.7651 (4)	0.5774 (5)	0.3714 (2)	0.0558 (9)
C7	0.6260 (5)	0.5489 (5)	0.4033 (3)	0.0683 (11)
H7A	0.6337	0.4577	0.4403	0.082*
C8	0.4748 (5)	0.6523 (5)	0.3816 (3)	0.0707 (11)
H8A	0.3826	0.6297	0.4042	0.085*
C9	0.9276 (5)	0.4658 (5)	0.3923 (2)	0.0566 (9)
C10	1.1844 (5)	0.3506 (5)	0.3835 (2)	0.0577 (9)
C11	1.3619 (5)	0.2919 (5)	0.3645 (3)	0.0637 (10)
C12	1.4409 (5)	0.3316 (5)	0.2846 (3)	0.0679 (11)
C13	1.6095 (5)	0.2761 (6)	0.2669 (3)	0.0818 (14)
H13A	1.6604	0.3045	0.2134	0.098*
C14	1.7009 (5)	0.1783 (6)	0.3296 (3)	0.0862 (14)
H14A	1.8146	0.1402	0.3183	0.103*
C15	1.6277 (5)	0.1367 (6)	0.4075 (3)	0.0837 (14)
H15A	1.6918	0.0700	0.4489	0.100*
C16	1.4578 (5)	0.1921 (5)	0.4267 (3)	0.0696 (11)
H16A	1.4087	0.1628	0.4806	0.084*
C17	1.4010 (4)	0.5052 (5)	0.1516 (3)	0.0656 (11)
H17A	1.4829	0.4271	0.1122	0.079*

H17B	1.4504	0.5719	0.1701	0.079*
C18	1.2550 (4)	0.6091 (5)	0.1056 (2)	0.0556 (9)
C19	0.9582 (4)	0.6882 (4)	0.1122 (2)	0.0496 (8)
C20	0.8857 (4)	0.5827 (4)	0.1007 (2)	0.0550 (9)
C21	0.7401 (5)	0.6480 (5)	0.0645 (3)	0.0667 (11)
H21A	0.6889	0.5809	0.0555	0.080*
C22	0.6711 (5)	0.8103 (6)	0.0420 (3)	0.0760 (13)
H22A	0.5747	0.8516	0.0171	0.091*
C23	0.7425 (5)	0.9115 (5)	0.0558 (3)	0.0724 (12)
H23A	0.6928	1.0213	0.0407	0.087*
C24	0.8885 (4)	0.8547 (4)	0.0920 (2)	0.0554 (9)
C25	0.9578 (5)	0.9673 (5)	0.1131 (3)	0.0716 (11)
H25A	0.8938	1.0752	0.0929	0.107*
H25B	1.0688	0.9365	0.0844	0.107*
H25C	0.9557	0.9632	0.1756	0.107*
C26	0.9577 (5)	0.4057 (5)	0.1276 (3)	0.0721 (12)
H26A	1.0581	0.3811	0.1503	0.108*
H26B	0.9792	0.3434	0.0774	0.108*
H26C	0.8817	0.3794	0.1723	0.108*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.067	0.067	0.067	−0.026	−0.009	−0.004
O2	0.0446 (15)	0.131 (3)	0.080 (2)	−0.0251 (17)	−0.0207 (14)	0.0476 (19)
O3	0.0594 (16)	0.0797 (19)	0.0633 (17)	−0.0231 (14)	−0.0103 (13)	0.0086 (15)
N1	0.056 (2)	0.115 (3)	0.109 (3)	−0.018 (2)	−0.028 (2)	0.025 (3)
N2	0.051 (2)	0.096 (3)	0.072 (2)	−0.0196 (19)	−0.0139 (17)	0.017 (2)
N3	0.0488 (17)	0.065 (2)	0.0557 (19)	−0.0150 (15)	−0.0166 (14)	0.0045 (15)
N4	0.0425 (16)	0.066 (2)	0.0545 (18)	−0.0178 (14)	−0.0153 (13)	0.0073 (15)
C1	0.048 (3)	0.151 (5)	0.133 (5)	−0.028 (3)	−0.027 (3)	0.021 (4)
C2	0.078 (3)	0.088 (4)	0.112 (4)	−0.024 (3)	−0.042 (3)	0.020 (3)
C3	0.051 (2)	0.074 (3)	0.066 (3)	−0.015 (2)	−0.0146 (19)	−0.008 (2)
C4	0.056 (2)	0.069 (3)	0.080 (3)	−0.013 (2)	−0.014 (2)	0.002 (2)
C5	0.053 (2)	0.069 (3)	0.067 (3)	−0.021 (2)	−0.0071 (19)	−0.002 (2)
C6	0.049 (2)	0.062 (2)	0.052 (2)	−0.0168 (18)	−0.0066 (16)	−0.0055 (18)
C7	0.061 (2)	0.076 (3)	0.068 (3)	−0.026 (2)	−0.015 (2)	0.006 (2)
C8	0.055 (2)	0.081 (3)	0.078 (3)	−0.026 (2)	−0.020 (2)	0.003 (2)
C9	0.054 (2)	0.064 (2)	0.049 (2)	−0.0192 (18)	−0.0127 (17)	0.0008 (18)
C10	0.058 (2)	0.067 (2)	0.047 (2)	−0.0236 (19)	−0.0141 (17)	0.0106 (18)
C11	0.052 (2)	0.066 (3)	0.062 (2)	−0.0055 (19)	−0.0252 (19)	−0.0010 (19)
C12	0.047 (2)	0.079 (3)	0.069 (3)	−0.013 (2)	−0.0200 (19)	0.008 (2)
C13	0.046 (2)	0.102 (4)	0.084 (3)	−0.011 (2)	−0.021 (2)	0.001 (3)
C14	0.053 (3)	0.093 (4)	0.096 (4)	−0.008 (2)	−0.026 (2)	0.007 (3)
C15	0.066 (3)	0.079 (3)	0.091 (4)	−0.002 (2)	−0.042 (3)	0.004 (3)
C16	0.067 (3)	0.069 (3)	0.065 (3)	−0.014 (2)	−0.026 (2)	0.007 (2)
C17	0.046 (2)	0.080 (3)	0.062 (2)	−0.018 (2)	−0.0085 (18)	0.007 (2)
C18	0.047 (2)	0.066 (2)	0.053 (2)	−0.0202 (18)	−0.0104 (17)	−0.0003 (18)

