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2-Amino-4-(4-methoxyphenyl)-1-(4-methylphenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carbonitrile

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Keywords: crystal structure; hexahydroquinoline ring; dimers; hydroquinones; multicomponent reactions.

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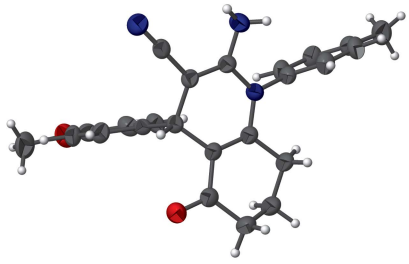
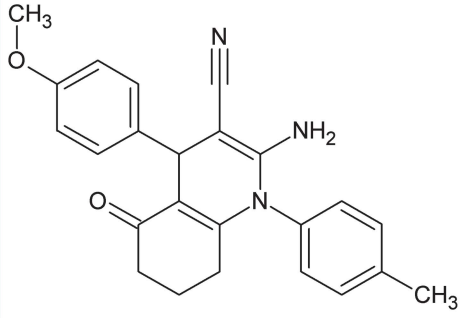
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{24}H_{23}N_3O_2$, the cyclohexene and 1,4-dihydropyridine rings of the 1,4,5,6,7,8-hexahydroquinoline ring system each adopt a twisted-boat conformation. The dihedral angle between the benzene rings is 13.89 (10)°. In the crystal, molecules are linked through pairs of amino–nitrile N—H···N hydrogen bonds, forming inversion dimers. Weak C—H···O and C—H···π interactions connect the dimers, forming a three-dimensional network.

3D view



Chemical scheme



Structure description

Studies have shown that 1,4,5,6,7,8-hexahydroquinolines have significant cytotoxic activity against different human cancer cell lines (Mohamed *et al.*, 2012; Al-Said *et al.*, 2011; Alqasoumi *et al.*, 2009). In recent years, hexahydroquinoline derivatives attracted more interest because of their biological and pharmacological activities, *e.g.* antimicrobial (Muli *et al.*, 2014; Shah *et al.*, 2012), antioxidant (Yang *et al.*, 2011), antimalarial (Kalaria *et al.*, 2014) and antiosteoporotic (Sashidhara *et al.*, 2013). In addition, hexahydroquinolines have been used as calcium channel blockers for the treatment of cardiovascular diseases including hypertension (Joshi & Pawar, 2013; Gunduz *et al.*, 2009; Aydin *et al.*, 2006; Simsek *et al.*, 2006).

As shown in Fig. 1, the cyclohexene (C4–C9) and 1,4-dihydropyridine (N1/C1–C4/C9) rings of the 1,4,5,6,7,8- hexahydroquinoline ring system (N1/C1–C9) each adopt a twisted-boat conformation [puckering parameters Q_T = 0.467 (2) Å, θ = 122.5 (2)°, φ = 354.0 (3)° and Q_T = 0.2541 (19) Å, θ = 106.6 (4)°, φ = 1.1 (5)°, respectively]. The

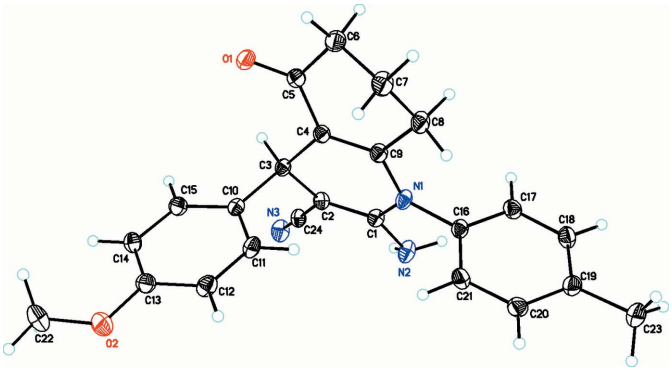


Figure 1
The title molecule, showing the atom-numbering scheme, with displacement ellipsoids drawn at the 50% probability level.

methylbenzene and methoxybenzene rings form a dihedral angle of 13.89 (10)°. This angle is similar to the value of 11.52 (7)° found in the closely related structure of 2-amino-4-(4-chlorophenyl)-1-(4-methylphenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carbonitrile (Mohamed *et al.*, 2015).

