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4-({4-[1-(Methoxyimino)ethyl]anilino}-(phenyl)methylene)-3-methyl-2-phenyl-1*H*-pyrazol-5(4*H*)-one

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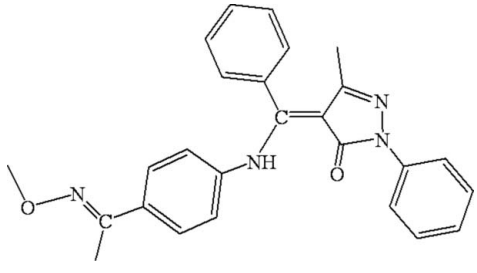
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.077; wR factor = 0.246; data-to-parameter ratio = 13.0.

In the title compound, $C_{26}H_{24}N_4O_2$, the dihedral angles between the central pyrazole ring and the other three benzene rings are 40.02 (3), 77.51 (5) and 55.72 (3)°. A strong intramolecular N—H···O hydrogen bond forms a six-membered ring with an S(6) motif. In the crystal structure, a weak intermolecular C—H···N interaction with graph-set motif $R_2^2(8)$ and C—H···O hydrogen bonds link each molecule to three others, forming an infinite two-dimensional supramolecular structure.

Related literature

For background to 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone, see: Lahiri *et al.* (2003). For related structures, see: Bomfim *et al.* (2005); Wang *et al.* (2008). For bond-length data, see: Allen *et al.* (1987). For graph-set notation, see: Bernstein *et al.* (1995). For the synthesis, see: Rafiq *et al.* (2008); Zhao *et al.* (2009); Dong *et al.* (2008).



Experimental

Crystal data

$C_{26}H_{24}N_4O_2$
M_r = 424.49
Triclinic, $P\overline{1}$
a = 7.3550 (6) Å
b = 11.1609 (13) Å
c = 14.9700 (12) Å
α = 68.536 (1)°
β = 76.654 (2)°
γ = 76.182 (2)°
V = 1096.46 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.50 × 0.49 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.992
5654 measured reflections
3781 independent reflections
1861 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.246
S = 1.03
3781 reflections
290 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1	0.86	1.95	2.683 (4)	142
C26—H26*C*···N4^{i}	0.96	2.72	3.643 (9)	163
C9—H9···O1^{ii}	0.93	2.67	3.398 (6)	135

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2280).

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Zhao, L., Dong, W.-K., Wu, J.-C., Sun, Y.-X. & Xu, L. (2009). *Acta Cryst.* E**65**, o2462.

supporting information

Acta Cryst. (2009). E**65**, o3122–o3123 [doi:10.1107/S1600536809048326]

4-({4-[1-(Methoxyimino)ethyl]anilino}(phenyl)methylene)-3-methyl-2-phenyl-1*H*-pyrazol-5(4*H*)-one

Jian Yao, Su-Xia Gao, Wen-Kui Dong, Jun-Feng Tong and Shang-Sheng Gong

S1. Comment

1-Phenyl-3-methyl-4-benzoyl-5-pyrazolone (PMBP) is an efficient extractant of metal ions, and has the potential to form different types of compounds (Lahiri *et al.*, 2003). Some structures of oxime compounds, similar to the title compound (Fig. 1), formed by Schiff base reactions have been reported (Bomfim *et al.*, 2005; Wang *et al.*, 2008).

The title compound is a potential tridentate mono-oxime ligand. The bond lengths and angles in the molecule are within normal ranges (Allen *et al.*, 1987). In the molecule, the dihedral angles between the central pyrazole ring and the other three benzene rings (C5—C10), (C12—C17) and (C18—C23) are 40.02 (3)°, 77.51 (5)° and 55.72 (3)°, respectively.

In the crystal, a strong intramolecular N3—H3···O1 hydrogen bond forms a six-membered ring, producing a S(6) ring motif (Table 1, Fig. 1). A weak intermolecular C26—H26C···N4 interacation with the graph-set motif of $R_2^2(8)$ (Bernstein *et al.*, 1995) and C9—H9···O1 hydrogen bonds, link each molecule to three others, forming an infinite two-dimensional supramolecular structure along the diagonal of the unit cell (Table 1, Fig. 2).

