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Crystal structure of 2-amino-4-(4-chlorophenyl)-1-(4-methylphenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carbonitrile

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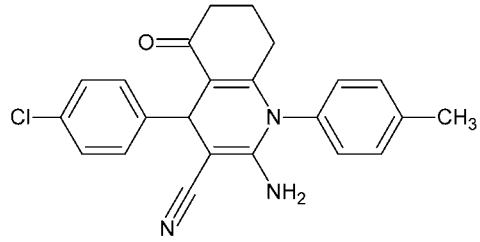
In the title compound, $C_{23}H_{20}ClN_3O$, each of the cyclohexene and 1,4-dihydropyridine rings of the 1,4,5,6,7,8-hexahydroquinoline ring system adopts a twisted-boat conformation. The dihedral angle between the two benzene rings is 11.52 (7)°. In the crystal, molecules are linked through a pair of amino–nitrile N—H···N hydrogen bonds, forming inversion dimers. These assemble into a three-dimensional network *via* C—H···O and C—H···π interactions.

Keywords: crystal structure; dihydropyridines; annelated dihydropyridines; hydrogen bonding; inversion dimers.

CCDC reference: 1436038

1. Related literature

For the synthesis and pharmaceutical applications of dihydropyridines, see: Kumar & Maurya (2007); Kendre *et al.* (2008); Heydari *et al.* (2009).



2. Experimental

2.1. Crystal data

$C_{23}H_{20}ClN_3O$
M_r = 389.87
Monoclinic, $P2_1/c$
a = 8.7759 (3) Å
b = 10.6399 (3) Å
c = 20.7929 (7) Å
β = 93.842 (3)°
V = 1937.17 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 K
0.46 × 0.42 × 0.38 mm

2.2. Data collection

Agilent Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min} = 0.841, T_{max} = 1.000
15538 measured reflections
6453 independent reflections
4853 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.144
S = 1.04
6453 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

*Cg*3 and *Cg*4 are the centroids of the methyl- and chloro-benzene rings (C10–C15 and C18–C23), respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*N*···N3^{i}	0.91	2.17	3.013 (2)	153
C14—H14···O1^{ii}	0.93	2.58	3.4577 (19)	156
C3—H3*A*···*Cg*4^{iii}	0.97	2.93	3.7210 (16)	139
C16—H16*B*···*Cg*3^{iv}	0.96	2.81	3.6464 (18)	146

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

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5407).

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supporting information

Acta Cryst. (2015). E**71**, o949–o950 [doi:10.1107/S2056989015021313]

Crystal structure of 2-amino-4-(4-chlorophenyl)-1-(4-methylphenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carbonitrile

Shaaban K. Mohamed, Mehmet Akkurt, Jerry P. Jasinski, Omyma A. A. Abd Allah and Mustafa R. Albayati

S1. Comment

Dihydropiridines (DHP's) are a significant class of heterocyclic molecules due to their important biological activities (Kumar & Maurya, 2007). Dihydropyridine drugs, such as nifedipine, nicardipine and amlodipine are well known as cardiovascular agents for the treatment of hypertension (Kendre *et al*., 2008), calcium channel modulators and for cardiovascular disease treatment (Heydari *et al.*, 2009). In this context, we report here the synthesis and crystal structure of the title compound.

In the title compound (Fig. 1), the cyclohexene (C1–C6) and 1,4-dihydropyridine (N1/C5–C9) rings of the 1,4,5,6,7,8-hexahydroquinoline ring system (N1/C1–C9) each adopt a twisted-boat conformation (the puckering parameters are Q_T = 0.4813 (16) Å, θ = 123.31 (18)°, φ = 283.9 (2)° and Q_T = 0.2182 (14) Å, θ = 103.7 (4)°, φ = 353.5 (4)°, respectively). The dihedral angle between the methyl- and chloro-benzene rings is 11.52 (7)°.