In the crystal, molecules are linked by pairs of N—H···N hydrogen bonds with an $R_2^2(12)$ ring motif (Table 1), forming centrosymmetric dimers (Fig. 2). These dimers are assembled into a three-dimensional network *via* C—H···O and C—H···π interactions.

Synthesis and crystallization

To a solution of 1,3-cyclohexanedione (3.36 g, 0.03 mol) and *p*-toluidine (3.21 g, 0.03 mol) in ethanol (40 ml), a catalytic amount of triethylamine was added and the mixture was heated under reflux for 3 h. 4-Methoxybenzylidenemalononitrile (5.53 g, 0.03 mol) was added to the reaction mixture while refluxing for another 3 h. The reaction mixture was then cooled to room temperature. The precipitate that formed was filtered, dried and recrystallized from ethanol solution as orange crystals, yield 67%; m.p. 525 K.

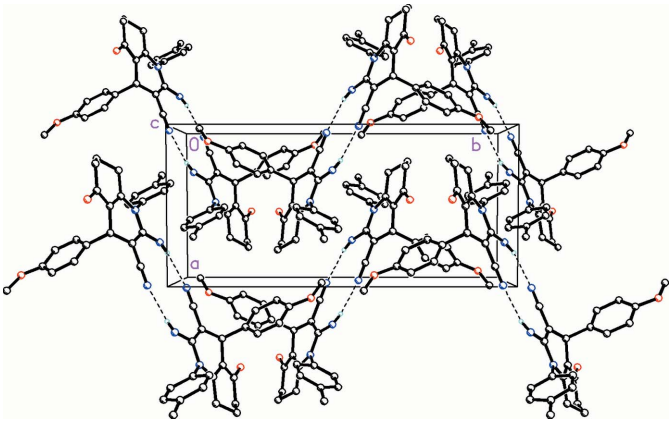


Figure 2
The molecular packing, viewed along the *c* axis, showing the intermolecular hydrogen bonds as dashed lines.

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

*Cg*3 and *Cg*4 are the centroids of the C10–C15 and C16–C21 benzene rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*A*···N3^{i}	0.86	2.31	3.016 (3)	140
C11—H11···O1^{ii}	0.95	2.70	3.408 (2)	132
C21—H21···O1^{ii}	0.95	2.68	3.433 (3)	136
C22—H22*C*···N3^{iii}	0.98	2.81	3.407 (4)	120
C23—H23*B*···O2^{iv}	0.98	2.76	3.484 (3)	131
C21—H21···*Cg*3^{v}	0.95	2.99	3.571 (2)	120
C22—H22*B*···*Cg*4^{vi}	0.98	2.92	3.695 (3)	137

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (v) $x, -y+\frac{1}{2}, z-\frac{3}{2}$; (vi) $x+1, -y+\frac{1}{2}, z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{23}N_3O_2$
M_r	385.45
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, *b*, *c* (Å)	9.1066 (4), 19.6406 (9), 11.2901 (5)
β (°)	94.343 (4)
V (Å^3)	2013.54 (16)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.66
Crystal size (mm)	0.38 × 0.28 × 0.22
Data collection	
Diffractometer	Rigaku Oxford Diffraction Xcalibur Eos Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku Oxford Diffraction, 2015)
T_{min}, T_{max}	0.813, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7397, 3793, 2933
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.614
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.149, 1.05
No. of reflections	3793
No. of parameters	265
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.25

Computer programs: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. 28 reflections were omitted as clear outlier data.