C19	0.0403 (18)	0.057 (2)	0.050 (2)	−0.0147 (16)	−0.0126 (15)	0.0002 (16)
C20	0.056 (2)	0.055 (2)	0.057 (2)	−0.0242 (18)	−0.0067 (17)	−0.0036 (17)
C21	0.060 (2)	0.084 (3)	0.070 (3)	−0.040 (2)	−0.015 (2)	−0.005 (2)
C22	0.053 (2)	0.091 (3)	0.081 (3)	−0.021 (2)	−0.030 (2)	0.010 (3)
C23	0.060 (2)	0.065 (3)	0.084 (3)	−0.010 (2)	−0.029 (2)	0.004 (2)
C24	0.054 (2)	0.053 (2)	0.056 (2)	−0.0153 (17)	−0.0133 (17)	−0.0032 (17)
C25	0.085 (3)	0.062 (3)	0.073 (3)	−0.029 (2)	−0.025 (2)	−0.002 (2)
C26	0.080 (3)	0.061 (3)	0.078 (3)	−0.032 (2)	−0.009 (2)	0.001 (2)

Geometric parameters (Å, °)

O1—C10	1.338 (4)	C10—C11	1.453 (5)
O1—N2	1.427 (4)	C11—C12	1.392 (5)
O2—C12	1.358 (4)	C11—C16	1.395 (5)
O2—C17	1.415 (4)	C12—C13	1.380 (5)
O3—C18	1.230 (4)	C13—C14	1.376 (6)
N1—C3	1.387 (5)	C13—H13A	0.9300
N1—C2	1.423 (6)	C14—C15	1.352 (6)
N1—C1	1.431 (6)	C14—H14A	0.9300
N2—C9	1.308 (5)	C15—C16	1.391 (6)
N3—C10	1.312 (4)	C15—H15A	0.9300
N3—C9	1.384 (5)	C16—H16A	0.9300
N4—C18	1.338 (4)	C17—C18	1.516 (5)
N4—C19	1.437 (4)	C17—H17A	0.9700
N4—H4A	0.8600	C17—H17B	0.9700
C1—H1A	0.9600	C19—C20	1.393 (5)
C1—H1B	0.9600	C19—C24	1.399 (5)
C1—H1C	0.9600	C20—C21	1.392 (5)
C2—H2B	0.9600	C20—C26	1.503 (5)
C2—H2C	0.9600	C21—C22	1.372 (6)
C2—H2D	0.9600	C21—H21A	0.9300
C3—C8	1.378 (6)	C22—C23	1.362 (6)
C3—C4	1.390 (5)	C22—H22A	0.9300
C4—C5	1.383 (5)	C23—C24	1.398 (5)
C4—H4B	0.9300	C23—H23A	0.9300
C5—C6	1.365 (5)	C24—C25	1.478 (5)
C5—H5A	0.9300	C25—H25A	0.9600
C6—C7	1.371 (5)	C25—H25B	0.9600
C6—C9	1.473 (5)	C25—H25C	0.9600
C7—C8	1.381 (5)	C26—H26A	0.9600
C7—H7A	0.9300	C26—H26B	0.9600
C8—H8A	0.9300	C26—H26C	0.9600
C10—O1—N2	107.7 (3)	C14—C13—C12	118.9 (5)
C12—O2—C17	121.2 (3)	C14—C13—H13A	120.5
C3—N1—C2	120.6 (4)	C12—C13—H13A	120.5
C3—N1—C1	121.0 (4)	C15—C14—C13	120.8 (4)
C2—N1—C1	118.0 (4)	C15—C14—H14A	119.6
C9—N2—O1	102.0 (3)	C13—C14—H14A	119.6
C10—N3—C9	102.8 (3)	C14—C15—C16	121.1 (4)

