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4-[(*Z*)-(*n*-Butylamino)(2-furyl)methylene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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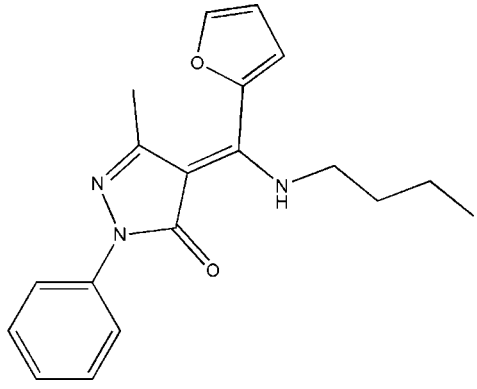
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.128; data-to-parameter ratio = 18.9.

In the title compound, $C_{19}H_{21}N_3O_2$, the pyrazolone ring and the attached C—NH group are essentially coplanar. The compound is in an enamine–keto form and its structure is stabilized by one strong intramolecular N—H···O hydrogen bond.

Related literature

For general background, see: Dong *et al.* (1983); Jensen (1959); Li *et al.* (1997, 2000); Nishihama *et al.* (2001).



Experimental

Crystal data

$C_{19}H_{21}N_3O_2$
M_r = 323.39
Orthorhombic, *Pbca*
a = 15.1910 (6) Å
b = 14.5509 (6) Å
c = 15.4249 (6) Å
V = 3409.6 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.26 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2005)
T_{min} = 0.884, T_{max} = 0.980
32853 measured reflections
4225 independent reflections
2326 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.128
S = 1.00
4225 reflections
223 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1	0.891 (19)	2.022 (19)	2.750 (2)	138.0 (16)
C2—H2···O1	0.93	2.30	2.939 (2)	125
C15—H15···O1^{i}	0.93	2.57	3.374 (2)	145

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: HG2259).

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supplementary materials

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4-[(*Z*)-(*n*-Butylamino)(2-furyl)methylene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

H.-Q. Zhang, J.-Z. Li, Y. Zhang, D. Zhang and Z.-H. Su

Comment

4-Acylpyrazolones are an interesting class of β-diketones, containing a pyrazole-bearing chelating arm. Thus, their metal complexes are used for the separation of elements with similar properties (Nishihama *et al.*, 2001). 1-phenyl-3-methyl-4-(2-furoyl)-5-pyrazolone(HPMFP), is a member of a family of 4-heterocyclic acylpyrazolones, first synthesized in 1983 (Dong *et al.*, 1983). In recent years, we have reported the Schiff bases derived from HPMFP and its complexes, which possess high antibacterial activation(Li *et al.*, 1997; Li *et al.*, 2000). Knowledge of the crystal structure of such 4-heterocyclic acylpyrazolones derivatives gives us not only information about nuclearity of the complex molecule, but is important in understanding the behaviour of this compounds in the vapour phase, and the mechanisms of sublimation and decomposition. Therefore, we have synthesized the title compound, (I), and report its crystal structure here.

The molecular structure of (I) is shown in Fig.1. Atoms O1, C7, C8 and C11 of the PMFP moiety and atom N3 of n-butylamine group are coplanar, the largest deviation being 0.0417 (11)Å for atom C11. The dihedral angle between this mean plane and pyrazole ring of PMFP is 3.35 (3)°. The bond length of C8—C11 (1.393 (2) Å) between the usual C—C and C=C bonds indicates the delocalization of the electrons because of the addition of a proton to N3 is more favorable than to O2. The atom O2 of 1-phenyl-3-methyl-4-(α-furoyl)-pyrazolone-5 moiety and the N3 atom of the n-butylamine group are on the same side of C8—C11 bond, which are available for coordination with metal cations. A strong intramolecular hydrogen bond N3—H3A···O1 (Table 1) is also indicative of the enamine-keto form. Another intramolecular hydrogen bond(C2—H2···O1) and an intermolelular hydrogen bond [C15—H15···O1^{i}; symmetry code(i): *x*, –y+1/2, *z* + 1/2] are also found, stabilizing the structure.