S2. Experimental

1-(4-Aminophenyl)ethanone *O*-methyl oxime (I) was prepared using 1-(4-aminophenyl)ethanone and methoxyamine (Rafiq *et al.*, 2008; Zhao *et al.*, 2009). The title compound was prepared according to a previously reported procedure (Dong *et al.*, 2008). To an ethanol solution (7 ml) of (I) (164.1 mg, 1.00 mmol) was added dropwise an ethanol solution (7 ml) of 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone (278.3 mg,1.00 mmol). The mixture was stirred at 333–338 K for 24 h. The solvent was removed under reduced pressure and the residue was recrystallized from ethanol to give the title compound. Yield, 68.9%. m. p. 454–456 K. Anal. Calcd. for $C_{26}H_{24}N_4O_2$: C, 73.56; H, 5.70; N, 13.20. Found: C,73.63; H,5.81; N,13.07.

Pale-yellow block-like single crystals suitable for X-ray diffraction studies were obtained by slow evaporation from a solution of dichloromethane at room temperature over a period of approximately one month.

S3. Refinement

H atoms were placed in calculated positions and non-H atoms were refined anisotropically. The remaining H atoms were treated as riding atoms with distances C—H=0.96 Å (CH_3), 0.93 Å (CH), 0.86 Å (NH), while U_{iso}(H)=1.20 U_{eq}(C) for methylidyne and 1.20 U_{eq}(N) for imino, 1.50 U_{eq}(C) for methyl. The H atom attached to N atom was located in a different density map and the atomic coordinates allowed to refine freely.

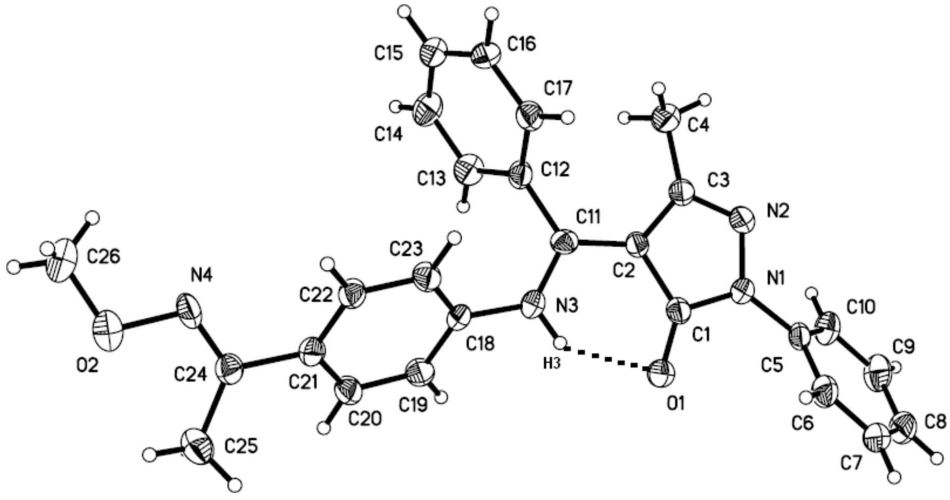

Figure 1

The molecular structure of the title compound with atom numbering scheme. Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level. Intramolecular hydrogen bond is shown as a dashed line.

