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2-(4-Aminophenyl)-3-[3,4-bis(pyridin-2-ylmethoxy)phenyl]acrylonitrile

Gang Liu,[a] Qingsong Liu,[a] Huihui Zhang[a] and Jianhua Yu[b]*

[a]Department of Chemistry, Anhui University, Hefei 230601, People's Republic of China, and [b]College of Chemistry and Chemical Engineering, Anhui University and Anhui Province Key Laboratory of Chemistry for Inorganic/Organic Hybrid Functionalized Materials, Hefei 230601, People's Republic of China. *Correspondence e-mail: iu_jh@163.com

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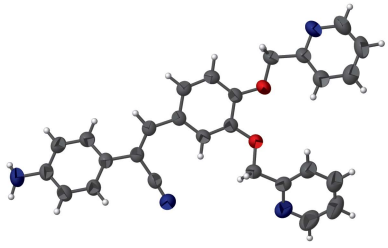
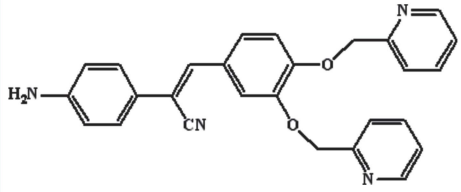
Structural data: full structural data are available from iucrdata.iucr.org

The crystal structure of $C_{27}H_{22}N_4O_2$ is characterized by N—H···N hydrogen bonds, which connect the molecules into zigzag chains running along the *b*-axis direction. The central ring subtends dihedral angles of 17.89 (6)° with the aminophenyl ring and of 8.75 (9) and 28.77 (7)° with the two pyridyl rings.

3D view



Chemical scheme



Structure description

A *D*–π–*A* structure formed from aniline and benzenenacrylonitrile has excellent luminescence properties (Zhang *et al.*, 2018). We report here the crystal structure of 2-(4-aminophenyl)-3-[3,4-bis(pyridin-2-ylmethoxy)phenyl]acrylonitrile (Fig. 1). The central ring subtends dihedral angles of 17.89 (6)° with the aminophenyl ring and 28.77 (7) and 8.75 (9)° with the N1- and N2-containing pyridyl rings.

In the crystal, the molecules are connected by N—H···N hydrogen bonds, forming zigzag chains running along the *b*-axis direction (Table 1, Fig. 2). Weak C—H···O interactions are also observed.

Synthesis and crystallization

To a solution of 3,4-dihydroxy-benzaldehyde (1.38 g, 10 mmol) in acetonitrile (50 ml) was added potassium carbonate (1.38 g, 10 mmol) and 2-bromomethyl-pyridine (3.44 g, 20 mmol). After the reaction mixture had been refluxed for 6 h, all the volatile components had completely evaporated and the residue was partitioned between dichloromethane and water. The organic phase was washed with water, then dried over calcium chloride, and concentrated *in vacuo*. The crude solid was recrystallized from petroleum ether–ethyl acetate (*v*/*v*= 1:1) solution to give a white solid. The white solid (0.5 g, 3.8 mmol) and (4-aminophenyl)acetonitrile (0.21 g, 3.8 mmol) were added to ethyl

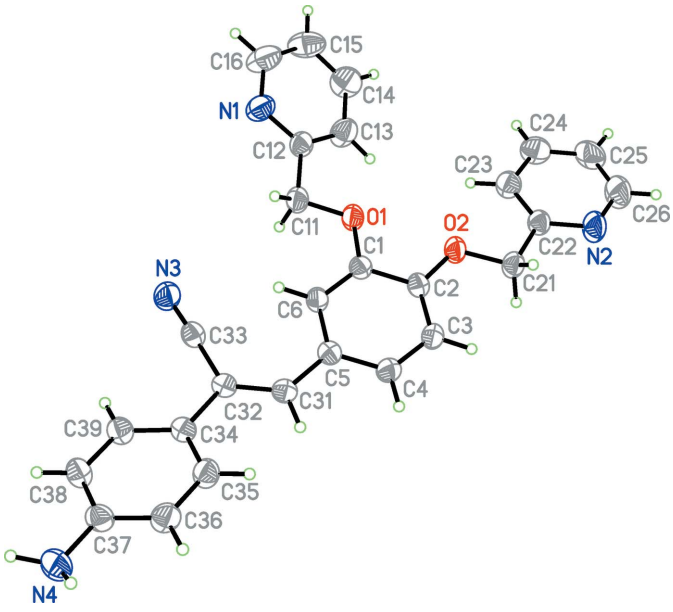


Figure 1
The structure of title molecule, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

alcohol. The mixture solution was refluxed for 8 h, and the resulting yellow residue was collected by filtration and then purified by silica gel column chromatography (petroleum ether: ethyl acetate = 2:1, *v*/*v*) to afford the title compound (0.29 g, 43%). Yellow single crystals were obtained by slow evaporation from acetonitrile solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

