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(*E*)-{4-Amino-3-[4-(dimethylamino)-benzylideneamino]phenyl}(phenyl)-methanone

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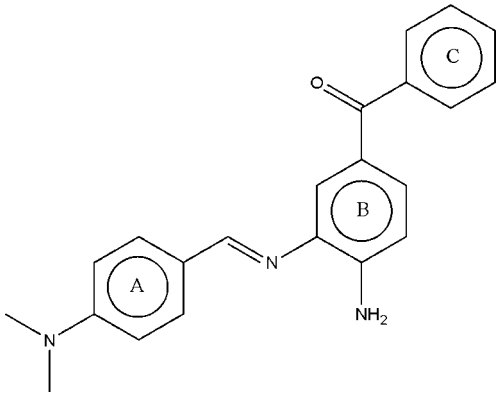
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.113; data-to-parameter ratio = 17.4.

The title compound, $C_{22}H_{21}N_3O$, crystallizes with two independent molecules in the asymmetric unit. The bond lengths and angles in both molecules are within normal ranges. The dihedral angles between benzene rings within the molecule are 32.4 (3) and 52.6 (3)° between the central and outer rings and 80.6 (3)° between the outer rings. The dihedral angles between benzene rings within the second molecule are 42.7 (3) and 57.0 (1)° between the central and outer rings and 82.8 (8)° between the outer ring. The crystal packing is stabilised by N—H···O hydrogen bonds linking the molecules into layers.

Related literature

For related literature, see: Pal *et al.* (2005), Ueno *et al.* (2004) and Hou (2005) for background information; Wetmore *et al.* (2001), Sattari *et al.* (1992) and Ganeshpure *et al.* (1996) for biological activity; Downing & Urbach (1969), Bosnich (1968) and Costes *et al.* (1995) for chemistry.



Experimental

Crystal data

$C_{22}H_{21}N_3O$
M_r = 343.42
Triclinic, $P\overline{1}$
a = 8.5652 (10) Å
b = 13.1529 (16) Å
c = 16.849 (2) Å
α = 75.936 (2)°
β = 89.864 (2)°
γ = 84.039 (2)°
V = 1830.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 150 (2) K
0.32 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.975, T_{max} = 0.992
16409 measured reflections
8504 independent reflections
6072 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.113
S = 1.02
8504 reflections
489 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.91 (2)	1.92 (2)	2.831 (2)	172.5 (19)
N4—H4A···O2^{i}	0.89 (2)	2.05 (2)	2.9368 (18)	171.5 (18)

Symmetry code: (i) $x+1, y, z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2126).

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supplementary materials

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(*E*)-{4-Amino-3-[4-(dimethylamino)benzylideneamino]phenyl}(phenyl)methanone

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Comment

Schiff bases readily form stable complexes with most transition metal ions (Pal *et al.*, 2005; Ueno *et al.*, 2004; Hou, 2005) and they have shown biological activity (Wetmore *et al.*, 2001; Sattari *et al.*, 1992; Ganeshpure *et al.*, 1996). In this paper, we report the crystal structure of the title Schiff base compound, (I) (Fig. 1). Compound (I) crystallizes with two independent molecules in the asymmetric unit. The bond lengths and angles in both molecules are within normal ranges. The N2–C14 bond length is 1.2804 (18), which is typical of C = N bonds. The torsion angles C15—C14—N2—C10 and C8—C7—C6—C1 are 173.35 (11) and 141.92 (15)° respectively. The dihedral angles between the various benzene rings within the molecule are: A/B = 32.43°, A/C = 80.63°, B/C = 52.63°. Crystal packing ia stabilized by N1—H1A···O1^{i} and N4—H4A···O2^{i} [symmetry code:i $x + 1$, y, z] hydrogen bonds that form layers of molecules with distances 1.92 (2), 2.05 (2) Å, respectively (Fig. 2).

.

Experimental

The title compound, (I), was prepared by reaction of 4-dimethylaminobenzaldehyde (1 mmol, 149 mg) and (3,4-diaminophenyl)(phenyl)methanone (1 mmol, 212 mg) which were dissolved in chloroform (10 ml). The mixture was stirred at room temperature for 4 h. Single crystals suitable for X-ray structure analysis which could be obtained by the crystallisationfrom ethanol and dichloromethane (1:1) solution, afforded yellow crystals.

Refinement

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95 and 0.98 Å, with U_{iso}(H) = 1.5Ueq(C).

Figures

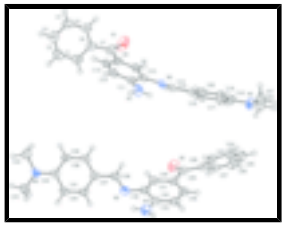


Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

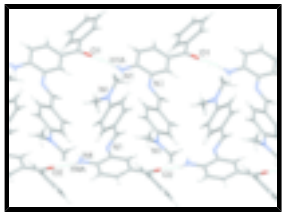


Fig. 2. The packing of (I), showing two layer of molecules connected by N—H···O hydrogen bonds.