In the crystal, a pair of N—H···N intermolecular hydrogen bonds connects two molecules by an $R_2^2(12)$ ring motif (Table 1), forming a centrosymmetric dimer (Fig. 2). Weak C—H···O and C—H···π interactions connect the dimers to each other, forming a three-dimensional network.

S2. Experimental

To a solution of 1.3-cyclohexanedione (3.36 g, 0.03 mol) in 40 ml ethanol, *p*-toluidine (3.21 g, 0.03 mol) and catalytic a amount of triethylamine were added. The mixture was heated under reflux for 3 h. (4-Chlorobenzylidene)malononitrile (5.68 g, 0.03 mol) was added to the reaction mixture and refluxed for another 3 h. The separated solid was filtered off while hot, dried and crystallized from DMF as colourless crystals. Yield: 49.7%; m.p. 573 K, IR (λ_{max}, cm^{-1}): 3472, 3325 (NH_2), 3209, 3032 ($CH_{arom.}$), 2972–2879 ($CH_{aliph.}$), 2177 (C≡N), 1631 (C=O); ^{1}H-NMR (DMSO-d_6), δ ppm: 7.39–7.29 (m, 8H, $CH_{arom.}$), 5.32 (s, 2H, NH_2, masked by D_2O), 4.51 (s, 1H, CH), 2.4 (s, 3H, CH_3), 2.23–2.19 (t, 2H, CH_2—C=O), 1.93–1.81 (t, 2H, CH_2—C=C), 1.67–1.62 (m, 2H, CH_2-CH_2-CH_2); ^{13}C-NMR (DMSO-d_6), δ ppm: 195.45, 153.14, 151.70, 146.07, 139.86, 133.96, 131.26, 131.03, 130.10, 129.13, 128.79, 121.78, 112.72, 60.26, 36.45, 36.21, 28.23, 21.22, 21.06.

S3. Refinement

All H atoms were placed in calculated positions with N2—H1N = 0.90 Å, N2—H2N = 0.91 Å, and C—H = 0.93 - 1.04 Å, and refined as riding with U_{iso}(H) = 1.2 or 1.5U_{eq}(C, N).

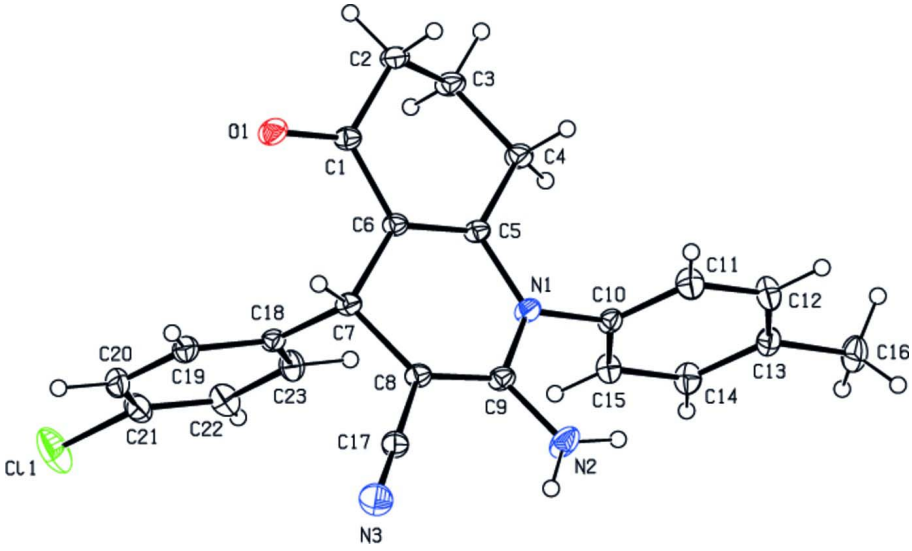

Figure 1

Molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level.