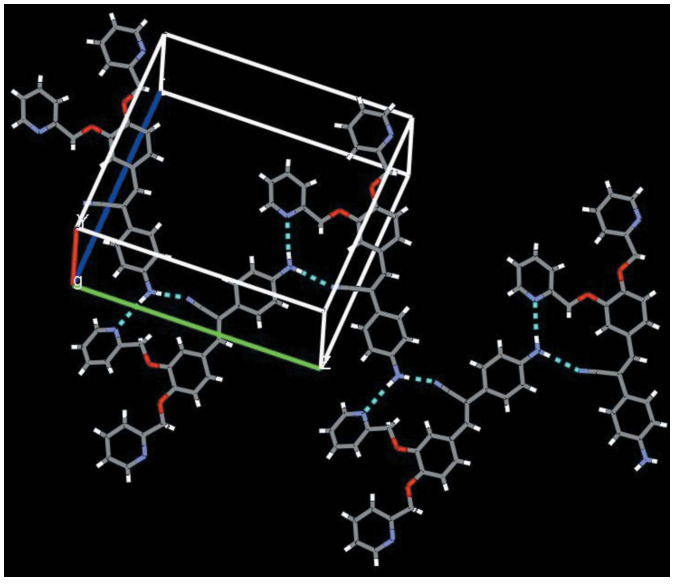


Figure 2
Hydrogen bonds in the crystal packing of the title compound. N—H···N hydrogen bonds are drawn with dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*B*···N1^{i}	0.95 (2)	2.35 (2)	3.293 (3)	172.8 (18)
N4—H4*A*···N3^{i}	0.89 (2)	2.52 (2)	3.390 (3)	165.5 (19)
C6—H6···N3	0.93	2.59	3.431 (2)	151
C26—H26···N2^{ii}	0.93	2.65	3.339 (3)	131

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{27}H_{22}N_4O_2$
M_r	434.49
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	8.0233 (15), 16.877 (3), 17.013 (3)
β (°)	101.021 (2)
V (Å^3)	2261.2 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.20 × 0.21 × 0.19
Data collection	
Diffractometer	Bruker SMART CCD area detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16528, 4222, 3016
R_{int}	0.025
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.041, 0.116, 1.07
No. of reflections	4222
No. of parameters	306
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.13, −0.12

Computer programs: *SMART* and *SAINT* (Bruker, 2000) and *SHELXS*, *SHELXL* and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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Funding information

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full crystallographic data

IUCrData (2018). **3**, x181329 [https://doi.org/10.1107/S2414314618013299]

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Crystal data

$C_{27}H_{22}N_4O_2$
M_r = 434.49
Monoclinic, $P2_1/c$
a = 8.0233 (15) Å
b = 16.877 (3) Å
c = 17.013 (3) Å
β = 101.021 (2)°
V = 2261.2 (7) Å^3
Z = 4
$F(000)$ = 912
D_x = 1.276 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4649 reflections
θ = 2.4–24.8°
μ = 0.08 mm^{-1}
T = 296 K
Block, yellow
0.21 × 0.20 × 0.19 mm