(*E*)-{4-Amino-3-[4-(dimethylamino)benzylideneamino]phenyl}(phenyl)methanone

Crystal data

$C_{22}H_{21}N_3O$	$Z = 4$
$M_r = 343.42$	$F_{000} = 728$
Triclinic, $P\overline{1}$	$D_x = 1.246$ Mg m^{-3}
$a = 8.5652$ (10) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 13.1529$ (16) Å	Cell parameters from 7407 reflections
$c = 16.849$ (2) Å	$\theta = 2.3$–28.3º
$\alpha = 75.936$ (2)º	$\mu = 0.08$ mm^{-1}
$\beta = 89.864$ (2)º	$T = 150$ (2) K
$\gamma = 84.039$ (2)º	Slab, yellow
$V = 1830.8$ (4) Å^3	0.32 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1K CCD diffractometer	8504 independent reflections
Radiation source: sealed tube	6072 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 150$(2) K	$\theta_{max} = 28.4$º
thin–slice ω scans	$\theta_{min} = 2.3$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -11 \rightarrow 11$
$T_{min} = 0.975$, $T_{max} = 0.992$	$k = -17 \rightarrow 17$
16409 measured reflections	$l = -21 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.113$	$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 0.4657P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
8504 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}

489 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.01998 (15)	0.49228 (14)	0.64740 (10)	0.0936 (6)
N1	0.72234 (17)	0.58249 (12)	0.57696 (11)	0.0489 (4)
H1A	0.814 (3)	0.5515 (16)	0.6040 (12)	0.070 (6)*
H1B	0.721 (2)	0.6314 (15)	0.5317 (12)	0.053 (5)*
N2	0.46183 (14)	0.68001 (9)	0.49105 (7)	0.0343 (3)
N3	0.36024 (17)	1.08459 (11)	0.18151 (8)	0.0494 (3)
C1	0.22074 (18)	0.24163 (14)	0.73783 (10)	0.0442 (4)
H1	0.3015	0.2419	0.6990	0.053*
C2	0.19895 (19)	0.14925 (14)	0.79468 (11)	0.0498 (4)
H2A	0.2639	0.0862	0.7945	0.060*
C3	0.08269 (19)	0.14856 (14)	0.85184 (11)	0.0491 (4)
H3A	0.0692	0.0854	0.8916	0.059*
C4	−0.01400 (18)	0.23979 (14)	0.85112 (10)	0.0453 (4)
H4	−0.0941	0.2391	0.8903	0.054*
C5	0.00560 (17)	0.33182 (13)	0.79367 (9)	0.0388 (3)
H5A	−0.0627	0.3938	0.7927	0.047*
C6	0.12506 (16)	0.33444 (13)	0.73698 (9)	0.0380 (3)
C7	0.14060 (18)	0.43615 (15)	0.67574 (10)	0.0494 (4)
C8	0.29519 (16)	0.46932 (12)	0.65070 (9)	0.0365 (3)
C9	0.30424 (16)	0.55217 (12)	0.58122 (9)	0.0360 (3)
H9A	0.2111	0.5821	0.5501	0.043*
C10	0.44430 (16)	0.59165 (11)	0.55654 (8)	0.0324 (3)
C11	0.58414 (17)	0.54672 (11)	0.60313 (9)	0.0349 (3)
C12	0.57379 (17)	0.46675 (11)	0.67442 (9)	0.0366 (3)
H12A	0.6653	0.4388	0.7074	0.044*
C13	0.43286 (17)	0.42815 (12)	0.69729 (9)	0.0358 (3)
H13A	0.4288	0.3729	0.7453	0.043*
C14	0.36401 (16)	0.70573 (11)	0.43034 (8)	0.0313 (3)
H14A	0.2862	0.6603	0.4271	0.038*
C15	0.36777 (15)	0.80215 (11)	0.36602 (8)	0.0303 (3)

