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1-(4-Methoxyphenyl)-3-[2-(4-methylpiperazin-1-yl)quinolin-3-yl]prop-2-en-1-one

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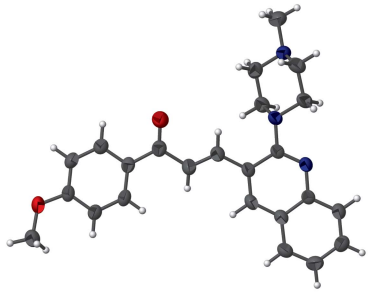
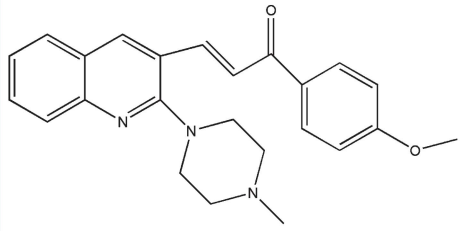
In the title molecule, $C_{24}H_{25}N_3O_2$, the piperazine ring adopts a chair conformation. The methoxyphenyl-substituted ring makes a dihedral angle of 6.79 (5)° with the quinoline ring system. In the crystal, molecules are consolidated in the crystal packing by a combination of weak C—H···N and C—H···O interactions. π–π stacking interactions also occur.

3D view



Chemical scheme



Structure description

Quinoline derivatives find importance owing to their wide occurrence in natural products and in biologically active compounds (Markees *et al.*, 1970; Campbell *et al.*, 1988; Kalluraya & Sreenivasa, 1998). Quinoline chalcone analogues have also attracted significant attention as a result of their bio-activity, *e.g.* anti-plasmodial, anti-microbial, anti-malarial and anti-cancer (Dimmock *et al.*, 1999; Wu *et al.*, 2006).

In the molecule of the title compound, (Fig. 1), bond lengths are in normal ranges and are comparable with related structures (Kaiser *et al.*, 2009; Prasath *et al.*, 2010, 2011). The piperazine ring adopts a chair conformation with best mirror plane passing through atoms C20 and C22 [asymmetry parameter ΔC_s(C20) = 2/3] and the best twofold rotational axis bisecting the C22—C23 and C20—C21 bonds [asymmetry parameter ΔC_2(C22—C23) = 0.43; Duax & Norton, 1975). The quinoline ring system is essentially planar with a maximum deviation of 0.0384 (1) Å for atom C17. The methoxyphenyl-substituted ring makes a dihedral angle of 6.79 (5)° with the quinoline ring system.

In the crystal, molecules are consolidated in the crystal packing by a combination of weak C—H···N and C—H···O interactions (Table 1, Fig. 2). The crystal structure also features π–π stacking interactions observed between the (C11–C13/C18/N1/C19) ring and the methoxyphenyl-substituted ring [centroid–centroid separation = 3.680 (1) Å, interplanar spacing = 3.350 Å and centroid shift = 1.52 Å] and the benzene ring (C13–

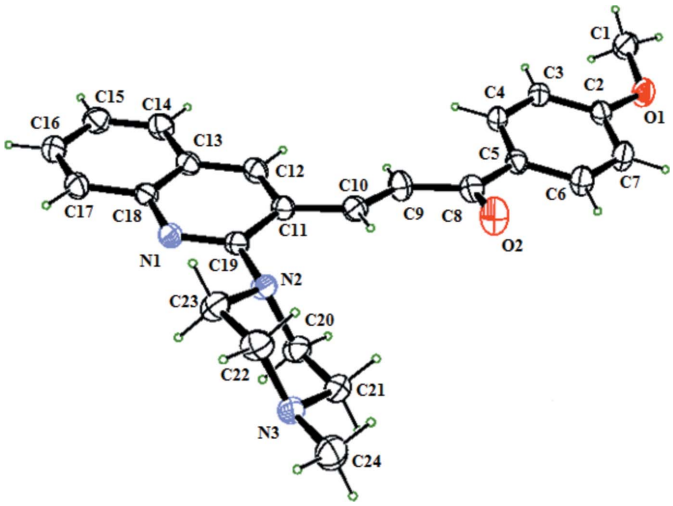


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.