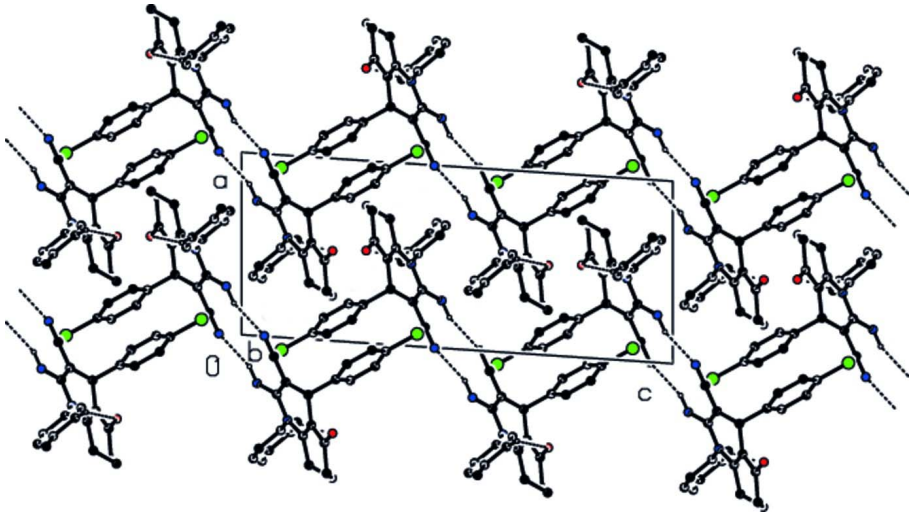

Figure 2

View of the dimers formed by N—H···N hydrogen bonds down the *b* axis.

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

Crystal data

$C_{23}H_{20}ClN_3O$
M_r = 389.87
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 8.7759 (3) Å
b = 10.6399 (3) Å
c = 20.7929 (7) Å
β = 93.842 (3)°
V = 1937.17 (11) Å^3
Z = 4
$F(000)$ = 816
D_x = 1.337 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4336 reflections
θ = 3.5–32.1°
μ = 0.22 mm^{-1}
T = 293 K
Irregular, colourless
0.46 × 0.42 × 0.38 mm

Data collection

Agilent Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min} = 0.841, T_{max} = 1.000
15538 measured reflections
6453 independent reflections
4853 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 32.8°, θ_{min} = 3.5°
h = −13→12
k = −15→13
l = −31→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.144
S = 1.04
6453 reflections
254 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.8789P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	−0.06881 (6)	1.08244 (7)	0.09288 (3)	0.0623 (2)
O1	0.50713 (13)	1.30415 (10)	0.28910 (6)	0.0326 (3)
N1	0.45035 (14)	0.91350 (11)	0.39374 (6)	0.0244 (3)
N2	0.26036 (17)	0.87555 (14)	0.46421 (7)	0.0396 (4)
N3	−0.00227 (17)	1.12750 (16)	0.44726 (8)	0.0423 (5)
C1	0.56260 (16)	1.20335 (12)	0.30796 (7)	0.0232 (3)
C2	0.72897 (16)	1.17417 (14)	0.30258 (8)	0.0276 (4)
C3	0.75310 (17)	1.03530 (14)	0.29019 (8)	0.0291 (4)
C4	0.69031 (16)	0.95720 (14)	0.34366 (8)	0.0282 (4)
C5	0.53218 (15)	0.99782 (12)	0.35801 (6)	0.0213 (3)
C6	0.47011 (15)	1.10911 (12)	0.33829 (6)	0.0206 (3)
C7	0.30491 (15)	1.14205 (12)	0.34566 (6)	0.0212 (3)
C8	0.24453 (15)	1.06023 (13)	0.39764 (6)	0.0221 (3)
C9	0.31330 (16)	0.95091 (13)	0.41841 (7)	0.0236 (3)
C10	0.50999 (16)	0.78952 (12)	0.40891 (7)	0.0223 (3)
C11	0.61730 (19)	0.77207 (14)	0.45979 (8)	0.0315 (4)
C12	0.67482 (19)	0.65278 (16)	0.47317 (8)	0.0340 (4)