C16	0.26080 (16)	0.82560 (11)	0.30039 (9)	0.0345 (3)
H16A	0.1882	0.7767	0.2972	0.041*
C17	0.25722 (18)	0.91793 (12)	0.23983 (9)	0.0379 (3)
H17A	0.1828	0.9312	0.1958	0.046*
C18	0.36223 (17)	0.99259 (11)	0.24235 (9)	0.0359 (3)
C19	0.47101 (16)	0.96889 (12)	0.30879 (9)	0.0358 (3)
H19A	0.5437	1.0175	0.3125	0.043*
C20	0.47305 (16)	0.87614 (11)	0.36830 (9)	0.0333 (3)
H20A	0.5479	0.8619	0.4122	0.040*
C21	0.4481 (2)	1.16902 (14)	0.19338 (11)	0.0538 (4)
H21A	0.5596	1.1429	0.2024	0.081*
H21B	0.4086	1.1931	0.2411	0.081*
H21C	0.4353	1.2279	0.1446	0.081*
C22	0.2325 (2)	1.11421 (14)	0.12156 (11)	0.0539 (4)
H22A	0.2269	1.0582	0.0928	0.081*
H22B	0.2506	1.1799	0.0821	0.081*
H22C	0.1334	1.1246	0.1492	0.081*
O2	0.34484 (14)	0.50869 (10)	0.10852 (8)	0.0566 (3)
N4	1.08012 (17)	0.38306 (14)	0.15495 (11)	0.0544 (4)
H4A	1.158 (3)	0.4213 (16)	0.1355 (12)	0.068 (6)*
H4B	1.093 (3)	0.3228 (18)	0.1948 (14)	0.080 (7)*
N5	0.84486 (15)	0.27592 (10)	0.23197 (8)	0.0394 (3)
N6	0.85759 (15)	−0.15406 (10)	0.51795 (8)	0.0422 (3)
C23	0.48287 (19)	0.75803 (12)	0.07612 (9)	0.0413 (4)
H23A	0.5656	0.7388	0.1161	0.050*
C24	0.4340 (2)	0.86335 (14)	0.04277 (10)	0.0511 (4)
H24A	0.4798	0.9163	0.0614	0.061*
C25	0.3181 (2)	0.89124 (16)	−0.01783 (11)	0.0577 (5)
H25A	0.2863	0.9635	−0.0420	0.069*
C26	0.2483 (2)	0.81371 (17)	−0.04336 (10)	0.0573 (5)
H26A	0.1696	0.8331	−0.0855	0.069*
C27	0.29241 (18)	0.70886 (15)	−0.00804 (9)	0.0454 (4)
H27A	0.2412	0.6562	−0.0243	0.054*
C28	0.41143 (17)	0.67979 (13)	0.05134 (8)	0.0377 (3)
C29	0.45286 (18)	0.56462 (12)	0.09044 (9)	0.0389 (3)
C30	0.61731 (17)	0.52142 (11)	0.10726 (9)	0.0351 (3)
C31	0.65249 (17)	0.42351 (11)	0.16287 (9)	0.0354 (3)
H31A	0.5689	0.3879	0.1897	0.042*
C32	0.80442 (17)	0.37709 (11)	0.17991 (9)	0.0365 (3)
C33	0.93019 (18)	0.42930 (12)	0.13883 (9)	0.0399 (3)
C34	0.89509 (18)	0.52650 (12)	0.08224 (9)	0.0412 (4)
H34A	0.9779	0.5617	0.0540	0.049*
C35	0.74296 (18)	0.57167 (12)	0.06700 (9)	0.0389 (3)
H35A	0.7221	0.6379	0.0287	0.047*
C36	0.76489 (17)	0.24686 (12)	0.29653 (9)	0.0369 (3)
H36A	0.6870	0.2968	0.3095	0.044*
C37	0.78650 (16)	0.14238 (11)	0.35071 (9)	0.0345 (3)
C38	0.70314 (17)	0.11965 (11)	0.42318 (9)	0.0359 (3)
H38A	0.6293	0.1727	0.4349	0.043*