C18) and the methoxyphenyl-substituted ring [centroid separation = 3.760 (1) Å, interplanar spacing = 3.625 Å and centroid shift = 1.00 Å].

Synthesis and crystallization

To a mixture of 9-acetylanthracene (0.01 mol) and 3-nitrobenzaldehyde (0.01 mol) in ethanol (50 ml), 15 ml of 10% sodium hydroxide solution was added and stirred at 273–278 K for 3 h. The precipitate formed was collected by filtration and purified by recrystallization from ethanol. Single crystals were grown from DMF by the slow evaporation method (m.p. 441–443 K).

Refinement

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

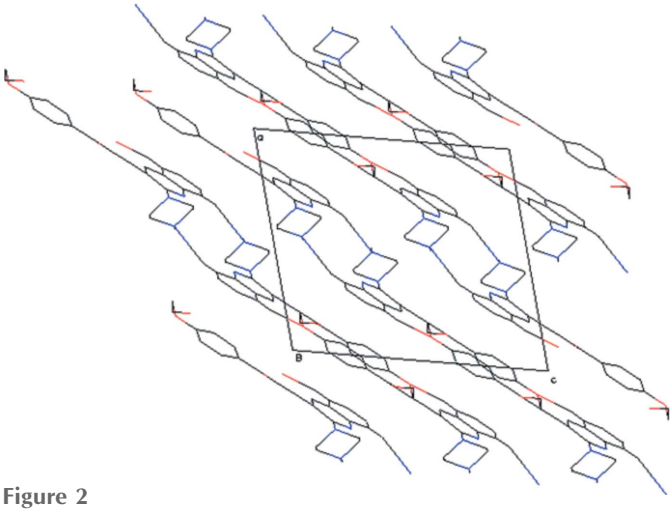


Figure 2
The packing arrangement of molecules viewed along the *b* axis.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O2^{i}	0.96	2.52	3.3096 (2)	139
C14—H14···O1^{i}	0.93	2.40	3.3112 (2)	165
C17—H17···N3^{ii}	0.93	2.54	3.4029 (3)	155

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{25}N_3O_2$
M_r	387.47
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	12.1054 (9), 12.5816 (8), 13.8151 (10)
β (°)	104.660 (8)
V (Å^3)	2035.6 (3)
Z	4
Radiation type	Mo $K\alpha$
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}	0.806, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7663, 3968, 2661
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.129, 1.03
No. of reflections	3968
No. of parameters	264
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.15, −0.16

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2010), *SHELXS97* (Sheldrick, 2008), *SHELXL2016/6* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek,2009).