Data collection

Bruker SMART CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
16528 measured reflections
4222 independent reflections
3016 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.5°, θ_{min} = 1.7°
h = −9→9
k = −20→20
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.116
S = 1.07
4222 reflections
306 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.1757P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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. All H-atom positions were taken from a Fourier map. The H atoms were refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.49999 (13)	0.35393 (6)	0.60726 (6)	0.0624 (3)
O2	0.64442 (13)	0.43936 (6)	0.72240 (6)	0.0640 (3)
N1	0.5073 (2)	0.18016 (8)	0.49938 (9)	0.0793 (4)
N2	0.9308 (2)	0.45055 (9)	0.90889 (9)	0.0839 (5)
N3	0.08360 (19)	0.41255 (8)	0.36157 (8)	0.0721 (4)
N4	−0.3243 (2)	0.75632 (11)	0.17390 (10)	0.0807 (5)
H4B	−0.383 (3)	0.7318 (13)	0.1266 (14)	0.114 (8)*
H4A	−0.276 (3)	0.8029 (14)	0.1678 (13)	0.115 (8)*
C1	0.44974 (17)	0.43157 (8)	0.60235 (8)	0.0484 (3)
C2	0.53138 (17)	0.47891 (8)	0.66594 (8)	0.0502 (3)
C3	0.49239 (19)	0.55817 (9)	0.66679 (9)	0.0560 (4)
H3	0.545197	0.590099	0.708799	0.067*
C4	0.37400 (19)	0.59051 (9)	0.60481 (8)	0.0555 (4)
H4	0.349164	0.644269	0.605985	0.067*
C5	0.29154 (17)	0.54486 (8)	0.54107 (8)	0.0484 (3)
C6	0.33223 (17)	0.46381 (8)	0.54156 (8)	0.0501 (4)
H6	0.278638	0.431542	0.500006	0.060*
C11	0.4137 (2)	0.30045 (9)	0.55064 (9)	0.0644 (4)
H11A	0.415632	0.318992	0.496858	0.077*
H11B	0.296336	0.295468	0.556604	0.077*
C12	0.50242 (19)	0.22186 (9)	0.56499 (9)	0.0592 (4)
C13	0.5746 (3)	0.19608 (10)	0.64029 (11)	0.0829 (6)
H13	0.564635	0.226012	0.685047	0.099*
C14	0.6619 (3)	0.12559 (12)	0.64889 (13)	0.0966 (7)
H14	0.713511	0.107670	0.699380	0.116*
C15	0.6716 (3)	0.08249 (12)	0.58249 (15)	0.1040 (7)
H15	0.731751	0.035105	0.586148	0.125*
C16	0.5897 (3)	0.11113 (13)	0.50989 (14)	0.1060 (7)
H16	0.591819	0.080287	0.464790	0.127*
C21	0.7269 (2)	0.47956 (9)	0.79186 (9)	0.0609 (4)
H21A	0.643897	0.504435	0.818532	0.073*
H21B	0.801109	0.520361	0.777763	0.073*
C22	0.82829 (19)	0.41938 (9)	0.84601 (8)	0.0566 (4)
C23	0.8152 (2)	0.33945 (10)	0.83217 (10)	0.0700 (5)
H23	0.742020	0.319653	0.787431	0.084*
C24	0.9128 (3)	0.28889 (11)	0.88595 (12)	0.0837 (5)
H24	0.908267	0.234429	0.877454	0.100*
C25	1.0158 (3)	0.31990 (13)	0.95159 (12)	0.0909 (6)