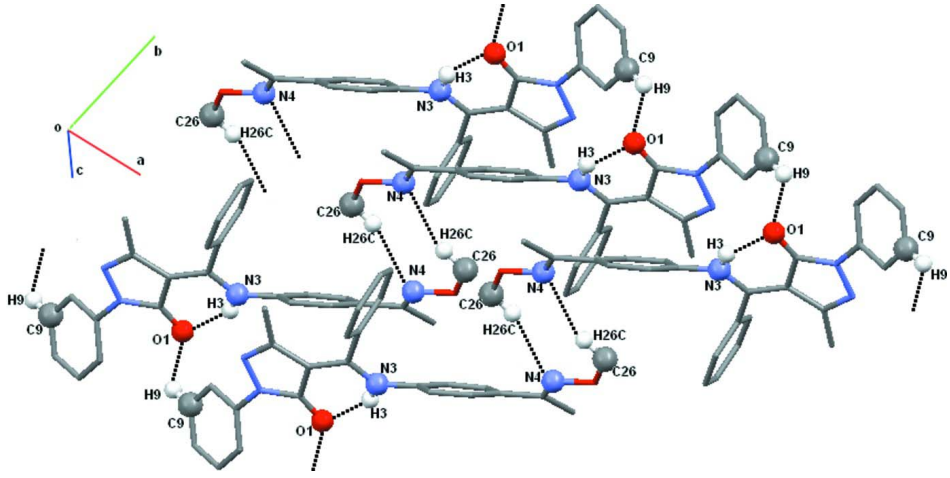

Figure 2

Part of two-dimensional supramolecular structure showing intermolecular hydrogen bonds interactions (dashed lines).

4-({4-[1-(Methoxyimino)ethyl]anilino}(phenyl)methylene)-3-methyl- 2-phenyl-1*H*-pyrazol-5(4*H*)-one

Crystal data

$C_{26}H_{24}N_4O_2$
$M_r = 424.49$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.3550\ (6)$ Å
$b = 11.1609\ (13)$ Å
$c = 14.9700\ (12)$ Å
$\alpha = 68.536\ (1)°$
$\beta = 76.654\ (2)°$
$\gamma = 76.182\ (2)°$
$V = 1096.46\ (18)$ Å^3
$Z = 2$
$F(000) = 448$
$D_x = 1.286$ Mg m^{-3}
Melting point = 454–456 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1018 reflections
$\theta = 2.9–22.3°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Block-like, yellow
0.50 × 0.49 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.992
5654 measured reflections
3781 independent reflections
1861 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −8→8
k = −13→13
l = −12→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.246
S = 1.03
3781 reflections
290 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
$w = 1/[\sigma^2(F_o^2) + (0.1078P)^2 + 0.3814P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.014 (5)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.5909 (5)	0.6071 (3)	0.1299 (3)	0.0443 (10)
N2	0.6863 (5)	0.5101 (4)	0.0891 (3)	0.0476 (10)
N3	0.1377 (5)	0.4355 (4)	0.2977 (3)	0.0498 (11)
H3	0.1605	0.5047	0.3025	0.060*
N4	−0.5909 (6)	0.1833 (5)	0.5239 (3)	0.0646 (13)
O1	0.3193 (4)	0.6395 (3)	0.2404 (2)	0.0505 (9)
O2	−0.7474 (6)	0.1375 (4)	0.5927 (3)	0.0817 (13)
C1	0.4246 (6)	0.5767 (4)	0.1894 (3)	0.0403 (11)
C2	0.4103 (6)	0.4552 (4)	0.1810 (3)	0.0384 (11)
C3	0.5784 (7)	0.4221 (4)	0.1177 (3)	0.0449 (12)
C4	0.6428 (7)	0.3052 (5)	0.0868 (4)	0.0602 (15)
H4A	0.7660	0.3094	0.0477	0.090*
H4B	0.5548	0.3022	0.0495	0.090*
H4C	0.6494	0.2281	0.1431	0.090*
C5	0.6829 (6)	0.7119 (4)	0.1179 (3)	0.0406 (11)