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Funding information

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full crystallographic data

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Crystal data

$C_{24}H_{25}N_3O_2$
M_r = 387.47
Monoclinic, $P2_1/c$
a = 12.1054 (9) Å
b = 12.5816 (8) Å
c = 13.8151 (10) Å
β = 104.660 (8)°
V = 2035.6 (3) Å^3
Z = 4
$F(000)$ = 824
D_x = 1.264 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2213 reflections
θ = 3.8–28.1°
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} = 0.806, T_{max} = 1.000
7663 measured reflections
3968 independent reflections
2661 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.0°, θ_{min} = 3.7°
h = −10→14
k = −15→9
l = −17→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.129
S = 1.03
3968 reflections
264 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.2064P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 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. 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}
N1	0.66324 (12)	0.04111 (11)	0.17671 (11)	0.0403 (4)
C19	0.68787 (15)	−0.02479 (13)	0.11184 (13)	0.0370 (4)
N2	0.65342 (12)	−0.13104 (11)	0.11343 (10)	0.0401 (4)
C13	0.75452 (15)	0.18349 (13)	0.10684 (13)	0.0399 (4)
C18	0.69723 (14)	0.14485 (13)	0.17632 (13)	0.0377 (4)
C11	0.75333 (15)	0.00475 (13)	0.04249 (13)	0.0381 (4)
C5	0.94339 (15)	−0.12384 (14)	−0.21987 (13)	0.0396 (4)
O1	1.11216 (12)	−0.07992 (10)	−0.44155 (10)	0.0572 (4)
N3	0.52218 (13)	−0.31851 (11)	0.11631 (12)	0.0464 (4)
C10	0.79570 (15)	−0.07570 (14)	−0.01499 (14)	0.0434 (5)
H10	0.786172	−0.146122	0.001693	0.052*
O2	0.86919 (14)	−0.24023 (10)	−0.11961 (11)	0.0661 (4)
C4	0.99289 (16)	−0.02680 (14)	−0.22924 (13)	0.0430 (5)
H4	0.987250	0.027752	−0.185317	0.052*
C17	0.67233 (16)	0.21571 (14)	0.24651 (14)	0.0466 (5)
H17	0.636395	0.191100	0.294237	0.056*
C23	0.62185 (18)	−0.16514 (14)	0.20369 (14)	0.0511 (5)
H23A	0.550435	−0.131980	0.206621	0.061*
H23B	0.680250	−0.143472	0.262350	0.061*
C12	0.78272 (16)	0.10930 (14)	0.04139 (13)	0.0431 (5)
H12	0.822651	0.131995	−0.004154	0.052*
C16	0.70063 (17)	0.32018 (14)	0.24486 (15)	0.0519 (5)
H16	0.682082	0.366850	0.290523	0.062*
C7	1.00681 (18)	−0.18600 (14)	−0.36065 (15)	0.0527 (5)
H7	1.010137	−0.239544	−0.406238	0.063*
C8	0.88595 (16)	−0.14806 (15)	−0.14025 (14)	0.0448 (5)
C2	1.05822 (16)	−0.08888 (14)	−0.36738 (14)	0.0430 (5)
C14	0.78453 (17)	0.29115 (14)	0.10835 (15)	0.0495 (5)
H14	0.823418	0.316742	0.063107	0.059*
C9	0.84587 (17)	−0.05991 (15)	−0.08776 (14)	0.0492 (5)
H9	0.856454	0.009486	−0.106793	0.059*
C22	0.60924 (18)	−0.28353 (15)	0.20268 (15)	0.0539 (5)
H22A	0.681542	−0.316235	0.201805	0.065*
H22B	0.589184	−0.306217	0.263146	0.065*
C21	0.55201 (18)	−0.28423 (14)	0.02596 (15)	0.0519 (5)
H21A	0.492652	−0.305925	−0.032006	0.062*
H21B	0.622716	−0.318125	0.022020	0.062*
C20	0.56593 (17)	−0.16596 (14)	0.02492 (14)	0.0476 (5)
H20A	0.587873	−0.144925	−0.035153	0.057*
H20B	0.493794	−0.131959	0.024143	0.057*
C3	1.05028 (16)	−0.00856 (14)	−0.30169 (14)	0.0440 (5)
H3	1.083415	0.057313	−0.306325	0.053*
C6	0.95132 (18)	−0.20370 (15)	−0.28761 (15)	0.0514 (5)
H6	0.918482	−0.269727	−0.283015	0.062*
C15	0.75707 (17)	0.35818 (15)	0.17556 (16)	0.0530 (5)