C39	0.72481 (16)	0.02273 (11)	0.47797 (9)	0.0357 (3)
H39A	0.6661	0.0102	0.5267	0.043*
C40	0.83299 (16)	−0.05823 (11)	0.46278 (9)	0.0344 (3)
C41	0.91407 (17)	−0.03660 (12)	0.38827 (9)	0.0383 (3)
H41A	0.9854	−0.0901	0.3753	0.046*
C42	0.89088 (17)	0.06060 (12)	0.33466 (9)	0.0381 (3)
H42A	0.9471	0.0730	0.2852	0.046*
C43	0.97637 (18)	−0.23426 (12)	0.50329 (11)	0.0466 (4)
H43A	0.9452	−0.2578	0.4553	0.070*
H43B	0.9869	−0.2943	0.5512	0.070*
H43C	1.0771	−0.2048	0.4934	0.070*
C44	0.78409 (19)	−0.17104 (13)	0.59719 (10)	0.0449 (4)
H44A	0.6701	−0.1679	0.5897	0.067*
H44B	0.8082	−0.1163	0.6242	0.067*
H44C	0.8243	−0.2404	0.6311	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0305 (7)	0.1253 (13)	0.0850 (10)	0.0195 (7)	0.0028 (7)	0.0394 (10)
N1	0.0331 (7)	0.0471 (8)	0.0617 (10)	−0.0046 (6)	−0.0137 (7)	−0.0039 (7)
N2	0.0325 (6)	0.0321 (6)	0.0396 (6)	0.0046 (5)	−0.0022 (5)	−0.0143 (5)
N3	0.0539 (9)	0.0469 (8)	0.0460 (8)	−0.0205 (7)	−0.0011 (6)	−0.0021 (6)
C1	0.0319 (8)	0.0612 (11)	0.0438 (8)	−0.0004 (7)	0.0018 (7)	−0.0230 (8)
C2	0.0373 (8)	0.0489 (10)	0.0667 (11)	−0.0007 (7)	−0.0017 (8)	−0.0225 (9)
C3	0.0405 (9)	0.0506 (10)	0.0564 (10)	−0.0125 (7)	−0.0023 (8)	−0.0101 (8)
C4	0.0355 (8)	0.0613 (11)	0.0443 (9)	−0.0125 (7)	0.0070 (7)	−0.0203 (8)
C5	0.0273 (7)	0.0540 (9)	0.0398 (8)	−0.0033 (6)	−0.0010 (6)	−0.0208 (7)
C6	0.0265 (7)	0.0555 (9)	0.0333 (7)	−0.0010 (6)	−0.0031 (6)	−0.0144 (7)
C7	0.0288 (8)	0.0702 (11)	0.0402 (8)	0.0084 (7)	−0.0013 (7)	−0.0022 (8)
C8	0.0299 (7)	0.0446 (8)	0.0327 (7)	0.0079 (6)	−0.0012 (6)	−0.0097 (6)
C9	0.0294 (7)	0.0423 (8)	0.0342 (7)	0.0105 (6)	−0.0045 (6)	−0.0112 (6)
C10	0.0316 (7)	0.0318 (7)	0.0353 (7)	0.0062 (6)	−0.0039 (6)	−0.0151 (6)
C11	0.0321 (7)	0.0329 (7)	0.0433 (8)	0.0027 (6)	−0.0066 (6)	−0.0188 (6)
C12	0.0327 (7)	0.0382 (8)	0.0397 (8)	0.0078 (6)	−0.0120 (6)	−0.0161 (6)
C13	0.0370 (8)	0.0382 (8)	0.0312 (7)	0.0074 (6)	−0.0036 (6)	−0.0116 (6)
C14	0.0282 (7)	0.0315 (7)	0.0373 (7)	0.0010 (5)	0.0013 (6)	−0.0162 (6)
C15	0.0268 (6)	0.0329 (7)	0.0341 (7)	0.0001 (5)	0.0033 (5)	−0.0151 (6)
C16	0.0324 (7)	0.0356 (7)	0.0383 (7)	−0.0080 (6)	0.0005 (6)	−0.0129 (6)
C17	0.0368 (8)	0.0423 (8)	0.0356 (7)	−0.0092 (6)	−0.0027 (6)	−0.0091 (6)
C18	0.0355 (7)	0.0377 (8)	0.0362 (7)	−0.0080 (6)	0.0078 (6)	−0.0107 (6)
C19	0.0288 (7)	0.0410 (8)	0.0429 (8)	−0.0106 (6)	0.0062 (6)	−0.0178 (6)
C20	0.0268 (7)	0.0396 (8)	0.0376 (7)	−0.0019 (6)	0.0014 (6)	−0.0178 (6)
C21	0.0625 (11)	0.0469 (10)	0.0538 (10)	−0.0230 (8)	0.0111 (9)	−0.0086 (8)
C22	0.0643 (12)	0.0461 (10)	0.0464 (9)	−0.0115 (8)	−0.0037 (8)	0.0005 (8)
O2	0.0445 (7)	0.0639 (8)	0.0634 (8)	−0.0296 (6)	0.0041 (6)	−0.0095 (6)
N4	0.0375 (8)	0.0514 (9)	0.0751 (11)	−0.0168 (7)	0.0162 (7)	−0.0123 (8)
N5	0.0376 (7)	0.0385 (7)	0.0480 (7)	−0.0147 (5)	0.0099 (6)	−0.0173 (6)