C6	0.5761 (7)	0.8342 (5)	0.1089 (4)	0.0532 (13)
H6	0.4470	0.8489	0.1069	0.064*
C7	0.6606 (8)	0.9334 (5)	0.1030 (4)	0.0600 (15)
H7	0.5880	1.0155	0.0983	0.072*
C8	0.8494 (8)	0.9141 (6)	0.1040 (4)	0.0665 (16)
H8	0.9060	0.9825	0.0998	0.080*
C9	0.9571 (7)	0.7925 (6)	0.1112 (4)	0.0654 (16)
H9	1.0869	0.7792	0.1111	0.078*
C10	0.8737 (7)	0.6911 (5)	0.1184 (4)	0.0533 (14)
H10	0.9461	0.6089	0.1237	0.064*
C11	0.2609 (6)	0.3874 (4)	0.2346 (3)	0.0401 (11)
C12	0.2423 (6)	0.2628 (4)	0.2279 (3)	0.0422 (12)
C13	0.2792 (7)	0.1492 (5)	0.3045 (4)	0.0532 (13)
H13	0.3171	0.1517	0.3588	0.064*
C14	0.2592 (7)	0.0319 (5)	0.2996 (4)	0.0610 (15)
H14	0.2862	−0.0447	0.3506	0.073*
C15	0.2010 (7)	0.0263 (5)	0.2221 (4)	0.0613 (15)
H15	0.1853	−0.0529	0.2202	0.074*
C16	0.1653 (7)	0.1410 (5)	0.1456 (4)	0.0598 (15)
H16	0.1251	0.1385	0.0919	0.072*
C17	0.1881 (6)	0.2558 (5)	0.1483 (4)	0.0500 (13)
H17	0.1668	0.3313	0.0955	0.060*
C18	−0.0273 (6)	0.3889 (4)	0.3586 (3)	0.0408 (11)
C19	−0.0580 (7)	0.3782 (5)	0.4543 (4)	0.0500 (13)
H19	0.0328	0.3967	0.4792	0.060*
C20	−0.2214 (6)	0.3404 (4)	0.5147 (4)	0.0488 (13)
H20	−0.2408	0.3350	0.5796	0.059*
C21	−0.3560 (6)	0.3105 (4)	0.4794 (3)	0.0426 (12)
C22	−0.3236 (6)	0.3217 (4)	0.3821 (3)	0.0448 (12)
H22	−0.4128	0.3012	0.3574	0.054*
C23	−0.1635 (6)	0.3622 (4)	0.3211 (4)	0.0467 (12)
H23	−0.1463	0.3717	0.2555	0.056*
C24	−0.5294 (6)	0.2642 (4)	0.5452 (4)	0.0460 (12)
C25	−0.6082 (7)	0.3043 (6)	0.6314 (4)	0.0646 (15)
H25A	−0.7391	0.2944	0.6510	0.097*
H25B	−0.5983	0.3941	0.6161	0.097*
H25C	−0.5387	0.2506	0.6833	0.097*
C26	−0.7905 (10)	0.0306 (7)	0.5759 (6)	0.111 (3)
H26A	−0.8927	0.0611	0.5388	0.166*
H26B	−0.8271	−0.0336	0.6370	0.166*
H26C	−0.6806	−0.0079	0.5404	0.166*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.051 (2)	0.042 (2)	0.044 (2)	−0.0190 (19)	0.000 (2)	−0.0154 (19)
N2	0.050 (2)	0.053 (2)	0.041 (3)	−0.017 (2)	0.002 (2)	−0.017 (2)
N3	0.051 (2)	0.051 (2)	0.054 (3)	−0.027 (2)	0.005 (2)	−0.021 (2)

