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3-[6-(4-Methoxyphenyl)-2-methylpyrimidin-4-yl]-2-(4-methylpiperazin-1-yl)quinoline

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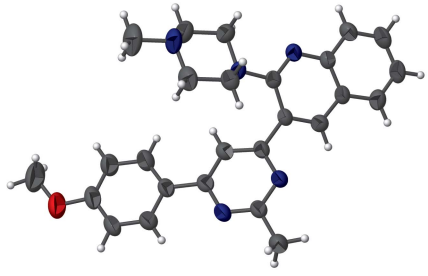
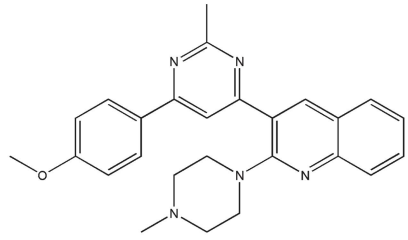
In the title compound, $C_{26}H_{27}N_5O$, the piperazine ring adopts a chair conformation. The pyrimidine ring makes a dihedral angle of 1.5 (1)° with the methoxyphenyl ring and 33.1 (1)° with the quinoline ring system. In the crystal, molecules are consolidated in the crystal packing by weak C—H···π interactions and π–π stacking interactions.

3D view



Chemical scheme



Structure description

Quinoline derivatives are important owing to their wide occurrence in natural products and in biologically active compounds (Markees *et al.*, 1970; Campbell *et al.*, 1988; Kalluraya & Sreenivasa, 1998). The pyrimidine nucleus also plays an important role in the medicinal chemistry and is reported to possess a broad spectrum of biological activities such as antimicrobial, anti-inflammatory, anthelmintic, anti HIV, antitubercular properties (Prasad *et al.*, 2008; Vaidya & Mathias 2005; Virsodia *et al.*, 2008). In a continuation of structural studies of these derivatives (Sharma *et al.*, 2017; Kaiser *et al.*, 2009; Prasath *et al.*, 2010) the title compound was investigated.

In the title molecule (Fig. 1), bond lengths are comparable with those in related structures (Prasath *et al.*, 2010, 2011; Sharma *et al.*, 2017). The piperazine ring adopts a chair conformation with best mirror plane passing through atoms N4 and N5 [asymmetry parameter C_s(N4) = 1.03] and the best twofold rotational axis bisecting the N4—C25 and N5—C23 bonds [asymmetry parameter C_2(N5—C25) = 1.27; Duax & Norton, 1975]. The quinoline ring system is essentially planar with a maximum deviation of 0.0583 (1) Å for atom C21. The methoxyphenyl ring makes a dihedral angle of 1.5 (1)° with the pyrimi-

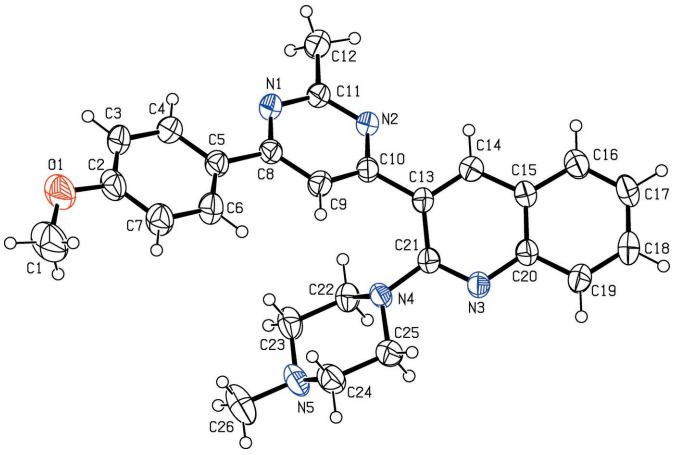


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.

dine ring while the dihedral angle between the pyrimidine ring and quinoline ring system is 33.1 (1)°.