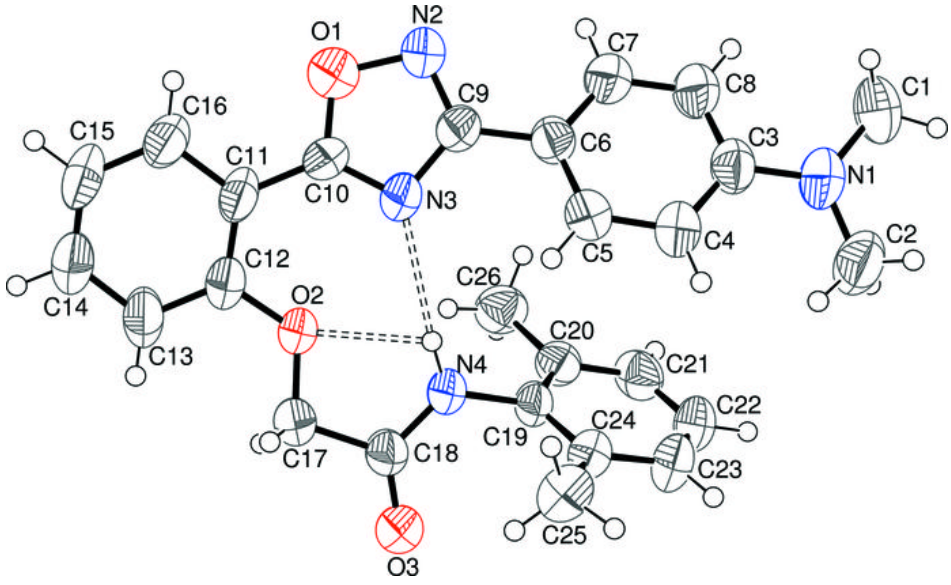
C18—N4—C19	124.7 (3)	C14—C15—H15A	119.5
C18—N4—H4A	117.6	C16—C15—H15A	119.5
C19—N4—H4A	117.6	C15—C16—C11	119.4 (4)
N1—C1—H1A	109.5	C15—C16—H16A	120.3
N1—C1—H1B	109.5	C11—C16—H16A	120.3
H1A—C1—H1B	109.5	O2—C17—C18	106.7 (3)
N1—C1—H1C	109.5	O2—C17—H17A	110.4
H1A—C1—H1C	109.5	C18—C17—H17A	110.4
H1B—C1—H1C	109.5	O2—C17—H17B	110.4
N1—C2—H2B	109.5	C18—C17—H17B	110.4
N1—C2—H2C	109.5	H17A—C17—H17B	108.6
H2B—C2—H2C	109.5	O3—C18—N4	125.8 (3)
N1—C2—H2D	109.5	O3—C18—C17	118.6 (3)
H2B—C2—H2D	109.5	N4—C18—C17	115.5 (3)
H2C—C2—H2D	109.5	C20—C19—C24	123.0 (3)
C8—C3—N1	120.5 (4)	C20—C19—N4	117.2 (3)
C8—C3—C4	117.8 (4)	C24—C19—N4	119.7 (3)
N1—C3—C4	121.7 (4)	C21—C20—C19	117.4 (3)
C5—C4—C3	120.3 (4)	C21—C20—C26	120.4 (4)
C5—C4—H4B	119.8	C19—C20—C26	122.2 (3)
C3—C4—H4B	119.8	C22—C21—C20	120.8 (4)
C6—C5—C4	121.7 (4)	C22—C21—H21A	119.6
C6—C5—H5A	119.2	C20—C21—H21A	119.6
C4—C5—H5A	119.2	C23—C22—C21	120.7 (4)
C5—C6—C7	117.9 (4)	C23—C22—H22A	119.7
C5—C6—C9	120.1 (4)	C21—C22—H22A	119.7
C7—C6—C9	122.0 (4)	C22—C23—C24	121.7 (4)
C6—C7—C8	121.6 (4)	C22—C23—H23A	119.1
C6—C7—H7A	119.2	C24—C23—H23A	119.1
C8—C7—H7A	119.2	C23—C24—C19	116.3 (4)
C3—C8—C7	120.7 (4)	C23—C24—C25	121.1 (4)
C3—C8—H8A	119.6	C19—C24—C25	122.4 (3)
C7—C8—H8A	119.6	C24—C25—H25A	109.5
N2—C9—N3	115.2 (3)	C24—C25—H25B	109.5
N2—C9—C6	122.1 (3)	H25A—C25—H25B	109.5
N3—C9—C6	122.7 (3)	C24—C25—H25C	109.5
N3—C10—O1	112.2 (3)	H25A—C25—H25C	109.5
N3—C10—C11	130.0 (3)	H25B—C25—H25C	109.5
O1—C10—C11	117.7 (3)	C20—C26—H26A	109.5
C12—C11—C16	118.3 (4)	C20—C26—H26B	109.5
C12—C11—C10	121.7 (3)	H26A—C26—H26B	109.5
C16—C11—C10	120.0 (4)	C20—C26—H26C	109.5
O2—C12—C13	122.8 (4)	H26A—C26—H26C	109.5
O2—C12—C11	115.7 (3)	H26B—C26—H26C	109.5
C13—C12—C11	121.5 (4)		
C10—O1—N2—C9	0.6 (4)	C16—C11—C12—O2	178.2 (4)
C2—N1—C3—C8	−165.1 (5)	C10—C11—C12—O2	−1.2 (6)
C1—N1—C3—C8	7.8 (7)	C16—C11—C12—C13	−0.8 (7)
C2—N1—C3—C4	15.3 (7)	C10—C11—C12—C13	179.8 (4)