C13	0.62493 (17)	0.54973 (14)	0.43663 (7)	0.0268 (4)
C14	0.51702 (19)	0.56892 (14)	0.38571 (7)	0.0296 (4)
C15	0.45943 (17)	0.68829 (14)	0.37163 (7)	0.0270 (4)
C16	0.6846 (2)	0.42010 (16)	0.45269 (8)	0.0369 (5)
C17	0.10810 (17)	1.09671 (14)	0.42500 (7)	0.0267 (4)
C18	0.21047 (15)	1.12918 (13)	0.28167 (7)	0.0215 (3)
C19	0.12277 (17)	1.22793 (14)	0.25608 (8)	0.0290 (4)
C20	0.03681 (18)	1.21482 (16)	0.19772 (8)	0.0351 (4)
C21	0.03801 (18)	1.10148 (18)	0.16578 (8)	0.0341 (5)
C22	0.12380 (19)	1.00150 (17)	0.19015 (8)	0.0334 (4)
C23	0.21025 (17)	1.01654 (14)	0.24800 (7)	0.0284 (4)
H1N	0.31260	0.80530	0.47550	0.0480*
H2A	0.78620	1.19830	0.34220	0.0330*
H2B	0.76720	1.22270	0.26760	0.0330*
H2N	0.17130	0.89510	0.48190	0.0480*
H3A	0.86130	1.01850	0.28810	0.0350*
H3B	0.70190	1.01210	0.24910	0.0350*
H4A	0.68820	0.86940	0.33100	0.0340*
H4B	0.75760	0.96510	0.38240	0.0340*
H7	0.29660	1.23540	0.36000	0.0250*
H11	0.65090	0.84010	0.48500	0.0380*
H12	0.74800	0.64170	0.50720	0.0410*
H14	0.48270	0.50090	0.36060	0.0350*
H15	0.38730	0.70000	0.33730	0.0320*
H16A	0.63750	0.36050	0.42290	0.0550*
H16B	0.66120	0.39850	0.49580	0.0550*
H16C	0.79330	0.41860	0.44960	0.0550*
H19	0.12140	1.30390	0.27820	0.0350*
H20	−0.02070	1.28170	0.18050	0.0420*
H22	0.12370	0.92540	0.16820	0.0400*
H23	0.26920	0.94990	0.26450	0.0340*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0483 (3)	0.0933 (5)	0.0424 (3)	0.0171 (3)	−0.0178 (2)	−0.0039 (3)
O1	0.0312 (6)	0.0215 (5)	0.0457 (6)	−0.0005 (4)	0.0073 (5)	0.0058 (4)
N1	0.0234 (6)	0.0192 (5)	0.0318 (6)	0.0035 (4)	0.0106 (4)	0.0033 (4)
N2	0.0389 (8)	0.0354 (7)	0.0476 (8)	0.0117 (6)	0.0251 (6)	0.0171 (6)
N3	0.0319 (7)	0.0531 (9)	0.0439 (8)	0.0113 (7)	0.0168 (6)	0.0056 (7)
C1	0.0228 (6)	0.0203 (6)	0.0267 (6)	−0.0028 (5)	0.0036 (5)	−0.0022 (5)
C2	0.0213 (6)	0.0253 (6)	0.0370 (8)	−0.0037 (5)	0.0069 (5)	0.0027 (6)
C3	0.0231 (7)	0.0277 (7)	0.0377 (8)	0.0004 (5)	0.0121 (6)	0.0016 (6)
C4	0.0222 (6)	0.0250 (6)	0.0383 (8)	0.0032 (5)	0.0095 (5)	0.0040 (6)
C5	0.0206 (6)	0.0200 (6)	0.0238 (6)	−0.0014 (5)	0.0058 (5)	−0.0011 (5)
C6	0.0190 (6)	0.0192 (6)	0.0242 (6)	−0.0001 (4)	0.0050 (4)	−0.0012 (5)
C7	0.0199 (6)	0.0179 (5)	0.0264 (6)	0.0012 (5)	0.0068 (5)	−0.0016 (5)
C8	0.0210 (6)	0.0237 (6)	0.0224 (6)	0.0007 (5)	0.0065 (5)	−0.0017 (5)