N4	0.053 (3)	0.090 (3)	0.056 (3)	−0.038 (2)	0.022 (2)	−0.031 (3)
O1	0.048 (2)	0.055 (2)	0.054 (2)	−0.0193 (16)	0.0039 (17)	−0.0249 (18)
O2	0.076 (3)	0.091 (3)	0.077 (3)	−0.041 (2)	0.017 (2)	−0.028 (2)
C1	0.043 (3)	0.051 (3)	0.032 (3)	−0.019 (2)	−0.005 (2)	−0.014 (2)
C2	0.043 (3)	0.043 (3)	0.031 (3)	−0.017 (2)	−0.002 (2)	−0.011 (2)
C3	0.051 (3)	0.050 (3)	0.039 (3)	−0.018 (2)	−0.005 (2)	−0.015 (2)
C4	0.060 (3)	0.059 (3)	0.067 (4)	−0.020 (3)	0.004 (3)	−0.029 (3)
C5	0.042 (3)	0.044 (3)	0.035 (3)	−0.017 (2)	0.000 (2)	−0.008 (2)
C6	0.046 (3)	0.056 (3)	0.056 (3)	−0.019 (3)	0.001 (3)	−0.015 (3)
C7	0.064 (4)	0.056 (3)	0.061 (4)	−0.024 (3)	0.012 (3)	−0.025 (3)
C8	0.077 (4)	0.074 (4)	0.062 (4)	−0.045 (3)	0.002 (3)	−0.025 (3)
C9	0.047 (3)	0.078 (4)	0.071 (4)	−0.029 (3)	−0.007 (3)	−0.014 (3)
C10	0.045 (3)	0.050 (3)	0.060 (4)	−0.014 (2)	−0.011 (3)	−0.006 (3)
C11	0.048 (3)	0.041 (3)	0.035 (3)	−0.007 (2)	−0.012 (2)	−0.014 (2)
C12	0.043 (3)	0.047 (3)	0.039 (3)	−0.018 (2)	−0.004 (2)	−0.011 (2)
C13	0.057 (3)	0.053 (3)	0.048 (3)	−0.009 (2)	−0.019 (3)	−0.009 (3)
C14	0.072 (4)	0.038 (3)	0.064 (4)	−0.010 (3)	−0.017 (3)	−0.004 (3)
C15	0.064 (3)	0.057 (3)	0.067 (4)	−0.026 (3)	0.010 (3)	−0.028 (3)
C16	0.072 (4)	0.072 (4)	0.053 (4)	−0.036 (3)	0.001 (3)	−0.033 (3)
C17	0.057 (3)	0.057 (3)	0.039 (3)	−0.021 (2)	−0.005 (2)	−0.013 (2)
C18	0.048 (3)	0.037 (2)	0.041 (3)	−0.018 (2)	−0.002 (2)	−0.013 (2)
C19	0.054 (3)	0.062 (3)	0.045 (3)	−0.022 (3)	−0.007 (3)	−0.024 (3)
C20	0.054 (3)	0.058 (3)	0.038 (3)	−0.018 (2)	−0.002 (2)	−0.018 (2)
C21	0.049 (3)	0.036 (2)	0.039 (3)	−0.010 (2)	−0.006 (2)	−0.008 (2)
C22	0.049 (3)	0.051 (3)	0.039 (3)	−0.020 (2)	−0.007 (2)	−0.013 (2)
C23	0.055 (3)	0.056 (3)	0.033 (3)	−0.018 (2)	−0.008 (2)	−0.013 (2)
C24	0.051 (3)	0.045 (3)	0.039 (3)	−0.012 (2)	−0.005 (2)	−0.009 (2)
C25	0.065 (4)	0.077 (4)	0.047 (4)	−0.016 (3)	0.001 (3)	−0.018 (3)
C26	0.113 (6)	0.106 (5)	0.127 (7)	−0.073 (5)	0.034 (5)	−0.052 (5)

Geometric parameters (Å, º)

N1—C1	1.371 (5)	C12—C17	1.374 (6)
N1—N2	1.401 (5)	C12—C13	1.383 (6)
N1—C5	1.424 (5)	C13—C14	1.381 (7)
N2—C3	1.298 (5)	C13—H13	0.9300
N3—C11	1.321 (6)	C14—C15	1.352 (8)
N3—C18	1.421 (5)	C14—H14	0.9300
N3—H3	0.8600	C15—C16	1.387 (7)
N4—C24	1.263 (6)	C15—H15	0.9300
N4—O2	1.412 (5)	C16—C17	1.348 (6)
O1—C1	1.239 (5)	C16—H16	0.9300
O2—C26	1.423 (7)	C17—H17	0.9300
C1—C2	1.436 (6)	C18—C19	1.361 (6)
C2—C11	1.403 (6)	C18—C23	1.390 (6)
C2—C3	1.435 (6)	C19—C20	1.379 (6)
C3—C4	1.479 (7)	C19—H19	0.9300
C4—H4A	0.9600	C20—C21	1.378 (6)