H15	0.775998	0.429808	0.175411	0.064*
C24	0.5069 (2)	−0.43288 (15)	0.11815 (19)	0.0685 (7)
H24A	0.447997	−0.454164	0.060792	0.103*
H24B	0.485380	−0.452479	0.178032	0.103*
H24C	0.577077	−0.467626	0.116856	0.103*
C1	1.17742 (19)	0.01359 (15)	−0.44464 (16)	0.0601 (6)
H1A	1.128690	0.074776	−0.451322	0.090*
H1B	1.210611	0.009934	−0.500733	0.090*
H1C	1.236977	0.019112	−0.383948	0.090*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0412 (9)	0.0439 (8)	0.0390 (9)	−0.0042 (7)	0.0159 (7)	−0.0015 (7)
C19	0.0351 (10)	0.0426 (10)	0.0330 (10)	−0.0027 (8)	0.0082 (8)	0.0027 (8)
N2	0.0437 (9)	0.0430 (8)	0.0341 (9)	−0.0088 (7)	0.0109 (7)	−0.0005 (7)
C13	0.0382 (10)	0.0431 (10)	0.0401 (11)	−0.0010 (8)	0.0131 (8)	0.0041 (8)
C18	0.0336 (9)	0.0414 (10)	0.0389 (10)	−0.0012 (8)	0.0108 (8)	0.0001 (8)
C11	0.0387 (10)	0.0437 (10)	0.0329 (10)	−0.0014 (8)	0.0112 (8)	0.0020 (8)
C5	0.0386 (10)	0.0427 (10)	0.0374 (10)	0.0080 (8)	0.0096 (8)	−0.0005 (8)
O1	0.0688 (10)	0.0589 (9)	0.0542 (9)	−0.0094 (7)	0.0349 (8)	−0.0149 (7)
N3	0.0481 (9)	0.0412 (9)	0.0540 (10)	−0.0087 (7)	0.0203 (8)	−0.0072 (7)
C10	0.0441 (11)	0.0459 (10)	0.0423 (11)	−0.0020 (9)	0.0145 (9)	−0.0002 (8)
O2	0.0970 (12)	0.0472 (8)	0.0651 (10)	0.0037 (8)	0.0410 (9)	0.0072 (7)
C4	0.0430 (11)	0.0469 (11)	0.0406 (11)	0.0040 (9)	0.0130 (9)	−0.0099 (9)
C17	0.0492 (12)	0.0503 (11)	0.0453 (12)	−0.0034 (9)	0.0211 (9)	−0.0028 (9)
C23	0.0645 (13)	0.0529 (11)	0.0379 (11)	−0.0167 (10)	0.0166 (10)	−0.0015 (9)
C12	0.0447 (11)	0.0504 (11)	0.0387 (11)	−0.0018 (9)	0.0188 (9)	0.0058 (9)
C16	0.0524 (12)	0.0487 (11)	0.0575 (14)	−0.0018 (10)	0.0193 (11)	−0.0114 (10)
C7	0.0696 (14)	0.0430 (11)	0.0516 (13)	−0.0004 (10)	0.0264 (11)	−0.0117 (9)
C8	0.0485 (11)	0.0462 (11)	0.0403 (11)	0.0068 (9)	0.0123 (9)	0.0023 (9)
C2	0.0419 (11)	0.0488 (11)	0.0408 (11)	0.0040 (9)	0.0153 (9)	−0.0055 (9)
C14	0.0533 (12)	0.0453 (10)	0.0551 (13)	−0.0043 (9)	0.0230 (10)	0.0056 (10)
C9	0.0597 (13)	0.0461 (11)	0.0476 (12)	0.0053 (10)	0.0243 (10)	0.0031 (9)
C22	0.0593 (13)	0.0537 (12)	0.0494 (13)	−0.0102 (10)	0.0149 (10)	0.0073 (10)
C21	0.0530 (12)	0.0560 (12)	0.0478 (12)	−0.0089 (10)	0.0149 (10)	−0.0133 (10)
C20	0.0492 (12)	0.0545 (11)	0.0382 (11)	−0.0078 (9)	0.0091 (9)	−0.0005 (9)
C3	0.0440 (11)	0.0437 (10)	0.0467 (12)	−0.0020 (9)	0.0161 (9)	−0.0082 (9)
C6	0.0646 (14)	0.0415 (10)	0.0534 (13)	0.0009 (10)	0.0246 (11)	−0.0033 (9)
C15	0.0527 (12)	0.0417 (11)	0.0657 (14)	−0.0058 (9)	0.0170 (11)	−0.0029 (10)
C24	0.0784 (17)	0.0465 (12)	0.0893 (18)	−0.0112 (11)	0.0370 (14)	−0.0112 (11)
C1	0.0659 (15)	0.0636 (13)	0.0588 (14)	−0.0145 (11)	0.0307 (12)	−0.0108 (11)

Geometric parameters (Å, º)

N1—C19	1.309 (2)	C23—H23B	0.9700
N1—C18	1.369 (2)	C12—H12	0.9300
C19—N2	1.402 (2)	C16—C15	1.394 (3)