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full crystallographic data

IUCrData (2018). **3**, x180167 [https://doi.org/10.1107/S2414314618001670]

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Crystal data

$C_{24}H_{23}N_3O_2$
M_r = 385.45
Monoclinic, $P2_1/c$
a = 9.1066 (4) Å
b = 19.6406 (9) Å
c = 11.2901 (5) Å
β = 94.343 (4)°
V = 2013.54 (16) Å^3
Z = 4
$F(000)$ = 816
D_x = 1.272 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 2845 reflections
θ = 4.0–71.1°
μ = 0.66 mm^{-1}
T = 173 K
Irregular, orange
0.38 × 0.28 × 0.22 mm

Data collection

Rigaku Oxford Diffraction **[model name?]** diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku Oxford Diffraction, 2015)
T_{min} = 0.813, T_{max} = 1.000
7397 measured reflections
3793 independent reflections
2933 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 71.3°, θ_{min} = 4.5°
h = −6→11
k = −19→23
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.149
S = 1.05
3793 reflections
265 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2 + 0.4388P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.46137 (17)	0.69821 (8)	0.77151 (12)	0.0500 (4)
O2	0.9254 (2)	0.90959 (8)	0.55490 (16)	0.0602 (4)
N1	0.52568 (18)	0.59661 (9)	0.39959 (14)	0.0402 (4)
N2	0.7293 (2)	0.52949 (10)	0.36461 (16)	0.0505 (5)
H2A	0.7936	0.5051	0.4054	0.061*
H2B	0.6629	0.5032	0.3309	0.061*
N3	0.9846 (2)	0.54847 (10)	0.61603 (17)	0.0531 (5)
C1	0.6661 (2)	0.57350 (9)	0.43835 (16)	0.0365 (4)
C2	0.7304 (2)	0.59502 (9)	0.54430 (16)	0.0344 (4)
C3	0.6644 (2)	0.65027 (9)	0.61721 (15)	0.0338 (4)
H3	0.6793	0.6369	0.7028	0.041*
C4	0.5003 (2)	0.65333 (9)	0.58438 (16)	0.0358 (4)
C5	0.4081 (2)	0.68142 (10)	0.67280 (18)	0.0410 (4)
C6	0.2453 (2)	0.68749 (14)	0.6401 (2)	0.0557 (6)
H6A	0.2061	0.7268	0.6825	0.067*
H6B	0.1953	0.6460	0.6664	0.067*
C7	0.2102 (2)	0.69671 (13)	0.5074 (2)	0.0557 (6)
H7A	0.2479	0.7414	0.4826	0.067*
H7B	0.1022	0.6962	0.4893	0.067*
C8	0.2800 (2)	0.64023 (12)	0.43862 (19)	0.0482 (5)
H8A	0.2273	0.5970	0.4506	0.058*
H8B	0.2697	0.6511	0.3528	0.058*
C9	0.4407 (2)	0.63125 (10)	0.47773 (17)	0.0381 (4)
C10	0.7382 (2)	0.71933 (9)	0.60276 (15)	0.0334 (4)
C11	0.7090 (2)	0.75732 (10)	0.49983 (16)	0.0421 (5)
H11	0.6434	0.7399	0.4377	0.051*
C12	0.7741 (3)	0.82000 (10)	0.48682 (18)	0.0472 (5)
H12	0.7530	0.8454	0.4160	0.057*
C13	0.8699 (2)	0.84605 (10)	0.57628 (19)	0.0439 (5)
C14	0.9020 (2)	0.80888 (11)	0.67871 (19)	0.0465 (5)
H14	0.9684	0.8262	0.7404	0.056*
C15	0.8356 (2)	0.74549 (10)	0.69038 (17)	0.0415 (4)
H15	0.8580	0.7197	0.7606	0.050*
C16	0.4724 (2)	0.58466 (10)	0.27725 (16)	0.0377 (4)
C17	0.4055 (2)	0.52317 (10)	0.24530 (18)	0.0440 (5)
H17	0.3950	0.4888	0.3033	0.053*
C18	0.3542 (3)	0.51228 (11)	0.1284 (2)	0.0493 (5)
H18	0.3111	0.4696	0.1063	0.059*
C19	0.3643 (2)	0.56241 (12)	0.04289 (18)	0.0465 (5)