N6	0.0373 (7)	0.0393 (7)	0.0493 (8)	0.0010 (5)	0.0086 (6)	−0.0117 (6)
C23	0.0453 (9)	0.0450 (9)	0.0324 (7)	−0.0118 (7)	−0.0021 (6)	−0.0042 (6)
C24	0.0566 (10)	0.0459 (10)	0.0488 (9)	−0.0127 (8)	0.0021 (8)	−0.0045 (8)
C25	0.0551 (11)	0.0585 (11)	0.0486 (10)	0.0017 (9)	0.0038 (8)	0.0043 (9)
C26	0.0398 (9)	0.0906 (15)	0.0361 (9)	−0.0005 (9)	−0.0018 (7)	−0.0075 (9)
C27	0.0362 (8)	0.0710 (12)	0.0327 (8)	−0.0099 (8)	0.0046 (6)	−0.0180 (8)
C28	0.0346 (7)	0.0528 (9)	0.0288 (7)	−0.0125 (7)	0.0072 (6)	−0.0130 (6)
C29	0.0414 (8)	0.0480 (9)	0.0338 (7)	−0.0200 (7)	0.0068 (6)	−0.0158 (7)
C30	0.0388 (8)	0.0381 (8)	0.0356 (7)	−0.0166 (6)	0.0095 (6)	−0.0178 (6)
C31	0.0388 (8)	0.0366 (8)	0.0387 (7)	−0.0179 (6)	0.0131 (6)	−0.0189 (6)
C32	0.0395 (8)	0.0359 (8)	0.0415 (8)	−0.0154 (6)	0.0117 (6)	−0.0193 (6)
C33	0.0387 (8)	0.0423 (8)	0.0468 (8)	−0.0167 (7)	0.0123 (7)	−0.0213 (7)
C34	0.0405 (8)	0.0450 (9)	0.0462 (8)	−0.0232 (7)	0.0164 (7)	−0.0193 (7)
C35	0.0455 (9)	0.0398 (8)	0.0371 (8)	−0.0178 (7)	0.0109 (7)	−0.0152 (6)
C36	0.0352 (8)	0.0380 (8)	0.0442 (8)	−0.0110 (6)	0.0056 (6)	−0.0201 (6)
C37	0.0313 (7)	0.0375 (8)	0.0406 (8)	−0.0103 (6)	0.0045 (6)	−0.0179 (6)
C38	0.0313 (7)	0.0379 (8)	0.0447 (8)	−0.0051 (6)	0.0063 (6)	−0.0214 (7)
C39	0.0312 (7)	0.0407 (8)	0.0388 (8)	−0.0055 (6)	0.0080 (6)	−0.0160 (6)
C40	0.0264 (7)	0.0383 (8)	0.0428 (8)	−0.0072 (6)	0.0028 (6)	−0.0169 (6)
C41	0.0300 (7)	0.0409 (8)	0.0489 (9)	−0.0026 (6)	0.0084 (6)	−0.0207 (7)
C42	0.0324 (7)	0.0446 (8)	0.0433 (8)	−0.0092 (6)	0.0116 (6)	−0.0202 (7)
C43	0.0336 (8)	0.0404 (9)	0.0655 (11)	−0.0006 (7)	0.0063 (7)	−0.0139 (8)
C44	0.0425 (9)	0.0449 (9)	0.0473 (9)	−0.0068 (7)	0.0051 (7)	−0.0100 (7)

Geometric parameters (Å, °)

O1—C7	1.2300 (19)	O2—C29	1.2333 (17)
N1—H1A	0.91 (2)	N4—H4A	0.89 (2)
N1—H1B	0.869 (19)	N4—H4B	0.90 (2)
N1—C11	1.352 (2)	N4—C33	1.361 (2)
N2—C10	1.4152 (18)	N5—C32	1.4136 (19)
N2—C14	1.2804 (18)	N5—C36	1.2836 (19)
N3—C18	1.3813 (19)	N6—C40	1.3687 (19)
N3—C21	1.457 (2)	N6—C43	1.4529 (19)
N3—C22	1.448 (2)	N6—C44	1.452 (2)
C1—H1	0.9500	C23—H23A	0.9500
C1—C2	1.382 (2)	C23—C24	1.383 (2)
C1—C6	1.395 (2)	C23—C28	1.396 (2)
C2—H2A	0.9500	C24—H24A	0.9500
C2—C3	1.383 (2)	C24—C25	1.382 (3)
C3—H3A	0.9500	C25—H25A	0.9500
C3—C4	1.383 (2)	C25—C26	1.387 (3)
C4—H4	0.9500	C26—H26A	0.9500
C4—C5	1.379 (2)	C26—C27	1.376 (3)
C5—H5A	0.9500	C27—H27A	0.9500
C5—C6	1.395 (2)	C27—C28	1.387 (2)
C6—C7	1.496 (2)	C28—C29	1.503 (2)
C7—C8	1.466 (2)	C29—C30	1.464 (2)
C8—C9	1.400 (2)	C30—C31	1.400 (2)