C19—C11	1.438 (2)	C16—H16	0.9300
N2—C23	1.458 (2)	C7—C6	1.365 (2)
N2—C20	1.468 (2)	C7—C2	1.385 (2)
C13—C14	1.401 (2)	C7—H7	0.9300
C13—C12	1.401 (2)	C8—C9	1.473 (2)
C13—C18	1.406 (2)	C2—C3	1.378 (2)
C18—C17	1.405 (2)	C14—C15	1.357 (3)
C11—C12	1.364 (2)	C14—H14	0.9300
C11—C10	1.458 (2)	C9—H9	0.9300
C5—C4	1.381 (2)	C22—H22A	0.9700
C5—C6	1.393 (2)	C22—H22B	0.9700
C5—C8	1.474 (2)	C21—C20	1.498 (2)
O1—C2	1.352 (2)	C21—H21A	0.9700
O1—C1	1.424 (2)	C21—H21B	0.9700
N3—C22	1.446 (2)	C20—H20A	0.9700
N3—C21	1.450 (2)	C20—H20B	0.9700
N3—C24	1.452 (2)	C3—H3	0.9300
C10—C9	1.315 (2)	C6—H6	0.9300
C10—H10	0.9300	C15—H15	0.9300
O2—C8	1.223 (2)	C24—H24A	0.9600
C4—C3	1.374 (2)	C24—H24B	0.9600
C4—H4	0.9300	C24—H24C	0.9600
C17—C16	1.360 (2)	C1—H1A	0.9600
C17—H17	0.9300	C1—H1B	0.9600
C23—C22	1.497 (2)	C1—H1C	0.9600
C23—H23A	0.9700		

C19—N1—C18	118.71 (14)	C9—C8—C5	119.22 (16)
N1—C19—N2	118.22 (15)	O1—C2—C3	124.44 (16)
N1—C19—C11	123.47 (15)	O1—C2—C7	115.85 (16)
N2—C19—C11	118.23 (15)	C3—C2—C7	119.70 (17)
C19—N2—C23	115.93 (14)	C15—C14—C13	120.24 (17)
C19—N2—C20	115.28 (14)	C15—C14—H14	119.9
C23—N2—C20	109.53 (14)	C13—C14—H14	119.9
C14—C13—C12	123.31 (16)	C10—C9—C8	122.43 (17)
C14—C13—C18	119.68 (16)	C10—C9—H9	118.8
C12—C13—C18	116.96 (15)	C8—C9—H9	118.8
N1—C18—C13	122.23 (15)	N3—C22—C23	111.21 (16)
N1—C18—C17	119.01 (15)	N3—C22—H22A	109.4
C13—C18—C17	118.75 (15)	C23—C22—H22A	109.4
C12—C11—C19	116.49 (15)	N3—C22—H22B	109.4
C12—C11—C10	122.34 (15)	C23—C22—H22B	109.4
C19—C11—C10	120.84 (15)	H22A—C22—H22B	108.0
C4—C5—C6	118.01 (17)	N3—C21—C20	110.90 (15)
C4—C5—C8	123.41 (16)	N3—C21—H21A	109.5
C6—C5—C8	118.55 (16)	C20—C21—H21A	109.5
C2—O1—C1	118.02 (14)	N3—C21—H21B	109.5
C22—N3—C21	109.36 (15)	C20—C21—H21B	109.5

C22—N3—C24	110.90 (16)	H21A—C21—H21B	108.0
C21—N3—C24	111.75 (15)	N2—C20—C21	110.39 (15)
C9—C10—C11	127.31 (17)	N2—C20—H20A	109.6
C9—C10—H10	116.3	C21—C20—H20A	109.6
C11—C10—H10	116.3	N2—C20—H20B	109.6
C3—C4—C5	121.83 (16)	C21—C20—H20B	109.6
C3—C4—H4	119.1	H20A—C20—H20B	108.1
C5—C4—H4	119.1	C4—C3—C2	119.31 (17)
C16—C17—C18	120.18 (17)	C4—C3—H3	120.3
C16—C17—H17	119.9	C2—C3—H3	120.3
C18—C17—H17	119.9	C7—C6—C5	120.64 (18)
N2—C23—C22	109.45 (15)	C7—C6—H6	119.7
N2—C23—H23A	109.8	C5—C6—H6	119.7
C22—C23—H23A	109.8	C14—C15—C16	120.30 (17)
N2—C23—H23B	109.8	C14—C15—H15	119.9
C22—C23—H23B	109.8	C16—C15—H15	119.9
H23A—C23—H23B	108.2	N3—C24—H24A	109.5
C11—C12—C13	121.92 (16)	N3—C24—H24B	109.5
C11—C12—H12	119.0	H24A—C24—H24B	109.5
C13—C12—H12	119.0	N3—C24—H24C	109.5
C17—C16—C15	120.82 (18)	H24A—C24—H24C	109.5
C17—C16—H16	119.6	H24B—C24—H24C	109.5
C15—C16—H16	119.6	O1—C1—H1A	109.5
C6—C7—C2	120.48 (17)	O1—C1—H1B	109.5
C6—C7—H7	119.8	H1A—C1—H1B	109.5
C2—C7—H7	119.8	O1—C1—H1C	109.5
O2—C8—C9	120.28 (17)	H1A—C1—H1C	109.5
O2—C8—C5	120.48 (16)	H1B—C1—H1C	109.5