In the crystal, π–π stacking interactions are observed between the pyrimidine ring and methoxyphenyl ring [centroid–centroid separation = 3.628 (1) Å, interplanar spacing = 3.588 Å and centroid shift = 0.54 Å; symmetry code: $1-x, -y, -z$]. Weak C—H$\cdots\pi$ interactions are also observed (Table 1). The above interaction combine to assemble the molecules into a three-dimensional network (Fig. 2).

Synthesis and crystallization

(2*E*)-3-[2-(4-Methylpiperazin-1-yl)quinolin-3-yl]-1-(4-methoxyphenyl)prop-2-en-1-one (1 g, 0.0026 mmol), acetamidine hydrochloride (243 mg, 0.0026 mmol) and NaOH (309 mg, 0.0077 mmol) were refluxed for 12 h in ethanol. The progress of reaction was monitored by thin layer chromatography. After the completion of reaction, the reaction mixture was poured into water and extracted with ethyl acetate. The organic layer was washed with water, dried and concentrated under vacuum using a rotary evaporator. The compound was purified by column chromatography by using 60–120 mesh silica gel and it was recrystallized from an ethyl acetate–petroleum ether mixture (7:3 *v*:*V*).

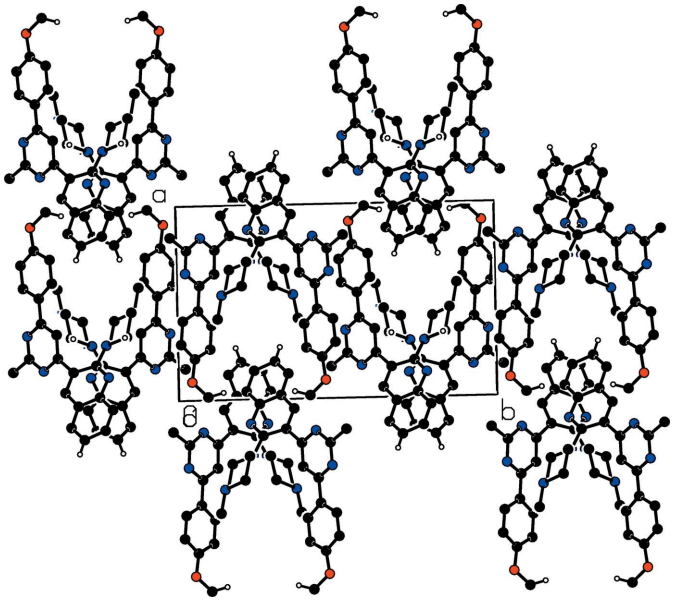


Figure 2
Part of the crystal structure. Only H atoms involved in the C—H$\cdots\pi$ interactions are shown.

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C15–C20, C8–C10/N2/C11/N2 and C2–C7 rings, respectively.

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
C1—H1*A*$\cdots$*Cg*1^{i}	0.96	3.10	3.867 (2)	138
C25—H25*A*$\cdots$*Cg*2^{ii}	0.97	2.96	3.706 (2)	134
C17—H17$\cdots$*Cg*3^{iii}	0.93	3.08	3.759 (2)	131

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{27}N_5O$
M_r	425.52
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	11.9896 (9), 18.4215 (13), 10.9903 (10)
β (°)	110.153 (9)
V (Å^3)	2278.8 (3)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Sapphire3
Absorption correction	Multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min}, T_{max}	0.776, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9015, 4461, 2193
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.064, 0.165, 1.00
No. of reflections	4461
No. of parameters	293
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.17

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2010), *SHELXS97* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015) and *PLATON* (Spek,2009).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x180030 [https://doi.org/10.1107/S2414314618000305]

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Crystal data

$C_{26}H_{27}N_5O$
M_r = 425.52
Monoclinic, $P2_1/c$
a = 11.9896 (9) Å
b = 18.4215 (13) Å
c = 10.9903 (10) Å
β = 110.153 (9)°
V = 2278.8 (3) Å^3
Z = 4
$F(000)$ = 904
D_x = 1.240 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1944 reflections
θ = 3.9–27.5°
μ = 0.08 mm^{-1}
T = 293 K
Block, white
0.30 × 0.20 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 6.1049 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2010)
T_{min} = 0.776, T_{max} = 1.000
9015 measured reflections
4461 independent reflections
2193 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 26.0°, θ_{min} = 3.6°
h = −14→10
k = −22→21
l = −13→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.165
S = 1.00
4461 reflections
293 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: SHELXL2016 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0065 (11)

