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1-(2,4-Dichlorophenyl)-5-(2-nitroanilino)-1*H*-pyrazole-4-carbonitrile

Ju Liu,[a] Zhi-Qiang Cai,[b]* Yang Wang,[a] Chun-Yan Li[c] and Li-Feng Xu[a]

[a]College of Pharmacy, Liaoning University, Shenyang 110036, People's Republic of China, [b]Tianjin Key Laboratory of Molecular Design and Drug Discovery, State Key Laboratory of Drug Delivery Technology and Pharmacokinetics, Tianjin Institute of Pharmaceutical Research, Tianjin 300193, People's Republic of China, and [c]Shenlong Pharmaceutical Limited Company, Shenyang 110141, People's Republic of China
Correspondence e-mail: caizq@tjipr.com

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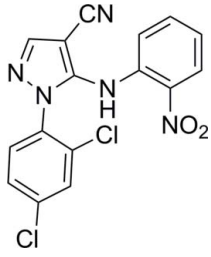
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.142; data-to-parameter ratio = 16.8.

In the title compound, $C_{16}H_9Cl_2N_5O_2$, the folded molecular conformation is characterized by a dihedral angle between the two benzene rings of 74.03 (5)°. An intramolecular N—H···O hydrogen bond is observed between the H atom of the amide group and a nitro-group O atom. Intermolecular C—H···O and N—H···N hydrogen bonds feature in the crystal packing.

Related literature

For general background to *N*-1-diaryl-1*H*-pyrazol-5-amine derivatives as synthetic intermediates in the preparation of medicinal compounds and the synthesis of the title compound, see: Markwalder *et al.* (2004); Mehdi *et al.* (2010). For the pharmacological activity of the 5-aminopyrazole nucleus, see: Nils *et al.* (2010); Aymn *et al.* (2005).



Experimental

Crystal data

$C_{16}H_9Cl_2N_5O_2$
M_r = 374.18
Orthorhombic, *Pbcn*
a = 13.878 (3) Å
b = 13.475 (3) Å
c = 17.421 (4) Å
V = 3257.7 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 293 K
0.20 × 0.18 × 0.12 mm

Data collection

Rigaku Saturn724 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.921, T_{max} = 0.951
31011 measured reflections
3888 independent reflections
2738 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.142
S = 1.04
3888 reflections
231 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O2^{i}	0.93	2.51	3.050 (3)	117
C5—H5···O1^{ii}	0.93	2.58	3.374 (3)	143
N4—H4···N3^{iii}	0.82 (3)	2.62 (3)	3.201 (3)	129 (2)
N4—H4···O1	0.82 (3)	2.02 (3)	2.608 (2)	128 (2)

Symmetry codes: (i) $x, -y+1, z+\frac{1}{2}$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, z$; (iii) $-x+1, -y+1, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2005); 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: KP2396).

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supplementary materials

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1-(2,4-Dichlorophenyl)-5-(2-nitroanilino)-1*H*-pyrazole-4-carbonitrile

Ju Liu, Zhi-Qiang Cai, Yang Wang, Chun-Yan Li and Li-Feng Xu

Comment

N-1-Diaryl-1*H*-pyrazol-5-amine derivatives possess therapeutic value. They are synthetic intermediates in the preparation of medicinal compounds (Markwalder *et al.*, 2004; Mehdi *et al.*, 2010). 5-Aminopyrazole nucleus is associated with several pharmacological activities such as selective adenosine A1 receptor antagonists (Nils *et al.*, 2010) and antimicrobial activity (Aymn *et al.*, 2005). In view of this biological importance a part of our ongoing studies of pyrazole derivatives includes the crystal structure determination of the title compound. The folded molecular conformation is characterised by the dihedral angle between the two benzene rings of 74.03 (5) ° (Fig. 1). Intramolecular N—H···O hydrogen bond between the hydrogen of the amide group and the nitro group O atom is observed. The crystal packing is stabilised by intermolecular C—H···O and N—H···N hydrogen bonds (Table 1).

Experimental

To a mixture of 5-amino-1-(2,4-dichlorophenyl)-1*H*-pyrazole-4-carbonitrile (3.0 g, 11.85 mmol) and *o*-nitrochloro-benzene (3.74 g, 23.74 mmol) in dimethyl sulfoxide (10 mL) lithium hydroxide monohydrate (0.74 g, 17.87 mmol) was added. The solution was heated at 343 K for 4.5 h. After cooling to 293 K, 50 mL of water was added to the reaction mixture. The resulting precipitate was collected by filtration, washed with ethanol to yield the title compound as a brown yellow solid (3.28 g, 73.95%). Crystals suitable for X-ray analysis were obtained from ethanol:acetone (1:1) solution by slow evaporation.