C9	0.0229 (6)	0.0235 (6)	0.0253 (6)	0.0004 (5)	0.0084 (5)	0.0001 (5)
C10	0.0235 (6)	0.0197 (6)	0.0242 (6)	0.0023 (5)	0.0063 (5)	0.0025 (5)
C11	0.0362 (8)	0.0255 (7)	0.0319 (7)	0.0001 (6)	−0.0049 (6)	−0.0045 (6)
C12	0.0364 (8)	0.0326 (8)	0.0315 (7)	0.0062 (6)	−0.0081 (6)	0.0014 (6)
C13	0.0302 (7)	0.0257 (6)	0.0249 (6)	0.0060 (5)	0.0054 (5)	0.0042 (5)
C14	0.0371 (8)	0.0230 (6)	0.0282 (7)	0.0024 (6)	−0.0007 (6)	−0.0032 (5)
C15	0.0296 (7)	0.0259 (7)	0.0250 (6)	0.0034 (5)	−0.0016 (5)	−0.0003 (5)
C16	0.0449 (10)	0.0304 (8)	0.0357 (8)	0.0127 (7)	0.0049 (7)	0.0060 (6)
C17	0.0242 (7)	0.0304 (7)	0.0260 (6)	0.0031 (5)	0.0054 (5)	0.0021 (5)
C18	0.0184 (6)	0.0213 (6)	0.0255 (6)	0.0017 (5)	0.0063 (5)	0.0028 (5)
C19	0.0257 (7)	0.0232 (6)	0.0385 (8)	0.0037 (5)	0.0059 (6)	0.0060 (6)
C20	0.0265 (7)	0.0384 (8)	0.0406 (8)	0.0081 (6)	0.0030 (6)	0.0150 (7)
C21	0.0234 (7)	0.0500 (10)	0.0287 (7)	0.0041 (7)	0.0007 (5)	0.0050 (7)
C22	0.0323 (8)	0.0378 (8)	0.0298 (7)	0.0057 (6)	0.0006 (6)	−0.0057 (6)
C23	0.0307 (7)	0.0267 (7)	0.0277 (7)	0.0074 (6)	0.0004 (5)	−0.0005 (5)

Geometric parameters (Å, º)

Cl1—C21	1.7399 (18)	C14—C15	1.391 (2)
O1—C1	1.2310 (17)	C18—C23	1.388 (2)
N1—C5	1.3943 (18)	C18—C19	1.387 (2)
N1—C9	1.3967 (19)	C19—C20	1.392 (2)
N1—C10	1.4462 (18)	C20—C21	1.377 (3)
N2—C9	1.351 (2)	C21—C22	1.380 (3)
N3—C17	1.149 (2)	C22—C23	1.388 (2)
C1—C2	1.504 (2)	C2—H2A	0.9700
C1—C6	1.4596 (19)	C2—H2B	0.9700
C2—C3	1.517 (2)	C3—H3A	0.9700
N2—H2N	0.9100	C3—H3B	0.9700
N2—H1N	0.9000	C4—H4A	0.9700
C3—C4	1.521 (2)	C4—H4B	0.9700
C4—C5	1.5024 (19)	C7—H7	1.0400
C5—C6	1.3554 (18)	C11—H11	0.9300
C6—C7	1.5093 (19)	C12—H12	0.9300
C7—C18	1.5259 (19)	C14—H14	0.9300
C7—C8	1.5112 (18)	C15—H15	0.9300
C8—C17	1.414 (2)	C16—H16A	0.9600
C8—C9	1.3670 (19)	C16—H16B	0.9600
C10—C15	1.383 (2)	C16—H16C	0.9600
C10—C11	1.381 (2)	C19—H19	0.9300
C11—C12	1.387 (2)	C20—H20	0.9300
C12—C13	1.388 (2)	C22—H22	0.9300
C13—C16	1.505 (2)	C23—H23	0.9300
C13—C14	1.388 (2)		
C5—N1—C9	119.95 (11)	Cl1—C21—C20	120.07 (14)
C5—N1—C10	120.75 (12)	C20—C21—C22	121.31 (15)
C9—N1—C10	119.20 (12)	C21—C22—C23	118.85 (16)