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. All H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances of 0.93–0.97 Å; and with U_{iso}(H) = 1.2U_{eq}(C), except for the methyl groups where U_{iso}(H) = 1.5U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N3	0.1267 (2)	0.72304 (11)	0.7034 (2)	0.0458 (6)
N2	0.16616 (19)	0.92591 (10)	0.9859 (2)	0.0472 (6)
N4	0.29090 (19)	0.72812 (11)	0.8926 (2)	0.0441 (6)
N1	0.3478 (2)	0.97474 (11)	1.1300 (2)	0.0499 (6)
C15	−0.0198 (2)	0.81946 (14)	0.6399 (3)	0.0459 (7)
C13	0.1555 (2)	0.83286 (13)	0.8309 (3)	0.0425 (7)
C5	0.5412 (3)	0.93685 (14)	1.1382 (3)	0.0484 (7)
C11	0.2301 (2)	0.97043 (13)	1.0800 (3)	0.0477 (7)
C10	0.2289 (2)	0.88089 (13)	0.9372 (3)	0.0429 (7)
C8	0.4107 (2)	0.93117 (13)	1.0799 (3)	0.0446 (7)
C21	0.1884 (2)	0.76059 (13)	0.8064 (3)	0.0404 (6)
C14	0.0510 (3)	0.85949 (14)	0.7484 (3)	0.0498 (7)
H14	0.025655	0.905167	0.763886	0.060*
C20	0.0242 (2)	0.75182 (14)	0.6186 (3)	0.0438 (7)
O1	0.9073 (2)	0.95927 (12)	1.3186 (3)	0.0891 (8)
C9	0.3520 (3)	0.88340 (13)	0.9812 (3)	0.0476 (7)
H9	0.394618	0.853403	0.945043	0.057*
C4	0.5930 (3)	0.98535 (14)	1.2376 (3)	0.0596 (9)
H4	0.544180	1.014562	1.266880	0.072*
C22	0.2925 (2)	0.71665 (14)	1.0246 (3)	0.0502 (8)
H22A	0.240969	0.676301	1.025978	0.060*
H22B	0.262964	0.759659	1.054419	0.060*
C19	−0.0409 (3)	0.71172 (16)	0.5084 (3)	0.0582 (8)
H19	−0.011218	0.667858	0.490842	0.070*
N5	0.4637 (2)	0.63727 (13)	1.0676 (3)	0.0655 (7)
C25	0.3320 (3)	0.66256 (14)	0.8466 (3)	0.0590 (8)
H25A	0.329712	0.669435	0.758258	0.071*
H25B	0.280934	0.621952	0.847932	0.071*
C2	0.7879 (3)	0.94946 (17)	1.2531 (3)	0.0628 (9)
C16	−0.1296 (3)	0.84345 (16)	0.5544 (3)	0.0603 (8)
H16	−0.159657	0.887878	0.568982	0.072*
C18	−0.1473 (3)	0.73667 (17)	0.4274 (3)	0.0667 (9)
H18	−0.190151	0.709160	0.355491	0.080*
C3	0.7132 (3)	0.99188 (15)	1.2944 (3)	0.0655 (9)
H3	0.744853	1.025074	1.361203	0.079*
C7	0.7395 (3)	0.90055 (17)	1.1532 (3)	0.0651 (9)
H7	0.788756	0.871573	1.124200	0.078*