H25	1.080498	0.287013	0.989461	0.109*
C26	1.0221 (3)	0.39952 (14)	0.96067 (12)	0.1004 (7)
H26	1.093962	0.420198	1.005379	0.120*
C31	0.17363 (17)	0.58435 (8)	0.47739 (8)	0.0517 (4)
H31	0.157669	0.637714	0.487389	0.062*
C32	0.08303 (17)	0.55909 (8)	0.40689 (8)	0.0482 (3)
C33	0.08525 (18)	0.47669 (9)	0.38329 (9)	0.0537 (4)
C34	−0.02236 (17)	0.61078 (8)	0.34649 (8)	0.0491 (3)
C35	−0.0004 (2)	0.69284 (9)	0.34669 (9)	0.0625 (4)
H35	0.082626	0.715972	0.385550	0.075*
C36	−0.0996 (2)	0.74018 (9)	0.29030 (10)	0.0697 (5)
H36	−0.083483	0.794767	0.292461	0.084*
C37	−0.2235 (2)	0.70805 (9)	0.23018 (9)	0.0601 (4)
C38	−0.24557 (19)	0.62686 (9)	0.22986 (9)	0.0609 (4)
H38	−0.328422	0.603694	0.190933	0.073*
C39	−0.14660 (19)	0.57983 (9)	0.28634 (9)	0.0565 (4)
H39	−0.163616	0.525305	0.284117	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0689 (7)	0.0464 (6)	0.0622 (6)	0.0023 (5)	−0.0119 (5)	−0.0040 (5)
O2	0.0697 (7)	0.0587 (6)	0.0540 (6)	0.0053 (5)	−0.0127 (5)	−0.0048 (5)
N1	0.0970 (11)	0.0676 (9)	0.0737 (9)	0.0127 (8)	0.0175 (8)	−0.0085 (8)
N2	0.0964 (11)	0.0797 (10)	0.0616 (9)	0.0045 (8)	−0.0206 (8)	−0.0027 (7)
N3	0.0823 (10)	0.0548 (8)	0.0724 (9)	0.0021 (7)	−0.0020 (7)	−0.0032 (7)
N4	0.0973 (12)	0.0680 (10)	0.0690 (10)	0.0147 (9)	−0.0039 (9)	0.0166 (8)
C1	0.0481 (8)	0.0462 (8)	0.0500 (8)	−0.0017 (6)	0.0071 (6)	0.0014 (6)
C2	0.0483 (8)	0.0537 (9)	0.0462 (8)	−0.0004 (7)	0.0033 (6)	0.0021 (6)
C3	0.0580 (9)	0.0552 (9)	0.0515 (8)	−0.0027 (7)	0.0020 (7)	−0.0073 (7)
C4	0.0599 (9)	0.0491 (8)	0.0564 (9)	0.0032 (7)	0.0086 (7)	−0.0023 (7)
C5	0.0466 (8)	0.0514 (8)	0.0475 (8)	−0.0001 (6)	0.0101 (6)	0.0023 (6)
C6	0.0502 (8)	0.0508 (8)	0.0469 (8)	−0.0024 (6)	0.0031 (7)	−0.0013 (6)
C11	0.0672 (10)	0.0542 (9)	0.0643 (10)	−0.0010 (8)	−0.0063 (8)	−0.0083 (7)
C12	0.0614 (10)	0.0494 (9)	0.0646 (10)	−0.0062 (7)	0.0063 (8)	−0.0049 (7)
C13	0.1142 (16)	0.0580 (11)	0.0711 (12)	0.0086 (10)	0.0041 (11)	0.0004 (8)
C14	0.1231 (18)	0.0708 (13)	0.0920 (15)	0.0152 (12)	0.0106 (13)	0.0205 (11)
C15	0.1274 (19)	0.0717 (13)	0.1205 (19)	0.0357 (13)	0.0428 (16)	0.0181 (13)
C16	0.144 (2)	0.0806 (14)	0.0999 (16)	0.0316 (14)	0.0405 (15)	−0.0108 (12)
C21	0.0706 (10)	0.0601 (9)	0.0474 (8)	0.0004 (8)	−0.0008 (7)	−0.0050 (7)
C22	0.0592 (9)	0.0615 (9)	0.0468 (8)	0.0004 (7)	0.0044 (7)	0.0006 (7)
C23	0.0766 (11)	0.0638 (11)	0.0662 (10)	0.0003 (8)	0.0051 (9)	0.0025 (8)
C24	0.0921 (14)	0.0663 (11)	0.0924 (14)	0.0089 (10)	0.0166 (11)	0.0132 (10)
C25	0.0896 (14)	0.0964 (16)	0.0806 (13)	0.0255 (12)	0.0008 (11)	0.0244 (12)
C26	0.1075 (17)	0.1034 (17)	0.0730 (13)	0.0144 (13)	−0.0259 (11)	0.0026 (12)
C31	0.0526 (9)	0.0480 (8)	0.0542 (9)	0.0032 (6)	0.0098 (7)	0.0021 (7)
C32	0.0468 (8)	0.0485 (8)	0.0499 (8)	0.0014 (6)	0.0111 (6)	0.0042 (6)
C33	0.0517 (9)	0.0554 (9)	0.0511 (8)	0.0011 (7)	0.0025 (7)	0.0063 (7)

C34	0.0495 (8)	0.0502 (8)	0.0482 (8)	0.0012 (6)	0.0112 (7)	0.0051 (6)
C35	0.0755 (11)	0.0532 (9)	0.0546 (9)	−0.0027 (8)	0.0021 (8)	0.0021 (7)
C36	0.0951 (13)	0.0473 (9)	0.0635 (10)	0.0031 (8)	0.0073 (9)	0.0056 (7)
C37	0.0675 (10)	0.0580 (9)	0.0541 (9)	0.0096 (8)	0.0097 (8)	0.0102 (7)
C38	0.0578 (9)	0.0624 (10)	0.0585 (9)	−0.0032 (8)	0.0006 (7)	0.0073 (7)
C39	0.0579 (9)	0.0493 (8)	0.0601 (9)	−0.0031 (7)	0.0059 (7)	0.0078 (7)