C4—H4B	0.9600	C20—H20	0.9300
C4—H4C	0.9600	C21—C22	1.383 (6)
C5—C10	1.368 (6)	C21—C24	1.492 (6)
C5—C6	1.379 (6)	C22—C23	1.371 (6)
C6—C7	1.360 (6)	C22—H22	0.9300
C6—H6	0.9300	C23—H23	0.9300
C7—C8	1.356 (7)	C24—C25	1.467 (7)
C7—H7	0.9300	C25—H25A	0.9600
C8—C9	1.378 (8)	C25—H25B	0.9600
C8—H8	0.9300	C25—H25C	0.9600
C9—C10	1.371 (7)	C26—H26A	0.9600
C9—H9	0.9300	C26—H26B	0.9600
C10—H10	0.9300	C26—H26C	0.9600
C11—C12	1.470 (6)		

C1—N1—N2	112.5 (3)	C14—C13—C12	119.4 (5)
C1—N1—C5	127.5 (4)	C14—C13—H13	120.3
N2—N1—C5	119.3 (4)	C12—C13—H13	120.3
C3—N2—N1	106.5 (4)	C15—C14—C13	121.3 (5)
C11—N3—C18	129.1 (4)	C15—C14—H14	119.4
C11—N3—H3	115.4	C13—C14—H14	119.4
C18—N3—H3	115.4	C14—C15—C16	118.7 (5)
C24—N4—O2	111.5 (4)	C14—C15—H15	120.6
N4—O2—C26	109.4 (5)	C16—C15—H15	120.6
O1—C1—N1	126.3 (4)	C17—C16—C15	120.8 (5)
O1—C1—C2	129.8 (4)	C17—C16—H16	119.6
N1—C1—C2	103.8 (4)	C15—C16—H16	119.6
C11—C2—C3	131.8 (4)	C16—C17—C12	120.8 (5)
C11—C2—C1	121.9 (4)	C16—C17—H17	119.6
C3—C2—C1	106.1 (4)	C12—C17—H17	119.6
N2—C3—C2	111.0 (4)	C19—C18—C23	119.5 (4)
N2—C3—C4	119.2 (4)	C19—C18—N3	119.2 (4)
C2—C3—C4	129.8 (4)	C23—C18—N3	121.2 (4)
C3—C4—H4A	109.5	C18—C19—C20	121.1 (4)
C3—C4—H4B	109.5	C18—C19—H19	119.5
H4A—C4—H4B	109.5	C20—C19—H19	119.5
C3—C4—H4C	109.5	C21—C20—C19	120.3 (5)
H4A—C4—H4C	109.5	C21—C20—H20	119.9
H4B—C4—H4C	109.5	C19—C20—H20	119.9
C10—C5—C6	120.2 (4)	C20—C21—C22	118.2 (4)
C10—C5—N1	120.6 (4)	C20—C21—C24	120.6 (4)
C6—C5—N1	119.1 (4)	C22—C21—C24	121.1 (4)
C7—C6—C5	119.7 (5)	C23—C22—C21	121.8 (4)
C7—C6—H6	120.2	C23—C22—H22	119.1
C5—C6—H6	120.2	C21—C22—H22	119.1
C8—C7—C6	120.8 (5)	C22—C23—C18	119.1 (4)
C8—C7—H7	119.6	C22—C23—H23	120.4
C6—C7—H7	119.6	C18—C23—H23	120.4

C7—C8—C9	119.6 (5)	N4—C24—C25	124.5 (4)
C7—C8—H8	120.2	N4—C24—C21	114.6 (4)
C9—C8—H8	120.2	C25—C24—C21	120.7 (4)
C10—C9—C8	120.3 (5)	C24—C25—H25A	109.5
C10—C9—H9	119.9	C24—C25—H25B	109.5
C8—C9—H9	119.9	H25A—C25—H25B	109.5
C5—C10—C9	119.4 (5)	C24—C25—H25C	109.5
C5—C10—H10	120.3	H25A—C25—H25C	109.5
C9—C10—H10	120.3	H25B—C25—H25C	109.5
N3—C11—C2	117.6 (4)	O2—C26—H26A	109.5
N3—C11—C12	119.0 (4)	O2—C26—H26B	109.5
C2—C11—C12	123.3 (4)	H26A—C26—H26B	109.5
C17—C12—C13	119.0 (4)	O2—C26—H26C	109.5
C17—C12—C11	122.1 (4)	H26A—C26—H26C	109.5
C13—C12—C11	118.9 (4)	H26B—C26—H26C	109.5