C17	−0.1932 (3)	0.80266 (17)	0.4500 (3)	0.0657 (9)
H17	−0.266549	0.818794	0.394481	0.079*
C6	0.6171 (3)	0.89510 (15)	1.0968 (3)	0.0608 (8)
H6	0.585050	0.862413	1.029274	0.073*
C24	0.4585 (3)	0.64721 (17)	0.9351 (3)	0.0660 (9)
H24A	0.487508	0.603801	0.905819	0.079*
H24B	0.509439	0.687366	0.931018	0.079*
C23	0.4171 (3)	0.70077 (16)	1.1133 (3)	0.0633 (9)
H23A	0.467516	0.742353	1.115965	0.076*
H23B	0.417257	0.692039	1.200358	0.076*
C12	0.1623 (3)	1.02123 (15)	1.1351 (3)	0.0710 (10)
H12A	0.178956	1.010145	1.224980	0.106*
H12B	0.078716	1.015809	1.088726	0.106*
H12C	0.185668	1.070310	1.126857	0.106*
C26	0.5859 (3)	0.6232 (2)	1.1512 (4)	0.0978 (13)
H26A	0.614351	0.580052	1.122464	0.147*
H26B	0.588714	0.616714	1.238847	0.147*
H26C	0.635150	0.663593	1.147165	0.147*
C1	0.9855 (3)	0.9098 (2)	1.2957 (4)	0.1088 (15)
H1A	0.963790	0.861485	1.311432	0.163*
H1B	1.064890	0.919991	1.352491	0.163*
H1C	0.981739	0.913863	1.207268	0.163*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N3	0.0408 (15)	0.0517 (13)	0.0405 (14)	0.0014 (11)	0.0086 (12)	−0.0049 (12)
N2	0.0432 (15)	0.0419 (12)	0.0480 (15)	−0.0009 (11)	0.0049 (13)	−0.0035 (11)
N4	0.0398 (15)	0.0507 (13)	0.0366 (13)	0.0098 (10)	0.0067 (12)	0.0003 (11)
N1	0.0438 (15)	0.0470 (13)	0.0503 (15)	−0.0057 (11)	0.0053 (13)	−0.0045 (12)
C15	0.0377 (17)	0.0517 (16)	0.0431 (17)	0.0011 (13)	0.0071 (15)	0.0009 (14)
C13	0.0352 (16)	0.0453 (15)	0.0420 (17)	−0.0023 (12)	0.0069 (14)	−0.0034 (13)
C5	0.0416 (18)	0.0468 (16)	0.0515 (19)	−0.0065 (13)	0.0091 (16)	0.0027 (15)
C11	0.0429 (18)	0.0408 (15)	0.0520 (19)	−0.0039 (13)	0.0070 (16)	−0.0004 (14)
C10	0.0395 (18)	0.0440 (15)	0.0401 (17)	−0.0028 (13)	0.0072 (15)	0.0010 (13)
C8	0.0463 (19)	0.0405 (15)	0.0411 (16)	−0.0022 (13)	0.0074 (15)	0.0050 (13)
C21	0.0367 (16)	0.0480 (15)	0.0363 (16)	−0.0003 (12)	0.0123 (14)	−0.0005 (13)
C14	0.0494 (19)	0.0477 (15)	0.0474 (18)	0.0026 (14)	0.0103 (16)	−0.0046 (15)
C20	0.0369 (17)	0.0514 (16)	0.0412 (17)	−0.0012 (13)	0.0111 (14)	−0.0017 (13)
O1	0.0451 (15)	0.0878 (16)	0.120 (2)	−0.0029 (12)	0.0106 (16)	0.0083 (16)
C9	0.0446 (19)	0.0483 (16)	0.0474 (18)	−0.0039 (13)	0.0128 (16)	−0.0034 (14)
C4	0.052 (2)	0.0491 (17)	0.068 (2)	−0.0036 (15)	0.0075 (18)	−0.0041 (16)
C22	0.049 (2)	0.0590 (17)	0.0398 (17)	−0.0035 (14)	0.0116 (16)	0.0015 (14)
C19	0.054 (2)	0.0626 (18)	0.048 (2)	−0.0024 (15)	0.0058 (17)	−0.0125 (16)
N5	0.0454 (17)	0.0750 (16)	0.0623 (18)	0.0086 (13)	0.0009 (15)	0.0191 (15)
C25	0.055 (2)	0.0588 (17)	0.058 (2)	0.0109 (15)	0.0121 (18)	−0.0059 (16)
C2	0.042 (2)	0.064 (2)	0.072 (2)	−0.0084 (16)	0.0058 (19)	0.0144 (18)
C16	0.048 (2)	0.0679 (19)	0.055 (2)	0.0085 (16)	0.0059 (18)	−0.0003 (16)