Experimental

HPMFP was synthesized according to the method proposed by Jensen (1959). A mixture of a 10 ml HPMFP (2 mmol, 0.5366 g) anhydrous ethanol solution, and a 0.2 ml n-butylamine (2 mmol, 0.1463 g) solution was refluxed for *ca*. 5 h, with addition of a few drops of glacial acetic acid as a catalyst. The ethanol was removed by evaporation and the resulting green precipitate formed was filtered off, washed with cold anhydrous ethanol and dried in air. Green block single crystals suitable for analysis were obtained by slow evaporation of a solution in anhydrous ethanol at room temperature for a few days.

Refinement

The H atom bonded to N3 was located in a difference map and refined freely. Other H atoms were placed in calculated positions, with C—H = 0.93Å for phenyl, 0.96Å for methyl and 0.97Å for methylene H atoms,and refined as riding, with U_{iso}(H)=1.2U_{eq} (C) for phenyl and methylene H, and 1.5$_{eq}$U(C) for methyl H.

Figures

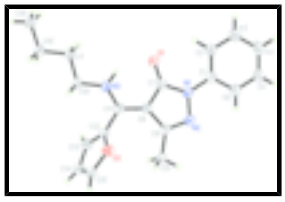


Fig. 1. The molecular structure of (I) (thermal ellipsoids are shown at 30% probability levels).

4-[(*Z*)-(*n*-Butylamino)(2-furyl)methylene]-3-methyl-1-phenyl- 1*H*-pyrazol-5(4*H*)-one

Crystal data

$C_{19}H_{21}N_3O_2$	F_{000} = 1376
M_r = 323.39	D_x = 1.260 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3467 reflections
a = 15.1910 (6) Å	θ = 2.6–21.8º
b = 14.5509 (6) Å	μ = 0.08 mm^{-1}
c = 15.4249 (6) Å	*T* = 295 (2) K
V = 3409.6 (2) Å^3	Block, green
Z = 8	0.26 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4225 independent reflections
Radiation source: fine-focus sealed tube	2326 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.060
T = 295(2) K	θ_{max} = 28.3º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 2005)	*h* = −20→20
T_{min} = 0.884, T_{max} = 0.980	*k* = −19→19
32853 measured reflections	*l* = −20→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.128	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.4662P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$

4225 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
223 parameters	$\Delta\rho_{min} = -0.19$ 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	0.06704 (8)	0.13250 (9)	0.41864 (8)	0.0560 (3)
N2	0.25340 (9)	0.11806 (10)	0.55284 (9)	0.0499 (4)
C8	0.10515 (10)	0.11395 (11)	0.57046 (11)	0.0431 (4)
O2	0.03838 (8)	0.17852 (8)	0.74500 (8)	0.0536 (3)
N1	0.21209 (9)	0.13090 (9)	0.47231 (9)	0.0475 (4)
N3	−0.04887 (9)	0.10498 (10)	0.55306 (11)	0.0493 (4)
C12	0.00469 (10)	0.10627 (11)	0.69884 (11)	0.0446 (4)
C17	−0.20167 (11)	0.12292 (12)	0.50373 (11)	0.0475 (4)
H17A	−0.1901	0.0783	0.4584	0.057*
H17B	−0.1898	0.1836	0.4805	0.057*
C11	0.02069 (10)	0.10832 (11)	0.60525 (11)	0.0429 (4)
C1	0.26506 (11)	0.14257 (11)	0.39802 (11)	0.0470 (4)
C18	−0.29717 (11)	0.11681 (13)	0.53097 (12)	0.0542 (5)
H18A	−0.3089	0.1644	0.5735	0.065*
H18B	−0.3070	0.0579	0.5588	0.065*
C9	0.19055 (10)	0.10845 (11)	0.61015 (11)	0.0446 (4)
C7	0.12121 (11)	0.12670 (11)	0.47977 (11)	0.0452 (4)
C6	0.35621 (12)	0.13823 (13)	0.40621 (13)	0.0599 (5)
H6	0.3816	0.1276	0.4602	0.072*
C16	−0.14156 (10)	0.10485 (12)	0.57981 (11)	0.0488 (4)
H16A	−0.1507	0.1518	0.6236	0.059*
H16B	−0.1560	0.0458	0.6053	0.059*
C2	0.22899 (13)	0.15950 (13)	0.31758 (12)	0.0593 (5)
H2	0.1682	0.1632	0.3112	0.071*
C15	0.01642 (12)	0.16258 (14)	0.82933 (12)	0.0600 (5)
H15	0.0306	0.2012	0.8753	0.072*
C13	−0.03612 (12)	0.04813 (14)	0.75253 (13)	0.0611 (5)
H13	−0.0646	−0.0061	0.7372	0.073*