C8—C13	1.4018 (19)	C30—C35	1.4077 (19)
C9—H9A	0.9500	C31—H31A	0.9500
C9—C10	1.380 (2)	C31—C32	1.378 (2)
C10—C11	1.4256 (19)	C32—C33	1.4249 (19)
C11—C12	1.401 (2)	C33—C34	1.401 (2)
C12—H12A	0.9500	C34—H34A	0.9500
C12—C13	1.376 (2)	C34—C35	1.372 (2)
C13—H13A	0.9500	C35—H35A	0.9500
C14—H14A	0.9500	C36—H36A	0.9500
C14—C15	1.4576 (19)	C36—C37	1.447 (2)
C15—C16	1.3920 (19)	C37—C38	1.397 (2)
C15—C20	1.4008 (19)	C37—C42	1.404 (2)
C16—H16A	0.9500	C38—H38A	0.9500
C16—C17	1.381 (2)	C38—C39	1.375 (2)
C17—H17A	0.9500	C39—H39A	0.9500
C17—C18	1.407 (2)	C39—C40	1.409 (2)
C18—C19	1.412 (2)	C40—C41	1.415 (2)
C19—H19A	0.9500	C41—H41A	0.9500
C19—C20	1.377 (2)	C41—C42	1.370 (2)
C20—H20A	0.9500	C42—H42A	0.9500
C21—H21A	0.9800	C43—H43A	0.9800
C21—H21B	0.9800	C43—H43B	0.9800
C21—H21C	0.9800	C43—H43C	0.9800
C22—H22A	0.9800	C44—H44A	0.9800
C22—H22B	0.9800	C44—H44B	0.9800
C22—H22C	0.9800	C44—H44C	0.9800
H1A—N1—H1B	121.8 (18)	H4A—N4—H4B	124 (2)
H1A—N1—C11	120.1 (13)	H4A—N4—C33	118.1 (13)
H1B—N1—C11	117.8 (12)	H4B—N4—C33	116.3 (14)
C10—N2—C14	120.60 (12)	C32—N5—C36	118.75 (13)
C18—N3—C21	119.76 (14)	C40—N6—C43	120.11 (13)
C18—N3—C22	119.87 (13)	C40—N6—C44	120.44 (12)
C21—N3—C22	116.62 (14)	C43—N6—C44	118.73 (13)
H1—C1—C2	119.8	H23A—C23—C24	119.8
H1—C1—C6	119.8	H23A—C23—C28	119.8
C2—C1—C6	120.48 (15)	C24—C23—C28	120.39 (15)
C1—C2—H2A	120.0	C23—C24—H24A	120.1
C1—C2—C3	120.02 (16)	C23—C24—C25	119.73 (17)
H2A—C2—C3	120.0	H24A—C24—C25	120.1
C2—C3—H3A	120.0	C24—C25—H25A	120.0
C2—C3—C4	120.06 (16)	C24—C25—C26	119.98 (17)
H3A—C3—C4	120.0	H25A—C25—C26	120.0
C3—C4—H4	119.9	C25—C26—H26A	119.8
C3—C4—C5	120.15 (15)	C25—C26—C27	120.41 (16)
H4—C4—C5	119.9	H26A—C26—C27	119.8
C4—C5—H5A	119.8	C26—C27—H27A	119.9
C4—C5—C6	120.46 (15)	C26—C27—C28	120.14 (16)
H5A—C5—C6	119.8	H27A—C27—C28	119.9
C1—C6—C5	118.79 (15)	C23—C28—C27	119.27 (15)

C1—C6—C7	122.89 (14)	C23—C28—C29	122.02 (13)
C5—C6—C7	118.27 (14)	C27—C28—C29	118.61 (14)
O1—C7—C6	118.27 (15)	O2—C29—C28	118.13 (15)
O1—C7—C8	120.55 (16)	O2—C29—C30	121.52 (15)
C6—C7—C8	121.17 (13)	C28—C29—C30	120.34 (12)
C7—C8—C9	118.69 (13)	C29—C30—C31	119.21 (12)
C7—C8—C13	122.79 (14)	C29—C30—C35	122.87 (14)
C9—C8—C13	118.27 (14)	C31—C30—C35	117.85 (14)
C8—C9—H9A	119.0	C30—C31—H31A	118.9
C8—C9—C10	122.01 (13)	C30—C31—C32	122.19 (13)
H9A—C9—C10	119.0	H31A—C31—C32	118.9
N2—C10—C9	125.55 (12)	N5—C32—C31	124.13 (12)
N2—C10—C11	115.25 (13)	N5—C32—C33	116.54 (13)
C9—C10—C11	119.03 (13)	C31—C32—C33	119.18 (14)
N1—C11—C10	118.96 (14)	N4—C33—C32	119.25 (15)
N1—C11—C12	122.21 (14)	N4—C33—C34	122.02 (14)
C10—C11—C12	118.84 (13)	C32—C33—C34	118.73 (14)
C11—C12—H12A	119.5	C33—C34—H34A	119.5
C11—C12—C13	120.92 (13)	C33—C34—C35	120.99 (13)
H12A—C12—C13	119.5	H34A—C34—C35	119.5
C8—C13—C12	120.85 (14)	C30—C35—C34	121.05 (14)
C8—C13—H13A	119.6	C30—C35—H35A	119.5
C12—C13—H13A	119.6	C34—C35—H35A	119.5
N2—C14—H14A	118.8	N5—C36—H36A	118.1
N2—C14—C15	122.37 (13)	N5—C36—C37	123.78 (14)
H14A—C14—C15	118.8	H36A—C36—C37	118.1
C14—C15—C16	120.20 (12)	C36—C37—C38	120.10 (13)
C14—C15—C20	122.49 (12)	C36—C37—C42	122.86 (13)
C16—C15—C20	117.27 (13)	C38—C37—C42	117.03 (14)
C15—C16—H16A	119.1	C37—C38—H38A	119.0
C15—C16—C17	121.83 (13)	C37—C38—C39	121.99 (13)
H16A—C16—C17	119.1	H38A—C38—C39	119.0
C16—C17—H17A	119.5	C38—C39—H39A	119.6
C16—C17—C18	120.94 (13)	C38—C39—C40	120.81 (13)
H17A—C17—C18	119.5	H39A—C39—C40	119.6
N3—C18—C17	121.19 (13)	N6—C40—C39	121.06 (13)
N3—C18—C19	121.48 (13)	N6—C40—C41	121.57 (13)
C17—C18—C19	117.32 (13)	C39—C40—C41	117.37 (14)
C18—C19—H19A	119.6	C40—C41—H41A	119.6
C18—C19—C20	120.79 (13)	C40—C41—C42	120.80 (13)
H19A—C19—C20	119.6	H41A—C41—C42	119.6
C15—C20—C19	121.84 (13)	C37—C42—C41	121.94 (13)
C15—C20—H20A	119.1	C37—C42—H42A	119.0
C19—C20—H20A	119.1	C41—C42—H42A	119.0
N3—C21—H21A	109.5	N6—C43—H43A	109.5
N3—C21—H21B	109.5	N6—C43—H43B	109.5
N3—C21—H21C	109.5	N6—C43—H43C	109.5
H21A—C21—H21B	109.5	H43A—C43—H43B	109.5
H21A—C21—H21C	109.5	H43A—C43—H43C	109.5