C18	0.055 (2)	0.081 (2)	0.048 (2)	−0.0054 (18)	−0.0043 (18)	−0.0075 (18)
C3	0.048 (2)	0.0594 (19)	0.070 (2)	−0.0101 (16)	−0.0034 (19)	−0.0057 (17)
C7	0.047 (2)	0.078 (2)	0.069 (2)	−0.0017 (17)	0.018 (2)	−0.0049 (19)
C17	0.049 (2)	0.078 (2)	0.053 (2)	0.0070 (17)	−0.0042 (17)	0.0073 (18)
C6	0.047 (2)	0.073 (2)	0.056 (2)	−0.0067 (16)	0.0108 (18)	−0.0074 (17)
C24	0.054 (2)	0.074 (2)	0.066 (2)	0.0158 (16)	0.0149 (19)	0.0020 (18)
C23	0.058 (2)	0.076 (2)	0.0449 (19)	0.0001 (17)	0.0038 (17)	0.0116 (16)
C12	0.053 (2)	0.0680 (19)	0.078 (3)	0.0034 (16)	0.0060 (19)	−0.0248 (18)
C26	0.063 (3)	0.125 (3)	0.085 (3)	0.019 (2)	−0.001 (2)	0.032 (2)
C1	0.052 (3)	0.127 (3)	0.146 (4)	0.009 (2)	0.031 (3)	0.011 (3)

Geometric parameters (Å, º)

N3—C21	1.315 (3)	C19—H19	0.9300
N3—C20	1.368 (3)	N5—C24	1.448 (4)
N2—C11	1.336 (3)	N5—C23	1.458 (4)
N2—C10	1.348 (3)	N5—C26	1.460 (4)
N4—C21	1.402 (3)	C25—C24	1.520 (4)
N4—C22	1.459 (3)	C25—H25A	0.9700
N4—C25	1.459 (3)	C25—H25B	0.9700
N1—C11	1.328 (3)	C2—C3	1.378 (4)
N1—C8	1.343 (3)	C2—C7	1.383 (4)
C15—C16	1.400 (4)	C16—C17	1.363 (4)
C15—C20	1.404 (3)	C16—H16	0.9300
C15—C14	1.410 (4)	C18—C17	1.392 (4)
C13—C14	1.360 (3)	C18—H18	0.9300
C13—C21	1.440 (3)	C3—H3	0.9300
C13—C10	1.488 (3)	C7—C6	1.387 (4)
C5—C6	1.382 (4)	C7—H7	0.9300
C5—C4	1.382 (4)	C17—H17	0.9300
C5—C8	1.477 (4)	C6—H6	0.9300
C11—C12	1.498 (4)	C24—H24A	0.9700
C10—C9	1.386 (3)	C24—H24B	0.9700
C8—C9	1.385 (3)	C23—H23A	0.9700
C14—H14	0.9300	C23—H23B	0.9700
C20—C19	1.404 (4)	C12—H12A	0.9600
O1—C2	1.376 (3)	C12—H12B	0.9600
O1—C1	1.391 (4)	C12—H12C	0.9600
C9—H9	0.9300	C26—H26A	0.9600
C4—C3	1.364 (4)	C26—H26B	0.9600
C4—H4	0.9300	C26—H26C	0.9600
C22—C23	1.504 (4)	C1—H1A	0.9600
C22—H22A	0.9700	C1—H1B	0.9600
C22—H22B	0.9700	C1—H1C	0.9600
C19—C18	1.360 (4)		
C21—N3—C20	119.3 (2)	N4—C25—H25B	110.0
C11—N2—C10	115.8 (2)	C24—C25—H25B	110.0