C10	0.21496 (12)	0.08888 (14)	0.70213 (11)	0.0590 (5)
H10A	0.2771	0.0776	0.7058	0.088*
H10B	0.1834	0.0357	0.7220	0.088*
H10C	0.2000	0.1408	0.7376	0.088*
C19	−0.36167 (13)	0.12711 (15)	0.45664 (14)	0.0694 (6)
H19A	−0.3558	0.1872	0.4316	0.104*
H19B	−0.4206	0.1192	0.4778	0.104*
H19C	−0.3495	0.0814	0.4133	0.104*
C5	0.40876 (14)	0.14969 (15)	0.33424 (14)	0.0702 (6)
H5	0.4696	0.1466	0.3402	0.084*
C14	−0.02789 (14)	0.08449 (15)	0.83679 (13)	0.0688 (6)
H14	−0.0494	0.0587	0.8877	0.083*
C4	0.37335 (14)	0.16551 (14)	0.25431 (14)	0.0697 (6)
H4	0.4095	0.1724	0.2061	0.084*
C3	0.28342 (15)	0.17102 (15)	0.24630 (13)	0.0693 (6)
H3	0.2587	0.1827	0.1922	0.083*
H3A	−0.0361 (12)	0.1030 (12)	0.4967 (13)	0.064 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0414 (7)	0.0769 (9)	0.0497 (8)	0.0025 (6)	−0.0059 (6)	0.0046 (6)
N2	0.0399 (8)	0.0599 (9)	0.0499 (9)	0.0007 (7)	−0.0033 (7)	0.0006 (7)
C8	0.0357 (9)	0.0468 (10)	0.0469 (10)	0.0019 (7)	−0.0011 (7)	0.0011 (7)
O2	0.0520 (7)	0.0551 (7)	0.0536 (8)	−0.0024 (6)	−0.0030 (6)	−0.0066 (6)
N1	0.0381 (8)	0.0576 (9)	0.0466 (9)	0.0006 (6)	−0.0007 (6)	0.0015 (6)
N3	0.0367 (8)	0.0660 (10)	0.0453 (9)	0.0018 (7)	−0.0008 (7)	−0.0032 (7)
C12	0.0359 (9)	0.0491 (9)	0.0488 (10)	0.0003 (7)	−0.0040 (7)	−0.0028 (8)
C17	0.0380 (9)	0.0528 (10)	0.0516 (10)	0.0018 (8)	−0.0029 (8)	−0.0054 (8)
C11	0.0373 (9)	0.0415 (9)	0.0499 (10)	0.0027 (7)	−0.0038 (8)	−0.0014 (7)
C1	0.0445 (10)	0.0463 (10)	0.0502 (10)	−0.0018 (7)	0.0043 (8)	−0.0017 (8)
C18	0.0392 (10)	0.0598 (12)	0.0635 (12)	−0.0014 (8)	−0.0033 (8)	−0.0013 (9)
C9	0.0378 (9)	0.0471 (10)	0.0488 (10)	0.0012 (7)	−0.0017 (8)	−0.0003 (8)
C7	0.0379 (9)	0.0456 (9)	0.0521 (11)	0.0020 (7)	−0.0023 (8)	0.0002 (8)
C6	0.0462 (11)	0.0714 (13)	0.0620 (12)	−0.0004 (9)	0.0045 (9)	0.0099 (10)
C16	0.0357 (9)	0.0586 (11)	0.0523 (11)	0.0010 (8)	−0.0005 (8)	−0.0026 (8)
C2	0.0520 (11)	0.0724 (13)	0.0536 (12)	−0.0025 (9)	0.0034 (9)	−0.0050 (9)
C15	0.0549 (11)	0.0806 (14)	0.0445 (11)	0.0075 (10)	−0.0050 (9)	−0.0094 (10)
C13	0.0615 (12)	0.0687 (12)	0.0531 (12)	−0.0185 (10)	−0.0049 (10)	0.0037 (10)
C10	0.0428 (10)	0.0812 (14)	0.0530 (12)	0.0065 (9)	−0.0070 (8)	0.0047 (10)
C19	0.0436 (11)	0.0901 (15)	0.0745 (14)	0.0001 (10)	−0.0103 (10)	−0.0080 (11)
C5	0.0499 (12)	0.0837 (15)	0.0771 (16)	−0.0035 (10)	0.0138 (11)	0.0048 (11)
C14	0.0635 (13)	0.0914 (16)	0.0514 (13)	−0.0126 (12)	−0.0007 (10)	0.0080 (11)
C4	0.0657 (14)	0.0785 (14)	0.0648 (14)	−0.0132 (11)	0.0212 (11)	−0.0046 (11)
C3	0.0768 (15)	0.0825 (15)	0.0487 (12)	−0.0076 (12)	0.0050 (11)	−0.0034 (10)