H21B—C21—H21C	109.5	H43B—C43—H43C	109.5
N3—C22—H22A	109.5	N6—C44—H44A	109.5
N3—C22—H22B	109.5	N6—C44—H44B	109.5
N3—C22—H22C	109.5	N6—C44—H44C	109.5
H22A—C22—H22B	109.5	H44A—C44—H44B	109.5
H22A—C22—H22C	109.5	H44A—C44—H44C	109.5
H22B—C22—H22C	109.5	H44B—C44—H44C	109.5
C6—C1—C2—C3	−0.7 (2)	C28—C23—C24—C25	−2.7 (2)
C1—C2—C3—C4	1.3 (3)	C23—C24—C25—C26	1.8 (3)
C2—C3—C4—C5	−0.3 (2)	C24—C25—C26—C27	0.8 (3)
C3—C4—C5—C6	−1.4 (2)	C25—C26—C27—C28	−2.4 (2)
C2—C1—C6—C5	−1.0 (2)	C26—C27—C28—C23	1.6 (2)
C2—C1—C6—C7	−178.53 (15)	C26—C27—C28—C29	178.08 (14)
C4—C5—C6—C1	2.1 (2)	C24—C23—C28—C27	1.0 (2)
C4—C5—C6—C7	179.69 (14)	C24—C23—C28—C29	−175.41 (14)
C1—C6—C7—O1	140.30 (19)	C23—C28—C29—O2	135.00 (16)
C1—C6—C7—C8	−40.5 (2)	C23—C28—C29—C30	−44.2 (2)
C5—C6—C7—O1	−37.2 (2)	C27—C28—C29—O2	−41.40 (19)
C5—C6—C7—C8	141.92 (15)	C27—C28—C29—C30	139.41 (14)
O1—C7—C8—C9	−14.6 (3)	O2—C29—C30—C31	−16.8 (2)
O1—C7—C8—C13	159.50 (18)	O2—C29—C30—C35	160.15 (14)
C6—C7—C8—C9	166.22 (14)	C28—C29—C30—C31	162.40 (12)
C6—C7—C8—C13	−19.6 (2)	C28—C29—C30—C35	−20.7 (2)
C7—C8—C9—C10	176.30 (14)	C29—C30—C31—C32	178.31 (13)
C13—C8—C9—C10	1.9 (2)	C35—C30—C31—C32	1.2 (2)
C8—C9—C10—N2	−174.91 (13)	C30—C31—C32—N5	−176.28 (13)
C8—C9—C10—C11	0.0 (2)	C30—C31—C32—C33	−1.0 (2)
C14—N2—C10—C9	−27.7 (2)	C36—N5—C32—C31	−37.7 (2)
C14—N2—C10—C11	157.16 (12)	C36—N5—C32—C33	146.94 (14)
N2—C10—C11—N1	−7.28 (19)	N5—C32—C33—N4	−3.7 (2)
N2—C10—C11—C12	172.89 (12)	N5—C32—C33—C34	175.63 (13)
C9—C10—C11—N1	177.26 (13)	C31—C32—C33—N4	−179.31 (14)
C9—C10—C11—C12	−2.58 (19)	C31—C32—C33—C34	0.0 (2)
N1—C11—C12—C13	−176.61 (14)	N4—C33—C34—C35	−179.97 (15)
C10—C11—C12—C13	3.2 (2)	C32—C33—C34—C35	0.7 (2)
C11—C12—C13—C8	−1.3 (2)	C33—C34—C35—C30	−0.5 (2)
C7—C8—C13—C12	−175.45 (14)	C29—C30—C35—C34	−177.44 (13)
C9—C8—C13—C12	−1.3 (2)	C31—C30—C35—C34	−0.5 (2)
C10—N2—C14—C15	173.35 (11)	C32—N5—C36—C37	174.66 (13)
N2—C14—C15—C16	178.71 (13)	N5—C36—C37—C38	174.95 (14)
N2—C14—C15—C20	−3.5 (2)	N5—C36—C37—C42	−4.2 (2)
C14—C15—C16—C17	177.68 (13)	C36—C37—C38—C39	−177.32 (13)
C20—C15—C16—C17	−0.2 (2)	C42—C37—C38—C39	1.9 (2)
C15—C16—C17—C18	−0.2 (2)	C37—C38—C39—C40	−0.1 (2)
C21—N3—C18—C17	168.15 (15)	C43—N6—C40—C39	−176.35 (14)
C21—N3—C18—C19	−12.8 (2)	C43—N6—C40—C41	4.0 (2)
C22—N3—C18—C17	10.7 (2)	C44—N6—C40—C39	−6.1 (2)
C22—N3—C18—C19	−170.32 (15)	C44—N6—C40—C41	174.22 (14)
C16—C17—C18—N3	179.33 (14)	C38—C39—C40—N6	178.53 (13)