C21—N4—C22	116.2 (2)	H25A—C25—H25B	108.4
C21—N4—C25	116.2 (2)	O1—C2—C3	115.5 (3)
C22—N4—C25	109.5 (2)	O1—C2—C7	125.2 (3)
C11—N1—C8	117.5 (2)	C3—C2—C7	119.3 (3)
C16—C15—C20	119.3 (3)	C17—C16—C15	121.0 (3)
C16—C15—C14	123.8 (3)	C17—C16—H16	119.5
C20—C15—C14	117.0 (3)	C15—C16—H16	119.5
C14—C13—C21	117.2 (2)	C19—C18—C17	121.1 (3)
C14—C13—C10	118.0 (2)	C19—C18—H18	119.4
C21—C13—C10	124.8 (2)	C17—C18—H18	119.4
C6—C5—C4	116.9 (3)	C4—C3—C2	120.2 (3)
C6—C5—C8	122.5 (3)	C4—C3—H3	119.9
C4—C5—C8	120.6 (3)	C2—C3—H3	119.9
N1—C11—N2	127.0 (3)	C2—C7—C6	119.4 (3)
N1—C11—C12	116.3 (2)	C2—C7—H7	120.3
N2—C11—C12	116.7 (3)	C6—C7—H7	120.3
N2—C10—C9	120.9 (2)	C16—C17—C18	119.4 (3)
N2—C10—C13	114.7 (2)	C16—C17—H17	120.3
C9—C10—C13	124.4 (2)	C18—C17—H17	120.3
N1—C8—C9	119.7 (3)	C5—C6—C7	121.9 (3)
N1—C8—C5	116.1 (2)	C5—C6—H6	119.1
C9—C8—C5	124.2 (3)	C7—C6—H6	119.1
N3—C21—N4	117.4 (2)	N5—C24—C25	110.8 (2)
N3—C21—C13	122.6 (3)	N5—C24—H24A	109.5
N4—C21—C13	120.1 (2)	C25—C24—H24A	109.5
C13—C14—C15	121.5 (3)	N5—C24—H24B	109.5
C13—C14—H14	119.2	C25—C24—H24B	109.5
C15—C14—H14	119.2	H24A—C24—H24B	108.1
N3—C20—C19	119.1 (2)	N5—C23—C22	110.2 (2)
N3—C20—C15	122.1 (3)	N5—C23—H23A	109.6
C19—C20—C15	118.8 (3)	C22—C23—H23A	109.6
C2—O1—C1	117.6 (3)	N5—C23—H23B	109.6
C8—C9—C10	119.1 (3)	C22—C23—H23B	109.6
C8—C9—H9	120.4	H23A—C23—H23B	108.1
C10—C9—H9	120.4	C11—C12—H12A	109.5
C3—C4—C5	122.3 (3)	C11—C12—H12B	109.5
C3—C4—H4	118.8	H12A—C12—H12B	109.5
C5—C4—H4	118.8	C11—C12—H12C	109.5
N4—C22—C23	110.0 (2)	H12A—C12—H12C	109.5
N4—C22—H22A	109.7	H12B—C12—H12C	109.5
C23—C22—H22A	109.7	N5—C26—H26A	109.5
N4—C22—H22B	109.7	N5—C26—H26B	109.5
C23—C22—H22B	109.7	H26A—C26—H26B	109.5
H22A—C22—H22B	108.2	N5—C26—H26C	109.5
C18—C19—C20	120.3 (3)	H26A—C26—H26C	109.5
C18—C19—H19	119.8	H26B—C26—H26C	109.5
C20—C19—H19	119.8	O1—C1—H1A	109.5
C24—N5—C23	110.9 (2)	O1—C1—H1B	109.5

C24—N5—C26	109.9 (3)	H1A—C1—H1B	109.5
C23—N5—C26	110.3 (3)	O1—C1—H1C	109.5
N4—C25—C24	108.3 (2)	H1A—C1—H1C	109.5
N4—C25—H25A	110.0	H1B—C1—H1C	109.5
C24—C25—H25A	110.0		