Geometric parameters (Å, º)

O1—C1	1.3688 (16)	C14—H14	0.9300
O1—C11	1.4023 (17)	C15—C16	1.371 (3)
O2—C2	1.3630 (16)	C15—H15	0.9300
O2—C21	1.4128 (17)	C16—H16	0.9300
N1—C12	1.3264 (19)	C21—C22	1.502 (2)
N1—C16	1.335 (2)	C21—H21A	0.9700
N2—C22	1.3271 (19)	C21—H21B	0.9700
N2—C26	1.345 (2)	C22—C23	1.370 (2)
N3—C33	1.1431 (18)	C23—C24	1.380 (2)
N4—C37	1.392 (2)	C23—H23	0.9300
N4—H4B	0.95 (2)	C24—C25	1.360 (3)
N4—H4A	0.89 (2)	C24—H24	0.9300
C1—C6	1.3718 (18)	C25—C26	1.352 (3)
C1—C2	1.4025 (19)	C25—H25	0.9300
C2—C3	1.374 (2)	C26—H26	0.9300
C3—C4	1.389 (2)	C31—C32	1.3473 (19)
C3—H3	0.9300	C31—H31	0.9300
C4—C5	1.3903 (19)	C32—C33	1.448 (2)
C4—H4	0.9300	C32—C34	1.4831 (18)
C5—C6	1.4060 (19)	C34—C39	1.3870 (19)
C5—C31	1.4564 (19)	C34—C35	1.396 (2)
C6—H6	0.9300	C35—C36	1.379 (2)
C11—C12	1.503 (2)	C35—H35	0.9300
C11—H11A	0.9700	C36—C37	1.393 (2)
C11—H11B	0.9700	C36—H36	0.9300
C12—C13	1.372 (2)	C37—C38	1.382 (2)
C13—C14	1.374 (3)	C38—C39	1.376 (2)
C13—H13	0.9300	C38—H38	0.9300
C14—C15	1.358 (3)	C39—H39	0.9300
C1—O1—C11	118.25 (11)	O2—C21—C22	107.48 (12)
C2—O2—C21	119.76 (11)	O2—C21—H21A	110.2
C12—N1—C16	116.36 (16)	C22—C21—H21A	110.2
C22—N2—C26	116.77 (17)	O2—C21—H21B	110.2
C37—N4—H4B	117.3 (13)	C22—C21—H21B	110.2
C37—N4—H4A	112.7 (15)	H21A—C21—H21B	108.5
H4B—N4—H4A	116.4 (19)	N2—C22—C23	122.97 (15)
O1—C1—C6	125.29 (12)	N2—C22—C21	113.95 (14)
O1—C1—C2	114.18 (12)	C23—C22—C21	123.08 (14)

C6—C1—C2	120.53 (13)	C22—C23—C24	118.67 (17)
O2—C2—C3	126.26 (13)	C22—C23—H23	120.7
O2—C2—C1	114.47 (12)	C24—C23—H23	120.7
C3—C2—C1	119.27 (13)	C25—C24—C23	119.00 (18)
C2—C3—C4	119.90 (13)	C25—C24—H24	120.5
C2—C3—H3	120.1	C23—C24—H24	120.5
C4—C3—H3	120.1	C26—C25—C24	118.67 (18)
C3—C4—C5	121.93 (14)	C26—C25—H25	120.7
C3—C4—H4	119.0	C24—C25—H25	120.7
C5—C4—H4	119.0	N2—C26—C25	123.89 (19)
C4—C5—C6	117.33 (13)	N2—C26—H26	118.1
C4—C5—C31	118.12 (13)	C25—C26—H26	118.1
C6—C5—C31	124.52 (13)	C32—C31—C5	132.90 (14)
C1—C6—C5	121.04 (13)	C32—C31—H31	113.6
C1—C6—H6	119.5	C5—C31—H31	113.6
C5—C6—H6	119.5	C31—C32—C33	121.16 (13)
O1—C11—C12	107.47 (12)	C31—C32—C34	124.73 (13)
O1—C11—H11A	110.2	C33—C32—C34	114.10 (12)
C12—C11—H11A	110.2	N3—C33—C32	177.17 (16)
O1—C11—H11B	110.2	C39—C34—C35	116.61 (13)
C12—C11—H11B	110.2	C39—C34—C32	121.59 (13)
H11A—C11—H11B	108.5	C35—C34—C32	121.80 (13)
N1—C12—C13	122.85 (15)	C36—C35—C34	121.17 (15)
N1—C12—C11	114.88 (14)	C36—C35—H35	119.4
C13—C12—C11	122.27 (15)	C34—C35—H35	119.4
C12—C13—C14	119.32 (18)	C35—C36—C37	121.43 (15)
C12—C13—H13	120.3	C35—C36—H36	119.3
C14—C13—H13	120.3	C37—C36—H36	119.3
C15—C14—C13	118.96 (19)	C38—C37—N4	121.36 (16)
C15—C14—H14	120.5	C38—C37—C36	117.52 (14)
C13—C14—H14	120.5	N4—C37—C36	121.09 (16)
C14—C15—C16	117.81 (19)	C39—C38—C37	120.87 (14)
C14—C15—H15	121.1	C39—C38—H38	119.6
C16—C15—H15	121.1	C37—C38—H38	119.6
N1—C16—C15	124.6 (2)	C38—C39—C34	122.39 (14)
N1—C16—H16	117.7	C38—C39—H39	118.8
C15—C16—H16	117.7	C34—C39—H39	118.8