Geometric parameters (Å, °)

O1—C7	1.2544 (19)	C9—C10	1.494 (2)

N2—C9	1.309 (2)	C7—O1	1.2544 (19)
N2—N1	1.4041 (19)	C6—C5	1.377 (3)
C8—C11	1.393 (2)	C6—H6	0.9300
C8—C7	1.432 (2)	C16—H16A	0.9700
C8—C9	1.437 (2)	C16—H16B	0.9700
O2—C15	1.363 (2)	C2—C3	1.386 (3)
O2—C12	1.3690 (19)	C2—H2	0.9300
N1—C7	1.387 (2)	C15—C14	1.326 (3)
N1—C1	1.410 (2)	C15—H15	0.9300
N3—C11	1.329 (2)	C13—C14	1.409 (3)
N3—C16	1.467 (2)	C13—H13	0.9300
N3—H3A	0.891 (19)	C10—H10A	0.9600
C12—C13	1.336 (2)	C10—H10B	0.9600
C12—C11	1.464 (2)	C10—H10C	0.9600
C17—C16	1.510 (2)	C19—H19A	0.9600
C17—C18	1.513 (2)	C19—H19B	0.9600
C17—H17A	0.9700	C19—H19C	0.9600
C17—H17B	0.9700	C5—C4	1.365 (3)
C1—C2	1.379 (2)	C5—H5	0.9300
C1—C6	1.392 (2)	C14—H14	0.9300
C18—C19	1.516 (3)	C4—C3	1.374 (3)
C18—H18A	0.9700	C4—H4	0.9300
C18—H18B	0.9700	C3—H3	0.9300
C9—N2—N1	106.61 (14)	C1—C6—H6	120.1
C11—C8—C7	122.74 (15)	N3—C16—C17	111.20 (14)
C11—C8—C9	131.62 (15)	N3—C16—H16A	109.4
C7—C8—C9	105.64 (14)	C17—C16—H16A	109.4
C15—O2—C12	105.91 (14)	N3—C16—H16B	109.4
C7—N1—N2	111.45 (13)	C17—C16—H16B	109.4
C7—N1—C1	129.85 (15)	H16A—C16—H16B	108.0
N2—N1—C1	118.67 (14)	C1—C2—C3	119.90 (19)
C11—N3—C16	126.34 (16)	C1—C2—H2	120.0
C11—N3—H3A	114.8 (12)	C3—C2—H2	120.0
C16—N3—H3A	118.9 (12)	C14—C15—O2	110.68 (17)
C13—C12—O2	109.71 (16)	C14—C15—H15	124.7
C13—C12—C11	134.50 (16)	O2—C15—H15	124.7
O2—C12—C11	115.79 (14)	C12—C13—C14	107.03 (17)
C16—C17—C18	110.72 (15)	C12—C13—H13	126.5
C16—C17—H17A	109.5	C14—C13—H13	126.5
C18—C17—H17A	109.5	C9—C10—H10A	109.5
C16—C17—H17B	109.5	C9—C10—H10B	109.5
C18—C17—H17B	109.5	H10A—C10—H10B	109.5
H17A—C17—H17B	108.1	C9—C10—H10C	109.5
N3—C11—C8	120.06 (16)	H10A—C10—H10C	109.5
N3—C11—C12	117.67 (15)	H10B—C10—H10C	109.5
C8—C11—C12	122.26 (14)	C18—C19—H19A	109.5
C2—C1—C6	119.02 (17)	C18—C19—H19B	109.5
C2—C1—N1	121.73 (16)	H19A—C19—H19B	109.5
C6—C1—N1	119.24 (16)	C18—C19—H19C	109.5