C8—N1—C11—N2	1.6 (4)	C14—C15—C20—C19	−177.2 (2)
C8—N1—C11—C12	−178.2 (2)	N1—C8—C9—C10	−0.8 (4)
C10—N2—C11—N1	−0.1 (4)	C5—C8—C9—C10	177.6 (2)
C10—N2—C11—C12	179.7 (2)	N2—C10—C9—C8	2.3 (4)
C11—N2—C10—C9	−1.8 (4)	C13—C10—C9—C8	179.1 (2)
C11—N2—C10—C13	−178.9 (2)	C6—C5—C4—C3	−0.7 (4)
C14—C13—C10—N2	34.1 (3)	C8—C5—C4—C3	179.7 (3)
C21—C13—C10—N2	−147.7 (2)	C21—N4—C22—C23	−164.8 (2)
C14—C13—C10—C9	−142.9 (3)	C25—N4—C22—C23	61.0 (3)
C21—C13—C10—C9	35.3 (4)	N3—C20—C19—C18	175.4 (3)
C11—N1—C8—C9	−1.0 (4)	C15—C20—C19—C18	−2.9 (4)
C11—N1—C8—C5	−179.5 (2)	C21—N4—C25—C24	165.0 (2)
C6—C5—C8—N1	179.7 (2)	C22—N4—C25—C24	−60.8 (3)
C4—C5—C8—N1	−0.7 (4)	C1—O1—C2—C3	169.6 (3)
C6—C5—C8—C9	1.2 (4)	C1—O1—C2—C7	−9.3 (5)
C4—C5—C8—C9	−179.1 (3)	C20—C15—C16—C17	−1.0 (4)
C20—N3—C21—N4	178.1 (2)	C14—C15—C16—C17	179.0 (3)
C20—N3—C21—C13	−3.1 (4)	C20—C19—C18—C17	1.0 (5)
C22—N4—C21—N3	−119.1 (3)	C5—C4—C3—C2	0.1 (5)
C25—N4—C21—N3	12.0 (3)	O1—C2—C3—C4	−178.7 (3)
C22—N4—C21—C13	62.1 (3)	C7—C2—C3—C4	0.3 (5)
C25—N4—C21—C13	−166.7 (2)	O1—C2—C7—C6	178.8 (3)
C14—C13—C21—N3	5.6 (4)	C3—C2—C7—C6	−0.1 (5)
C10—C13—C21—N3	−172.6 (2)	C15—C16—C17—C18	−0.9 (5)
C14—C13—C21—N4	−175.7 (2)	C19—C18—C17—C16	0.9 (5)
C10—C13—C21—N4	6.1 (4)	C4—C5—C6—C7	0.9 (4)
C21—C13—C14—C15	−2.8 (4)	C8—C5—C6—C7	−179.5 (3)
C10—C13—C14—C15	175.5 (2)	C2—C7—C6—C5	−0.5 (5)
C16—C15—C14—C13	178.0 (3)	C23—N5—C24—C25	−57.3 (3)
C20—C15—C14—C13	−2.0 (4)	C26—N5—C24—C25	−179.5 (2)
C21—N3—C20—C19	179.7 (2)	N4—C25—C24—N5	59.3 (3)
C21—N3—C20—C15	−2.1 (4)	C24—N5—C23—C22	56.2 (3)
C16—C15—C20—N3	−175.4 (2)	C26—N5—C23—C22	178.2 (2)
C14—C15—C20—N3	4.6 (4)	N4—C22—C23—N5	−57.9 (3)
C16—C15—C20—C19	2.9 (4)		

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg3 are the centroids of the C15–C20, C8–C10/N2/C11/N2 and C2–C7 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···*Cg*1^{i}	0.96	3.10	3.867 (2)	138

C25—H25*A*···*Cg*2^{ii}	0.97	2.96	3.706 (2)	134
C17—H17···*Cg*3^{iii}	0.93	3.08	3.759 (2)	131

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