Refinement

All H atoms were geometrically positioned (C—H 0.93–0.98 Å) and treated as riding, with U_{iso}(H) = 1.2Ueq(C).

Computing details

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO* (Rigaku, 1998); data reduction: *CrystalClear* (Rigaku/MSC, 2005); 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* (Sheldrick, 2008).

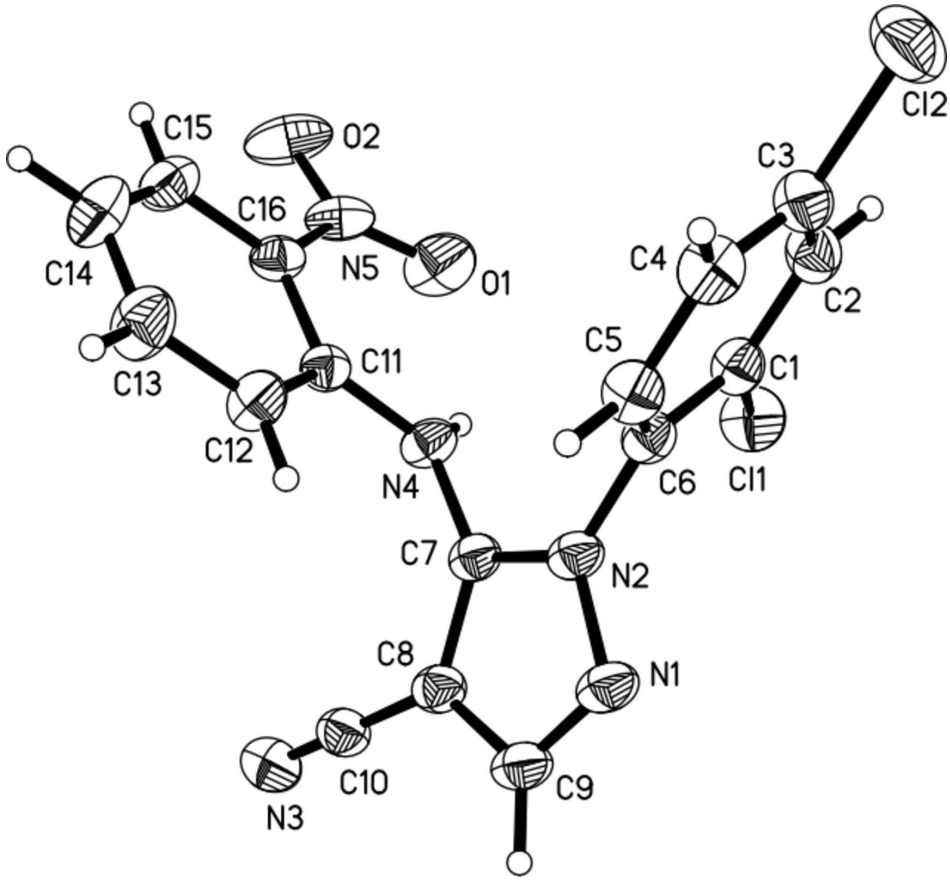

Figure 1

The structure of $C_{16}H_9Cl_2N_5O_2$ with all non-H atom-labelling scheme and ellipsoids drawn at the 50% probability level.

1-(2,4-Dichlorophenyl)-5-(2-nitroanilino)-1*H*-pyrazole-4-carbonitrile

Crystal data

$C_{16}H_9Cl_2N_5O_2$
M_r = 374.18
Orthorhombic, *Pbcn*
Hall symbol: -P2n2ab
a = 13.878 (3) Å
b = 13.475 (3) Å
c = 17.421 (4) Å
V = 3257.7 (11) Å^3
Z = 8
$F(000)$ = 1520
D_x = 1.526 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7017 reflections
θ = 2.4–28.0°
μ = 0.42 mm^{-1}
T = 293 K
Prism, yellow
0.20 × 0.18 × 0.12 mm

Data collection

Rigaku Saturn724 CCD diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.921, T_{max} = 0.951
31011 measured reflections
3888 independent reflections
2738 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 27.9°, θ_{min} = 2.3°
h = −17→17
k = −17→16
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.142$
$S = 1.04$
3888 reflections
231 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0759P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0166 (13)