O1—C1—C2	121.42 (13)	C18—C23—C22	121.27 (14)
O1—C1—C6	121.11 (13)	C1—C2—H2A	109.00
C2—C1—C6	117.45 (12)	C1—C2—H2B	109.00
C1—C2—C3	111.15 (12)	C3—C2—H2A	109.00
C9—N2—H1N	119.00	C3—C2—H2B	109.00
C9—N2—H2N	120.00	H2A—C2—H2B	108.00
H1N—N2—H2N	121.00	C2—C3—H3A	110.00
C2—C3—C4	110.27 (13)	C2—C3—H3B	110.00
C3—C4—C5	111.89 (12)	C4—C3—H3A	110.00
N1—C5—C6	120.83 (12)	C4—C3—H3B	110.00
N1—C5—C4	115.87 (12)	H3A—C3—H3B	108.00
C4—C5—C6	123.31 (12)	C3—C4—H4A	109.00
C1—C6—C5	120.47 (12)	C3—C4—H4B	109.00
C1—C6—C7	116.75 (11)	C5—C4—H4A	109.00
C5—C6—C7	122.78 (12)	C5—C4—H4B	109.00
C6—C7—C18	111.10 (10)	H4A—C4—H4B	108.00
C8—C7—C18	112.08 (11)	C6—C7—H7	110.00
C6—C7—C8	108.91 (11)	C8—C7—H7	108.00
C7—C8—C17	118.46 (12)	C18—C7—H7	107.00
C7—C8—C9	123.20 (12)	C10—C11—H11	120.00
C9—C8—C17	118.31 (13)	C12—C11—H11	120.00
N1—C9—N2	115.79 (13)	C11—C12—H12	119.00
N1—C9—C8	119.95 (13)	C13—C12—H12	119.00
N2—C9—C8	124.22 (13)	C13—C14—H14	119.00
C11—C10—C15	120.10 (13)	C15—C14—H14	120.00
N1—C10—C11	120.53 (12)	C10—C15—H15	120.00
N1—C10—C15	119.37 (13)	C14—C15—H15	120.00
C10—C11—C12	119.80 (14)	C13—C16—H16A	109.00
C11—C12—C13	121.05 (15)	C13—C16—H16B	109.00
C12—C13—C14	118.40 (14)	C13—C16—H16C	109.00
C14—C13—C16	120.92 (14)	H16A—C16—H16B	110.00
C12—C13—C16	120.68 (14)	H16A—C16—H16C	109.00
C13—C14—C15	120.99 (14)	H16B—C16—H16C	109.00
C10—C15—C14	119.66 (13)	C18—C19—H19	120.00
N3—C17—C8	179.36 (17)	C20—C19—H19	120.00
C7—C18—C19	121.43 (13)	C19—C20—H20	120.00
C7—C18—C23	119.98 (12)	C21—C20—H20	120.00
C19—C18—C23	118.59 (14)	C21—C22—H22	121.00
C18—C19—C20	120.84 (14)	C23—C22—H22	121.00
C19—C20—C21	119.14 (15)	C18—C23—H23	119.00
Cl1—C21—C22	118.62 (14)	C22—C23—H23	119.00