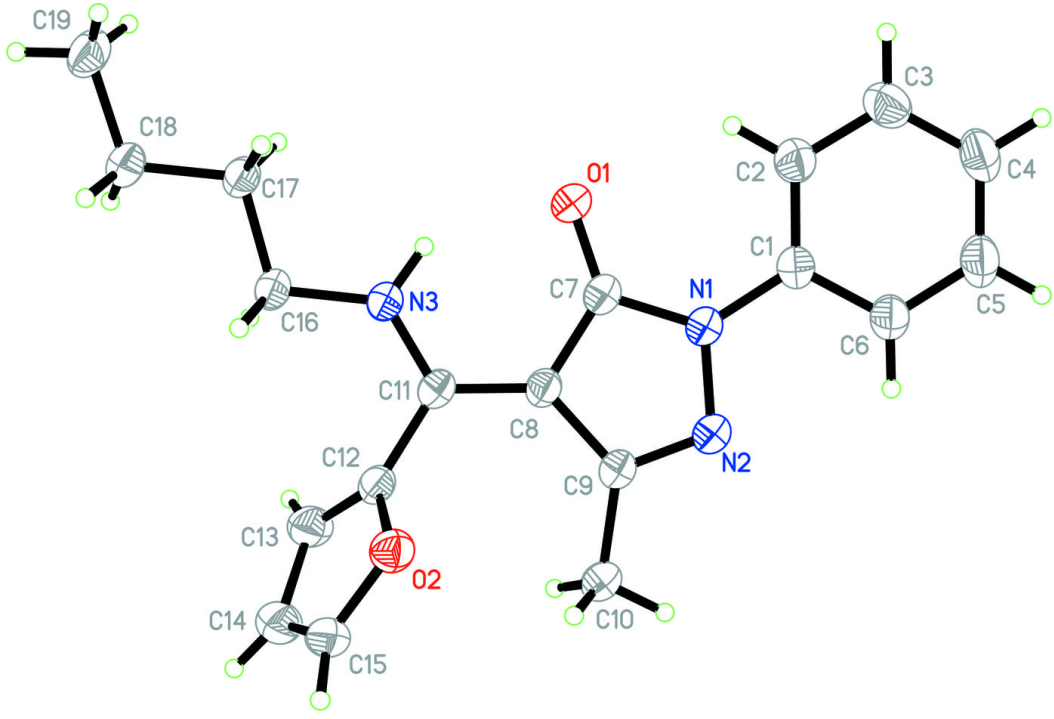
C17—C18—C19	113.83 (17)	H19A—C19—H19C	109.5
C17—C18—H18A	108.8	H19B—C19—H19C	109.5
C19—C18—H18A	108.8	C4—C5—C6	121.3 (2)
C17—C18—H18B	108.8	C4—C5—H5	119.3
C19—C18—H18B	108.8	C6—C5—H5	119.3
H18A—C18—H18B	107.7	C15—C14—C13	106.66 (18)
N2—C9—C8	111.41 (15)	C15—C14—H14	126.7
N2—C9—C10	118.75 (15)	C13—C14—H14	126.7
C8—C9—C10	129.75 (15)	C5—C4—C3	118.89 (19)
O1—C7—N1	126.00 (16)	C5—C4—H4	120.6
O1—C7—C8	129.15 (15)	C3—C4—H4	120.6
N1—C7—C8	104.86 (14)	C4—C3—C2	121.0 (2)
C5—C6—C1	119.87 (19)	C4—C3—H3	119.5
C5—C6—H6	120.1	C2—C3—H3	119.5
C9—N2—N1—C7	−1.61 (18)	N2—N1—C7—O1	−177.39 (15)
C9—N2—N1—C1	−179.57 (14)	C1—N1—C7—O1	0.3 (3)
C15—O2—C12—C13	−0.15 (19)	N2—N1—C7—O1	−177.39 (15)
C15—O2—C12—C11	−179.74 (14)	C1—N1—C7—O1	0.3 (3)
C16—N3—C11—C8	−175.87 (15)	N2—N1—C7—C8	2.20 (18)
C16—N3—C11—C12	3.9 (2)	C1—N1—C7—C8	179.87 (15)
C7—C8—C11—N3	7.2 (2)	C11—C8—C7—O1	−1.9 (3)
C9—C8—C11—N3	−172.23 (16)	C9—C8—C7—O1	177.67 (17)
C7—C8—C11—C12	−172.57 (15)	C11—C8—C7—O1	−1.9 (3)
C9—C8—C11—C12	8.0 (3)	C9—C8—C7—O1	177.67 (17)