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}
Cl1	0.15552 (5)	0.60779 (4)	0.46994 (4)	0.0673 (2)
Cl2	−0.14562 (5)	0.48959 (6)	0.30041 (5)	0.0881 (3)
O1	0.35014 (15)	0.63038 (12)	0.30863 (12)	0.0858 (6)
O2	0.41521 (15)	0.62525 (14)	0.19700 (10)	0.0914 (6)
N1	0.20172 (14)	0.33598 (13)	0.53423 (10)	0.0540 (5)
N2	0.20985 (13)	0.39203 (11)	0.46920 (9)	0.0467 (4)
N3	0.54146 (17)	0.37889 (14)	0.51865 (12)	0.0667 (5)
N4	0.32727 (13)	0.46781 (13)	0.38776 (9)	0.0477 (4)
N5	0.37959 (14)	0.58365 (14)	0.25298 (11)	0.0609 (5)
C1	0.09266 (15)	0.51444 (13)	0.42412 (12)	0.0481 (5)
C2	0.00946 (15)	0.53705 (15)	0.38503 (13)	0.0558 (6)
H2A	−0.0128	0.6021	0.3830	0.067*
C3	−0.04013 (16)	0.46247 (16)	0.34907 (13)	0.0556 (6)
C4	−0.00852 (16)	0.36558 (16)	0.35107 (13)	0.0575 (6)
H4A	−0.0428	0.3158	0.3261	0.069*
C5	0.07443 (15)	0.34366 (14)	0.39045 (12)	0.0521 (5)
H5	0.0962	0.2785	0.3925	0.063*
C6	0.12581 (15)	0.41746 (14)	0.42708 (11)	0.0446 (5)
C7	0.30239 (15)	0.41365 (13)	0.45245 (11)	0.0438 (5)
C8	0.35782 (15)	0.37153 (15)	0.50928 (12)	0.0476 (5)
C9	0.29092 (16)	0.32434 (15)	0.55794 (11)	0.0536 (5)
H9	0.3079	0.2890	0.6018	0.064*
C10	0.45966 (19)	0.37500 (15)	0.51458 (12)	0.0516 (5)
C11	0.34423 (13)	0.42402 (14)	0.31790 (11)	0.0407 (4)