C5—N1—C10—C11	81.13 (18)	C6—C7—C8—C17	162.97 (12)
C9—N1—C10—C11	−95.26 (17)	C18—C7—C8—C9	104.62 (15)
C5—N1—C10—C15	−98.38 (16)	C18—C7—C8—C17	−73.69 (15)
C5—N1—C9—N2	−165.14 (13)	C6—C7—C18—C23	55.07 (16)
C10—N1—C9—N2	11.28 (19)	C8—C7—C18—C19	112.49 (15)
C5—N1—C9—C8	12.5 (2)	C8—C7—C18—C23	−67.03 (16)

C10—N1—C9—C8	−171.05 (13)	C6—C7—C18—C19	−125.41 (14)
C9—N1—C5—C4	169.55 (13)	C7—C8—C9—N1	3.4 (2)
C10—N1—C5—C4	−6.82 (18)	C17—C8—C9—N1	−178.31 (13)
C9—N1—C5—C6	−10.23 (19)	C17—C8—C9—N2	−0.8 (2)
C10—N1—C5—C6	173.41 (12)	C7—C8—C9—N2	−179.15 (13)
C9—N1—C10—C15	85.23 (17)	N1—C10—C11—C12	−179.16 (14)
C6—C1—C2—C3	35.47 (18)	C15—C10—C11—C12	0.4 (2)
O1—C1—C6—C5	179.08 (13)	N1—C10—C15—C14	179.60 (13)
C2—C1—C6—C7	177.66 (12)	C11—C10—C15—C14	0.1 (2)
O1—C1—C2—C3	−146.41 (15)	C10—C11—C12—C13	−0.8 (2)
C2—C1—C6—C5	−2.80 (19)	C11—C12—C13—C14	0.7 (2)
O1—C1—C6—C7	−0.5 (2)	C11—C12—C13—C16	−178.22 (15)
C1—C2—C3—C4	−57.68 (17)	C12—C13—C14—C15	−0.3 (2)
C2—C3—C4—C5	47.83 (16)	C16—C13—C14—C15	178.66 (14)
C3—C4—C5—C6	−16.04 (19)	C13—C14—C15—C10	−0.1 (2)
C3—C4—C5—N1	164.19 (12)	C7—C18—C19—C20	−179.83 (14)
N1—C5—C6—C1	172.36 (12)	C23—C18—C19—C20	−0.3 (2)
N1—C5—C6—C7	−8.13 (19)	C7—C18—C23—C22	179.08 (14)
C4—C5—C6—C7	172.11 (12)	C19—C18—C23—C22	−0.5 (2)
C4—C5—C6—C1	−7.4 (2)	C18—C19—C20—C21	0.9 (2)
C1—C6—C7—C8	−159.39 (11)	C19—C20—C21—Cl1	179.82 (13)
C1—C6—C7—C18	76.69 (14)	C19—C20—C21—C22	−0.7 (2)
C5—C6—C7—C8	21.09 (17)	Cl1—C21—C22—C23	179.45 (12)
C5—C6—C7—C18	−102.84 (14)	C20—C21—C22—C23	−0.1 (2)
C6—C7—C8—C9	−18.72 (17)	C21—C22—C23—C18	0.6 (2)

Hydrogen-bond geometry (Å, º)

Cg3 and Cg4 are the centroids of the methyl- and chloro-benzene rings (C10–C15 and C18–C23), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*···N3^{i}	0.91	2.17	3.013 (2)	153
C14—H14···O1^{ii}	0.93	2.58	3.4577 (19)	156
C3—H3*A*···*Cg*4^{iii}	0.97	2.93	3.7210 (16)	139
C16—H16*B*···*Cg*3^{iv}	0.96	2.81	3.6464 (18)	146

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