C1—N1—C3—C4	−171.8 (5)	O2—C12—C13—C14	−178.3 (5)
C8—C3—C4—C5	0.7 (6)	C11—C12—C13—C14	0.6 (7)
N1—C3—C4—C5	−179.7 (4)	C12—C13—C14—C15	0.0 (8)
C3—C4—C5—C6	0.5 (7)	C13—C14—C15—C16	−0.3 (8)
C4—C5—C6—C7	−1.4 (6)	C14—C15—C16—C11	0.1 (7)
C4—C5—C6—C9	178.3 (4)	C12—C11—C16—C15	0.4 (6)
C5—C6—C7—C8	1.2 (6)	C10—C11—C16—C15	179.9 (4)
C9—C6—C7—C8	−178.5 (4)	C12—O2—C17—C18	−175.1 (4)
N1—C3—C8—C7	179.5 (4)	C19—N4—C18—O3	11.1 (6)
C4—C3—C8—C7	−0.9 (6)	C19—N4—C18—C17	−168.8 (3)
C6—C7—C8—C3	−0.1 (7)	O2—C17—C18—O3	−171.0 (4)
O1—N2—C9—N3	0.1 (5)	O2—C17—C18—N4	8.9 (5)
O1—N2—C9—C6	179.3 (3)	C18—N4—C19—C20	112.1 (4)
C10—N3—C9—N2	−0.8 (5)	C18—N4—C19—C24	−69.8 (5)
C10—N3—C9—C6	−180.0 (4)	C24—C19—C20—C21	2.2 (5)
C5—C6—C9—N2	162.5 (4)	N4—C19—C20—C21	−179.8 (3)
C7—C6—C9—N2	−17.8 (6)	C24—C19—C20—C26	−176.4 (4)
C5—C6—C9—N3	−18.4 (6)	N4—C19—C20—C26	1.6 (5)
C7—C6—C9—N3	161.3 (4)	C19—C20—C21—C22	−0.5 (6)
C9—N3—C10—O1	1.2 (4)	C26—C20—C21—C22	178.2 (4)
C9—N3—C10—C11	−179.2 (4)	C20—C21—C22—C23	−1.0 (7)
N2—O1—C10—N3	−1.2 (4)	C21—C22—C23—C24	0.8 (7)
N2—O1—C10—C11	179.1 (3)	C22—C23—C24—C19	0.8 (6)
N3—C10—C11—C12	−14.3 (7)	C22—C23—C24—C25	−175.1 (4)
O1—C10—C11—C12	165.3 (4)	C20—C19—C24—C23	−2.4 (5)
N3—C10—C11—C16	166.3 (4)	N4—C19—C24—C23	179.7 (3)
O1—C10—C11—C16	−14.1 (6)	C20—C19—C24—C25	173.5 (4)
C17—O2—C12—C13	−16.0 (7)	N4—C19—C24—C25	−4.4 (5)
C17—O2—C12—C11	165.0 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4A···O2	0.86	2.10	2.513 (4)	109
N4—H4A···N3	0.86	2.32	3.170 (4)	171

Fig. 1


O1
N2
C7
C8
C1
C16
C9
C15
C6
C3
C11
C10
N3
N1
C5
C4
C2
C12
C26
C14
O2
C20
C13
N4
C21
C22
C19
C24
C17
C18
C23
C25
O3