C20	0.4346 (2)	0.62267 (11)	0.07619 (19)	0.0471 (5)
H20	0.4450	0.6571	0.0183	0.057*
C21	0.4898 (2)	0.63388 (10)	0.19185 (19)	0.0442 (5)
H21	0.5395	0.6752	0.2126	0.053*
C22	1.0145 (3)	0.93964 (14)	0.6489 (3)	0.0714 (8)
H22A	1.0443	0.9853	0.6254	0.107*
H22B	1.1024	0.9116	0.6668	0.107*
H22C	0.9587	0.9428	0.7196	0.107*
C23	0.2984 (3)	0.55176 (15)	−0.0820 (2)	0.0655 (7)
H23A	0.2000	0.5722	−0.0907	0.098*
H23B	0.2910	0.5029	−0.0988	0.098*
H23C	0.3612	0.5733	−0.1380	0.098*
C24	0.8710 (2)	0.56923 (9)	0.58305 (17)	0.0382 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0454 (8)	0.0660 (9)	0.0386 (7)	−0.0022 (7)	0.0023 (6)	−0.0111 (7)
O2	0.0724 (11)	0.0429 (8)	0.0654 (10)	−0.0117 (8)	0.0065 (8)	0.0014 (7)
N1	0.0349 (8)	0.0502 (9)	0.0343 (8)	0.0089 (7)	−0.0056 (6)	−0.0083 (7)
N2	0.0458 (10)	0.0572 (10)	0.0466 (10)	0.0162 (8)	−0.0088 (8)	−0.0144 (8)
N3	0.0421 (10)	0.0568 (11)	0.0581 (11)	0.0144 (9)	−0.0115 (8)	−0.0075 (9)
C1	0.0336 (10)	0.0381 (9)	0.0371 (9)	0.0060 (7)	−0.0013 (7)	−0.0007 (7)
C2	0.0316 (9)	0.0349 (9)	0.0357 (9)	0.0037 (7)	−0.0035 (7)	0.0014 (7)
C3	0.0336 (9)	0.0382 (9)	0.0286 (8)	0.0025 (7)	−0.0034 (7)	0.0000 (7)
C4	0.0303 (9)	0.0405 (9)	0.0360 (9)	0.0011 (7)	−0.0010 (7)	−0.0013 (7)
C5	0.0366 (10)	0.0455 (10)	0.0408 (10)	−0.0016 (8)	0.0022 (8)	−0.0026 (8)
C6	0.0351 (11)	0.0765 (15)	0.0558 (13)	0.0034 (10)	0.0059 (9)	−0.0201 (12)
C7	0.0354 (11)	0.0706 (15)	0.0597 (13)	0.0117 (10)	−0.0049 (10)	−0.0143 (11)
C8	0.0324 (10)	0.0657 (13)	0.0451 (11)	0.0077 (9)	−0.0068 (8)	−0.0106 (10)
C9	0.0320 (10)	0.0439 (10)	0.0378 (9)	0.0035 (8)	−0.0020 (7)	−0.0022 (8)
C10	0.0315 (9)	0.0371 (9)	0.0314 (8)	0.0043 (7)	0.0009 (7)	−0.0027 (7)
C11	0.0536 (12)	0.0398 (10)	0.0316 (9)	0.0038 (9)	−0.0060 (8)	−0.0026 (7)
C12	0.0633 (14)	0.0403 (10)	0.0375 (10)	0.0057 (9)	0.0010 (9)	0.0030 (8)
C13	0.0467 (11)	0.0379 (10)	0.0479 (11)	0.0001 (8)	0.0089 (9)	−0.0024 (8)
C14	0.0403 (11)	0.0545 (12)	0.0437 (11)	−0.0078 (9)	−0.0036 (9)	−0.0047 (9)
C15	0.0387 (10)	0.0493 (11)	0.0355 (9)	−0.0012 (8)	−0.0035 (8)	0.0043 (8)
C16	0.0336 (9)	0.0431 (10)	0.0357 (9)	0.0021 (8)	−0.0026 (7)	−0.0025 (7)
C17	0.0452 (11)	0.0409 (10)	0.0450 (11)	−0.0061 (8)	−0.0026 (9)	0.0063 (8)
C18	0.0514 (13)	0.0439 (11)	0.0513 (12)	−0.0087 (9)	−0.0038 (10)	−0.0053 (9)
C19	0.0422 (11)	0.0561 (12)	0.0406 (10)	0.0000 (9)	−0.0004 (9)	−0.0019 (9)
C20	0.0460 (12)	0.0511 (11)	0.0437 (11)	−0.0058 (9)	−0.0001 (9)	0.0095 (9)
C21	0.0439 (11)	0.0380 (10)	0.0494 (11)	−0.0071 (8)	−0.0043 (9)	0.0018 (8)
C22	0.0638 (17)	0.0592 (15)	0.090 (2)	−0.0223 (13)	−0.0006 (14)	−0.0020 (14)
C23	0.0625 (16)	0.0885 (18)	0.0436 (12)	−0.0079 (14)	−0.0076 (11)	−0.0030 (12)
C24	0.0376 (11)	0.0369 (9)	0.0390 (9)	0.0016 (8)	−0.0041 (8)	−0.0028 (7)