C13—C12—C11—N3	57.2 (3)	C11—C8—C7—N1	178.57 (14)
O2—C12—C11—N3	−123.33 (16)	C9—C8—C7—N1	−1.90 (17)
C13—C12—C11—C8	−123.1 (2)	C2—C1—C6—C5	−0.8 (3)
O2—C12—C11—C8	56.4 (2)	N1—C1—C6—C5	−179.87 (17)
C7—N1—C1—C2	5.4 (3)	C11—N3—C16—C17	166.66 (16)
N2—N1—C1—C2	−177.10 (16)	C18—C17—C16—N3	176.50 (14)
C7—N1—C1—C6	−175.58 (16)	C6—C1—C2—C3	0.6 (3)
N2—N1—C1—C6	1.9 (2)	N1—C1—C2—C3	179.66 (17)
C16—C17—C18—C19	−175.67 (15)	C12—O2—C15—C14	0.5 (2)
N1—N2—C9—C8	0.30 (18)	O2—C12—C13—C14	−0.3 (2)
N1—N2—C9—C10	176.99 (15)	C11—C12—C13—C14	179.22 (18)
C11—C8—C9—N2	−179.51 (16)	C1—C6—C5—C4	0.1 (3)
C7—C8—C9—N2	1.03 (19)	O2—C15—C14—C13	−0.7 (2)
C11—C8—C9—C10	4.3 (3)	C12—C13—C14—C15	0.6 (2)
C7—C8—C9—C10	−175.19 (18)	C6—C5—C4—C3	0.7 (3)
O1—O1—C7—N1	0.00 (9)	C5—C4—C3—C2	−0.9 (3)
O1—O1—C7—C8	0.00 (5)	C1—C2—C3—C4	0.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O1	0.891 (19)	2.022 (19)	2.750 (2)	138.0 (16)
C2—H2···O1	0.93	2.30	2.939 (2)	125
C15—H15···O1^{i}	0.93	2.57	3.374 (2)	145

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2.

Fig. 1


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