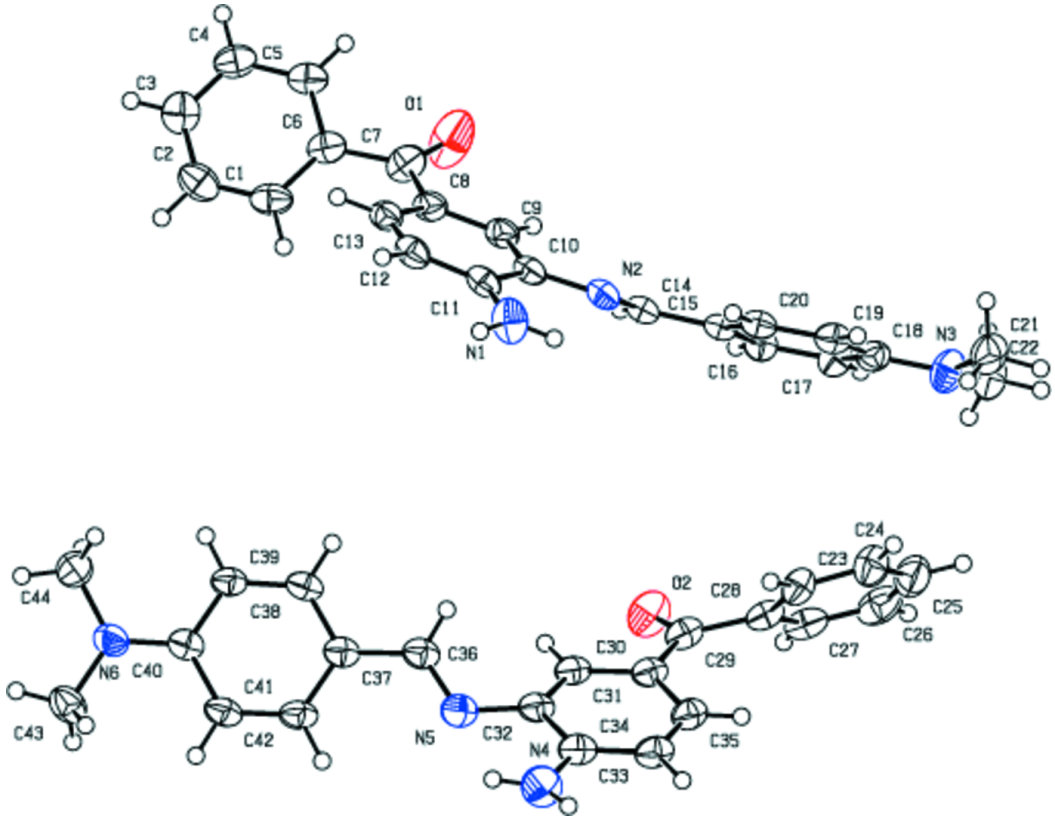
C16—C17—C18—C19	0.3 (2)	C38—C39—C40—C41	−1.8 (2)
N3—C18—C19—C20	−179.02 (13)	N6—C40—C41—C42	−178.38 (14)
C17—C18—C19—C20	0.0 (2)	C39—C40—C41—C42	2.0 (2)
C18—C19—C20—C15	−0.4 (2)	C40—C41—C42—C37	−0.2 (2)
C14—C15—C20—C19	−177.32 (12)	C36—C37—C42—C41	177.45 (14)
C16—C15—C20—C19	0.53 (19)	C38—C37—C42—C41	−1.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.91 (2)	1.92 (2)	2.831 (2)	172.5 (19)
N4—H4A···O2^{i}	0.89 (2)	2.05 (2)	2.9368 (18)	171.5 (18)

Symmetry codes: (i) *x*+1, *y*, *z*.

Fig. 1


C4
C5
C3
C6
O1
C7
C2
C1
C8
C9
C13
C10
C12
N2
C14
C11
C15
C20
C19
C18
N3
C21
C22
N1
C16
C17
C24
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C39
C44
O2
C28
C25
C38
C30
C26
C29
C27
N6
C40
C36
C31
C37
C41
C34
C43
C42
N5
C32
C35
N4
C33

Fig. 2