Geometric parameters (Å, º)

O1—C5	1.227 (2)	C10—C11	1.390 (3)
O2—C13	1.375 (2)	C10—C15	1.377 (3)
O2—C22	1.416 (3)	C11—H11	0.9500
N1—C1	1.396 (2)	C11—C12	1.379 (3)
N1—C9	1.394 (2)	C12—H12	0.9500
N1—C16	1.448 (2)	C12—C13	1.382 (3)
N2—H2A	0.8618	C13—C14	1.380 (3)
N2—H2B	0.8621	C14—H14	0.9500
N2—C1	1.358 (2)	C14—C15	1.395 (3)
N3—C24	1.148 (3)	C15—H15	0.9500
C1—C2	1.359 (3)	C16—C17	1.388 (3)
C2—C3	1.514 (2)	C16—C21	1.383 (3)
C2—C24	1.414 (3)	C17—H17	0.9500
C3—H3	1.0000	C17—C18	1.383 (3)
C3—C4	1.513 (3)	C18—H18	0.9500
C3—C10	1.528 (3)	C18—C19	1.387 (3)
C4—C5	1.461 (3)	C19—C20	1.384 (3)
C4—C9	1.354 (3)	C19—C23	1.505 (3)
C5—C6	1.505 (3)	C20—H20	0.9500
C6—H6A	0.9900	C20—C21	1.381 (3)
C6—H6B	0.9900	C21—H21	0.9500
C6—C7	1.518 (3)	C22—H22A	0.9800
C7—H7A	0.9900	C22—H22B	0.9800
C7—H7B	0.9900	C22—H22C	0.9800
C7—C8	1.521 (3)	C23—H23A	0.9800
C8—H8A	0.9900	C23—H23B	0.9800
C8—H8B	0.9900	C23—H23C	0.9800
C8—C9	1.507 (3)		
C13—O2—C22	116.38 (19)	C15—C10—C11	118.20 (18)
C1—N1—C16	118.64 (15)	C10—C11—H11	119.6
C9—N1—C1	119.96 (15)	C12—C11—C10	120.78 (18)
C9—N1—C16	121.40 (15)	C12—C11—H11	119.6
H2A—N2—H2B	109.2	C11—C12—H12	119.8
C1—N2—H2A	109.2	C11—C12—C13	120.35 (19)
C1—N2—H2B	109.7	C13—C12—H12	119.8
N2—C1—N1	115.82 (16)	O2—C13—C12	115.33 (19)
N2—C1—C2	124.27 (17)	O2—C13—C14	124.8 (2)
C2—C1—N1	119.91 (17)	C14—C13—C12	119.91 (19)
C1—C2—C3	122.61 (16)	C13—C14—H14	120.5
C1—C2—C24	118.73 (17)	C13—C14—C15	119.03 (19)
C24—C2—C3	118.42 (15)	C15—C14—H14	120.5
C2—C3—H3	107.9	C10—C15—C14	121.71 (18)
C2—C3—C10	112.45 (15)	C10—C15—H15	119.1
C4—C3—C2	108.71 (15)	C14—C15—H15	119.1
C4—C3—H3	107.9	C17—C16—N1	119.85 (18)