C18—N1—C19—N2	179.50 (15)	C4—C5—C8—O2	−161.56 (18)
C18—N1—C19—C11	2.8 (3)	C6—C5—C8—O2	16.5 (3)
N1—C19—N2—C23	−16.4 (2)	C4—C5—C8—C9	20.2 (3)
C11—C19—N2—C23	160.47 (16)	C6—C5—C8—C9	−161.74 (18)
N1—C19—N2—C20	113.40 (18)	C1—O1—C2—C3	8.3 (3)
C11—C19—N2—C20	−69.7 (2)	C1—O1—C2—C7	−172.89 (18)
C19—N1—C18—C13	1.9 (3)	C6—C7—C2—O1	179.19 (18)
C19—N1—C18—C17	−179.23 (16)	C6—C7—C2—C3	−2.0 (3)
C14—C13—C18—N1	178.29 (17)	C12—C13—C14—C15	−178.26 (19)
C12—C13—C18—N1	−4.2 (3)	C18—C13—C14—C15	−0.9 (3)
C14—C13—C18—C17	−0.5 (3)	C11—C10—C9—C8	179.61 (17)
C12—C13—C18—C17	176.95 (17)	O2—C8—C9—C10	2.9 (3)
N1—C19—C11—C12	−4.9 (3)	C5—C8—C9—C10	−178.87 (18)
N2—C19—C11—C12	178.38 (15)	C21—N3—C22—C23	58.9 (2)
N1—C19—C11—C10	168.70 (16)	C24—N3—C22—C23	−177.45 (16)
N2—C19—C11—C10	−8.0 (3)	N2—C23—C22—N3	−59.8 (2)
C12—C11—C10—C9	−14.4 (3)	C22—N3—C21—C20	−57.6 (2)
C19—C11—C10—C9	172.4 (2)	C24—N3—C21—C20	179.26 (17)
C6—C5—C4—C3	−1.1 (3)	C19—N2—C20—C21	169.36 (14)

C8—C5—C4—C3	176.98 (17)	C23—N2—C20—C21	−57.75 (19)
N1—C18—C17—C16	−177.06 (17)	N3—C21—C20—N2	57.7 (2)
C13—C18—C17—C16	1.8 (3)	C5—C4—C3—C2	0.4 (3)
C19—N2—C23—C22	−169.17 (16)	O1—C2—C3—C4	179.83 (18)
C20—N2—C23—C22	58.3 (2)	C7—C2—C3—C4	1.1 (3)
C19—C11—C12—C13	2.3 (3)	C2—C7—C6—C5	1.3 (3)
C10—C11—C12—C13	−171.15 (17)	C4—C5—C6—C7	0.2 (3)
C14—C13—C12—C11	179.28 (18)	C8—C5—C6—C7	−177.96 (18)
C18—C13—C12—C11	1.9 (3)	C13—C14—C15—C16	1.2 (3)
C18—C17—C16—C15	−1.6 (3)	C17—C16—C15—C14	0.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O2^{i}	0.96	2.52	3.3096 (2)	139
C14—H14···O1^{i}	0.93	2.40	3.3112 (2)	165
C17—H17···N3^{ii}	0.93	2.54	3.4029 (3)	155

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