C1—N1—N2—C3	3.3 (5)	C3—C2—C11—C12	−5.7 (7)
C5—N1—N2—C3	174.7 (4)	C1—C2—C11—C12	−179.8 (4)
C24—N4—O2—C26	−169.8 (5)	N3—C11—C12—C17	110.5 (5)
N2—N1—C1—O1	174.2 (4)	C2—C11—C12—C17	−73.3 (6)
C5—N1—C1—O1	3.7 (7)	N3—C11—C12—C13	−69.0 (6)
N2—N1—C1—C2	−3.2 (5)	C2—C11—C12—C13	107.2 (5)
C5—N1—C1—C2	−173.8 (4)	C17—C12—C13—C14	−0.6 (7)
O1—C1—C2—C11	0.1 (7)	C11—C12—C13—C14	179.0 (4)
N1—C1—C2—C11	177.4 (4)	C12—C13—C14—C15	−1.2 (8)
O1—C1—C2—C3	−175.3 (5)	C13—C14—C15—C16	1.4 (8)
N1—C1—C2—C3	1.9 (5)	C14—C15—C16—C17	0.0 (8)
N1—N2—C3—C2	−1.8 (5)	C15—C16—C17—C12	−1.8 (8)
N1—N2—C3—C4	−179.4 (4)	C13—C12—C17—C16	2.0 (7)
C11—C2—C3—N2	−174.9 (4)	C11—C12—C17—C16	−177.5 (4)
C1—C2—C3—N2	−0.1 (5)	C11—N3—C18—C19	132.8 (5)
C11—C2—C3—C4	2.3 (8)	C11—N3—C18—C23	−51.4 (7)
C1—C2—C3—C4	177.1 (5)	C23—C18—C19—C20	0.5 (7)
C1—N1—C5—C10	133.8 (5)	N3—C18—C19—C20	176.3 (4)
N2—N1—C5—C10	−36.2 (6)	C18—C19—C20—C21	1.1 (7)
C1—N1—C5—C6	−44.1 (7)	C19—C20—C21—C22	−1.1 (7)
N2—N1—C5—C6	145.9 (4)	C19—C20—C21—C24	177.4 (4)
C10—C5—C6—C7	−1.6 (8)	C20—C21—C22—C23	−0.5 (7)
N1—C5—C6—C7	176.2 (5)	C24—C21—C22—C23	−179.0 (4)
C5—C6—C7—C8	1.3 (8)	C21—C22—C23—C18	2.0 (7)
C6—C7—C8—C9	−0.1 (9)	C19—C18—C23—C22	−2.0 (7)
C7—C8—C9—C10	−0.7 (9)	N3—C18—C23—C22	−177.8 (4)
C6—C5—C10—C9	0.8 (8)	O2—N4—C24—C25	0.9 (7)
N1—C5—C10—C9	−177.0 (5)	O2—N4—C24—C21	176.2 (4)
C8—C9—C10—C5	0.4 (9)	C20—C21—C24—N4	−146.8 (5)
C18—N3—C11—C2	178.2 (4)	C22—C21—C24—N4	31.6 (7)
C18—N3—C11—C12	−5.4 (7)	C20—C21—C24—C25	28.7 (7)
C3—C2—C11—N3	170.6 (5)	C22—C21—C24—C25	−152.9 (5)

C1—C2—C11—N3	−3.6 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O1	0.86	1.95	2.683 (4)	142
C26—H26*C*···N4^{i}	0.96	2.72	3.643 (9)	163
C9—H9···O1^{ii}	0.93	2.67	3.398 (6)	135

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