C4—C3—C10	111.90 (15)	C21—C16—N1	120.25 (18)
C10—C3—H3	107.9	C21—C16—C17	119.89 (18)
C5—C4—C3	117.12 (16)	C16—C17—H17	120.2
C9—C4—C3	121.81 (17)	C18—C17—C16	119.51 (19)
C9—C4—C5	121.07 (18)	C18—C17—H17	120.2
O1—C5—C4	120.93 (18)	C17—C18—H18	119.4
O1—C5—C6	121.09 (19)	C17—C18—C19	121.27 (19)
C4—C5—C6	117.97 (17)	C19—C18—H18	119.4
C5—C6—H6A	109.1	C18—C19—C23	120.7 (2)
C5—C6—H6B	109.1	C20—C19—C18	118.15 (19)
C5—C6—C7	112.41 (19)	C20—C19—C23	121.1 (2)
H6A—C6—H6B	107.9	C19—C20—H20	119.3
C7—C6—H6A	109.1	C21—C20—C19	121.40 (19)
C7—C6—H6B	109.1	C21—C20—H20	119.3
C6—C7—H7A	109.5	C16—C21—H21	120.2
C6—C7—H7B	109.5	C20—C21—C16	119.67 (18)
C6—C7—C8	110.6 (2)	C20—C21—H21	120.2
H7A—C7—H7B	108.1	O2—C22—H22A	109.5
C8—C7—H7A	109.5	O2—C22—H22B	109.5
C8—C7—H7B	109.5	O2—C22—H22C	109.5
C7—C8—H8A	109.3	H22A—C22—H22B	109.5
C7—C8—H8B	109.3	H22A—C22—H22C	109.5
H8A—C8—H8B	107.9	H22B—C22—H22C	109.5
C9—C8—C7	111.70 (17)	C19—C23—H23A	109.5
C9—C8—H8A	109.3	C19—C23—H23B	109.5
C9—C8—H8B	109.3	C19—C23—H23C	109.5
N1—C9—C8	116.42 (16)	H23A—C23—H23B	109.5
C4—C9—N1	120.99 (17)	H23A—C23—H23C	109.5
C4—C9—C8	122.56 (18)	H23B—C23—H23C	109.5
C11—C10—C3	120.53 (16)	N3—C24—C2	179.1 (2)
C15—C10—C3	121.27 (16)		

Hydrogen-bond geometry (Å, º)

Cg3 and Cg4 are the centroids of the C10–C15 and C16–C21 benzene rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···N3^{i}	0.86	2.31	3.016 (3)	140
C11—H11···O1^{ii}	0.95	2.70	3.408 (2)	132
C21—H21···O1^{ii}	0.95	2.68	3.433 (3)	136
C22—H22*C*···N3^{iii}	0.98	2.81	3.407 (4)	120
C23—H23*B*···O2^{iv}	0.98	2.76	3.484 (3)	131
C21—H21···*Cg*3^{v}	0.95	2.99	3.571 (2)	120
C22—H22*B*···*Cg*4^{vi}	0.98	2.92	3.695 (3)	137

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) *x*, −*y*+3/2, *z*−1/2; (iii) −*x*+2, *y*+1/2, −*z*+3/2; (iv) −*x*+1, *y*−1/2, −*z*+1/2; (v) *x*, −*y*+1/2, *z*−3/2; (vi) *x*+1, −*y*+1/2, *z*−1/2.