C12	0.33508 (16)	0.32211 (15)	0.30894 (12)	0.0559 (6)
H12	0.3164	0.2838	0.3508	0.067*
C13	0.35285 (19)	0.27656 (18)	0.24013 (15)	0.0735 (7)
H13	0.3455	0.2082	0.2360	0.088*
C14	0.3815 (2)	0.3305 (2)	0.17670 (14)	0.0750 (7)
H14	0.3942	0.2988	0.1304	0.090*
C15	0.39084 (16)	0.4299 (2)	0.18286 (12)	0.0608 (6)
H15	0.4098	0.4670	0.1404	0.073*
C16	0.37242 (14)	0.47708 (15)	0.25204 (11)	0.0453 (5)
H4	0.3360 (18)	0.528 (2)	0.3926 (15)	0.077 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0852 (5)	0.0448 (3)	0.0719 (4)	−0.0062 (3)	−0.0050 (3)	−0.0152 (3)
Cl2	0.0593 (4)	0.1038 (6)	0.1013 (6)	0.0108 (3)	−0.0192 (4)	−0.0065 (4)
O1	0.1372 (18)	0.0455 (10)	0.0746 (13)	−0.0036 (9)	0.0066 (11)	0.0082 (9)
O2	0.1296 (16)	0.0868 (13)	0.0577 (11)	−0.0414 (11)	−0.0163 (11)	0.0338 (9)
N1	0.0691 (13)	0.0515 (10)	0.0413 (9)	−0.0029 (8)	0.0045 (8)	0.0103 (7)
N2	0.0577 (11)	0.0429 (9)	0.0394 (9)	−0.0014 (7)	0.0013 (7)	0.0059 (6)
N3	0.0697 (15)	0.0613 (12)	0.0691 (14)	0.0055 (10)	−0.0084 (10)	0.0057 (9)
N4	0.0668 (11)	0.0363 (9)	0.0401 (9)	−0.0063 (8)	0.0028 (8)	0.0020 (7)
N5	0.0745 (13)	0.0594 (12)	0.0488 (12)	−0.0166 (10)	−0.0150 (10)	0.0172 (9)
C1	0.0547 (13)	0.0399 (10)	0.0499 (12)	−0.0017 (9)	0.0047 (10)	−0.0043 (8)
C2	0.0593 (14)	0.0464 (12)	0.0617 (14)	0.0075 (10)	0.0046 (11)	−0.0014 (10)
C3	0.0485 (13)	0.0607 (14)	0.0576 (14)	0.0001 (10)	0.0000 (10)	0.0011 (10)
C4	0.0570 (14)	0.0552 (13)	0.0603 (14)	−0.0137 (11)	0.0003 (11)	−0.0063 (10)
C5	0.0603 (13)	0.0374 (10)	0.0586 (13)	−0.0049 (9)	0.0041 (11)	−0.0001 (9)
C6	0.0504 (12)	0.0412 (10)	0.0421 (11)	−0.0031 (8)	0.0036 (9)	0.0022 (8)
C7	0.0556 (13)	0.0383 (10)	0.0375 (10)	0.0000 (8)	0.0012 (9)	0.0007 (7)
C8	0.0616 (14)	0.0411 (10)	0.0400 (11)	0.0023 (9)	−0.0034 (9)	−0.0011 (8)
C9	0.0733 (16)	0.0472 (12)	0.0401 (11)	0.0021 (10)	−0.0014 (10)	0.0068 (8)
C10	0.0625 (16)	0.0450 (11)	0.0472 (12)	0.0066 (10)	−0.0054 (10)	0.0006 (8)
C11	0.0394 (10)	0.0420 (10)	0.0406 (10)	−0.0025 (8)	−0.0020 (8)	0.0023 (8)
C12	0.0729 (14)	0.0439 (11)	0.0511 (13)	−0.0054 (10)	0.0077 (11)	−0.0017 (9)
C13	0.097 (2)	0.0552 (15)	0.0684 (17)	−0.0038 (12)	0.0093 (14)	−0.0156 (12)
C14	0.0862 (18)	0.0849 (19)	0.0540 (15)	−0.0084 (15)	0.0118 (13)	−0.0203 (13)
C15	0.0567 (14)	0.0836 (17)	0.0422 (12)	−0.0094 (12)	0.0042 (10)	0.0003 (11)
C16	0.0428 (11)	0.0514 (11)	0.0419 (11)	−0.0071 (9)	−0.0053 (8)	0.0061 (8)

Geometric parameters (Å, º)

Cl1—C1	1.726 (2)	C4—C5	1.372 (3)
Cl2—C3	1.731 (2)	C4—H4A	0.9300
O1—N5	1.226 (3)	C5—C6	1.380 (3)
O2—N5	1.229 (2)	C5—H5	0.9300
N1—C9	1.314 (3)	C7—C8	1.376 (3)
N1—N2	1.366 (2)	C8—C9	1.409 (3)
N2—C7	1.349 (3)	C8—C10	1.417 (3)
N2—C6	1.420 (3)	C9—H9	0.9300

N3—C10	1.139 (3)	C11—C12	1.388 (3)
N4—C11	1.373 (2)	C11—C16	1.407 (3)
N4—C7	1.386 (2)	C12—C13	1.369 (3)
N4—H4	0.82 (3)	C12—H12	0.9300
N5—C16	1.440 (3)	C13—C14	1.381 (3)
C1—C2	1.375 (3)	C13—H13	0.9300
C1—C6	1.386 (3)	C14—C15	1.350 (3)
C2—C3	1.370 (3)	C14—H14	0.9300
C2—H2A	0.9300	C15—C16	1.386 (3)
C3—C4	1.378 (3)	C15—H15	0.9300