C11—O1—C1—C6	−6.9 (2)	C26—N2—C22—C23	−1.0 (3)
C11—O1—C1—C2	173.89 (13)	C26—N2—C22—C21	178.49 (17)
C21—O2—C2—C3	3.6 (2)	O2—C21—C22—N2	171.32 (14)
C21—O2—C2—C1	−176.08 (13)	O2—C21—C22—C23	−9.2 (2)
O1—C1—C2—O2	−1.09 (18)	N2—C22—C23—C24	0.0 (3)
C6—C1—C2—O2	179.70 (12)	C21—C22—C23—C24	−179.40 (16)
O1—C1—C2—C3	179.23 (13)	C22—C23—C24—C25	1.4 (3)
C6—C1—C2—C3	0.0 (2)	C23—C24—C25—C26	−1.7 (3)
O2—C2—C3—C4	179.98 (14)	C22—N2—C26—C25	0.6 (3)
C1—C2—C3—C4	−0.4 (2)	C24—C25—C26—N2	0.8 (4)

C2—C3—C4—C5	0.3 (2)	C4—C5—C31—C32	175.56 (15)
C3—C4—C5—C6	0.1 (2)	C6—C5—C31—C32	−2.4 (3)
C3—C4—C5—C31	−177.94 (13)	C5—C31—C32—C33	3.3 (2)
O1—C1—C6—C5	−178.68 (13)	C5—C31—C32—C34	−175.23 (14)
C2—C1—C6—C5	0.4 (2)	C31—C32—C34—C39	−162.29 (14)
C4—C5—C6—C1	−0.5 (2)	C33—C32—C34—C39	19.11 (19)
C31—C5—C6—C1	177.43 (13)	C31—C32—C34—C35	18.4 (2)
C1—O1—C11—C12	175.28 (12)	C33—C32—C34—C35	−160.15 (14)
C16—N1—C12—C13	−1.1 (3)	C39—C34—C35—C36	0.9 (2)
C16—N1—C12—C11	178.01 (17)	C32—C34—C35—C36	−179.82 (14)
O1—C11—C12—N1	−144.35 (15)	C34—C35—C36—C37	−1.1 (3)
O1—C11—C12—C13	34.8 (2)	C35—C36—C37—C38	1.1 (2)
N1—C12—C13—C14	2.6 (3)	C35—C36—C37—N4	179.39 (16)
C11—C12—C13—C14	−176.45 (18)	N4—C37—C38—C39	−179.21 (15)
C12—C13—C14—C15	−1.2 (3)	C36—C37—C38—C39	−0.9 (2)
C13—C14—C15—C16	−1.4 (4)	C37—C38—C39—C34	0.8 (2)
C12—N1—C16—C15	−1.8 (3)	C35—C34—C39—C38	−0.7 (2)
C14—C15—C16—N1	3.1 (4)	C32—C34—C39—C38	179.97 (13)
C2—O2—C21—C22	174.24 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*B*···N1^{i}	0.95 (2)	2.35 (2)	3.293 (3)	172.8 (18)
N4—H4*A*···N3^{i}	0.89 (2)	2.52 (2)	3.390 (3)	165.5 (19)
C6—H6···N3	0.93	2.59	3.431 (2)	151
C26—H26···N2^{ii}	0.93	2.65	3.339 (3)	131

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