C9—N1—N2	104.40 (16)	N2—C7—C8	106.71 (18)
C7—N2—N1	112.17 (16)	N2—C7—N4	121.77 (18)
C7—N2—C6	128.19 (16)	C8—C7—N4	131.51 (19)
N1—N2—C6	119.60 (17)	C7—C8—C9	104.52 (19)
C11—N4—C7	122.49 (17)	C7—C8—C10	126.21 (19)
C11—N4—H4	119.2 (18)	C9—C8—C10	129.26 (19)
C7—N4—H4	118.1 (18)	N1—C9—C8	112.19 (18)
O1—N5—O2	121.8 (2)	N1—C9—H9	123.9
O1—N5—C16	119.88 (18)	C8—C9—H9	123.9
O2—N5—C16	118.3 (2)	N3—C10—C8	179.2 (2)
C2—C1—C6	120.40 (18)	N4—C11—C12	120.61 (17)
C2—C1—Cl1	119.47 (15)	N4—C11—C16	123.50 (17)
C6—C1—Cl1	120.13 (17)	C12—C11—C16	115.88 (18)
C3—C2—C1	119.08 (19)	C13—C12—C11	121.7 (2)
C3—C2—H2A	120.5	C13—C12—H12	119.1
C1—C2—H2A	120.5	C11—C12—H12	119.1
C2—C3—C4	121.6 (2)	C12—C13—C14	121.1 (2)
C2—C3—Cl2	119.61 (17)	C12—C13—H13	119.5
C4—C3—Cl2	118.80 (17)	C14—C13—H13	119.5
C5—C4—C3	118.9 (2)	C15—C14—C13	119.1 (2)
C5—C4—H4A	120.5	C15—C14—H14	120.4
C3—C4—H4A	120.5	C13—C14—H14	120.4
C4—C5—C6	120.63 (19)	C14—C15—C16	120.4 (2)
C4—C5—H5	119.7	C14—C15—H15	119.8
C6—C5—H5	119.7	C16—C15—H15	119.8
C5—C6—C1	119.4 (2)	C15—C16—C11	121.82 (19)
C5—C6—N2	119.31 (17)	C15—C16—N5	117.01 (19)
C1—C6—N2	121.28 (17)	C11—C16—N5	121.12 (18)

C9—N1—N2—C7	0.7 (2)	N4—C7—C8—C9	−178.5 (2)
C9—N1—N2—C6	178.77 (16)	N2—C7—C8—C10	179.56 (19)
C6—C1—C2—C3	0.0 (3)	N4—C7—C8—C10	0.3 (4)
Cl1—C1—C2—C3	−179.77 (17)	N2—N1—C9—C8	−0.3 (2)
C1—C2—C3—C4	−0.1 (3)	C7—C8—C9—N1	−0.3 (2)
C1—C2—C3—Cl2	179.38 (17)	C10—C8—C9—N1	−179.1 (2)
C2—C3—C4—C5	0.3 (3)	C7—C8—C10—N3	45 (19)
Cl2—C3—C4—C5	−179.17 (17)	C9—C8—C10—N3	−136 (19)
C3—C4—C5—C6	−0.4 (3)	C7—N4—C11—C12	1.3 (3)

C4—C5—C6—C1	0.3 (3)	C7—N4—C11—C16	−177.99 (18)
C4—C5—C6—N2	178.21 (19)	N4—C11—C12—C13	−179.1 (2)
C2—C1—C6—C5	−0.1 (3)	C16—C11—C12—C13	0.2 (3)
Cl1—C1—C6—C5	179.68 (16)	C11—C12—C13—C14	0.5 (4)
C2—C1—C6—N2	−177.94 (18)	C12—C13—C14—C15	−0.8 (4)
Cl1—C1—C6—N2	1.8 (3)	C13—C14—C15—C16	0.3 (4)
C7—N2—C6—C5	110.9 (2)	C14—C15—C16—C11	0.4 (3)
N1—N2—C6—C5	−66.7 (2)	C14—C15—C16—N5	−177.1 (2)
C7—N2—C6—C1	−71.2 (3)	N4—C11—C16—C15	178.6 (2)
N1—N2—C6—C1	111.1 (2)	C12—C11—C16—C15	−0.7 (3)
N1—N2—C7—C8	−0.9 (2)	N4—C11—C16—N5	−3.9 (3)
C6—N2—C7—C8	−178.74 (17)	C12—C11—C16—N5	176.78 (18)
N1—N2—C7—N4	178.39 (17)	O1—N5—C16—C15	168.9 (2)
C6—N2—C7—N4	0.6 (3)	O2—N5—C16—C15	−10.8 (3)
C11—N4—C7—N2	−88.3 (2)	O1—N5—C16—C11	−8.7 (3)
C11—N4—C7—C8	90.8 (3)	O2—N5—C16—C11	171.6 (2)
N2—C7—C8—C9	0.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2^{i}	0.93	2.51	3.050 (3)	117
C5—H5···O1^{ii}	0.93	2.58	3.374 (3)	143
N4—H4···N3^{iii}	0.82 (3)	2.62 (3)	3.201 (3)	129 (2)
N4—H4···O1	0.82 (3)	2.02 (3)	2.608 (2)	128 (2)

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