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N,*N*′-Di-*p*-tolylethylenediamine

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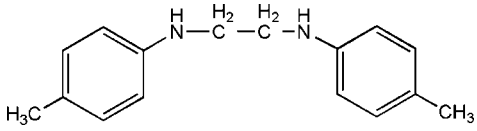
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.090; wR factor = 0.205; data-to-parameter ratio = 16.6.

The asymmetric unit of the title compound, $C_{16}H_{20}N_2$, contains two independent molecules. The rings in each molecule are oriented at dihedral angles of 78.94 (3) and 77.76 (3)°.

Related literature

For general background, see: Yang *et al.* (2004); Garcia-Marco *et al.* (2006). For related literature, see: Türkmen & Çetinkaya (2006); Grasa *et al.* (2001). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{16}H_{20}N_2$
M_r = 240.34
Monoclinic, $P2_1/n$
a = 8.9070 (18) Å
b = 25.252 (5) Å
c = 12.287 (3) Å
β = 90.30 (3)°
V = 2763.5 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.963, T_{max} = 0.987
5764 measured reflections
5408 independent reflections
2777 reflections with $I > 2\sigma(I)$
R_{int} = 0.073
3 standard reflections every 120 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.090
$wR(F^2)$ = 0.205
S = 1.00
5408 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2391).

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supporting information

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N,*N*′-Di-*p*-tolylethylenediamine

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S1. Comment

N,*N*-Disubstituted ethylenediamine compounds are important subunits present in a number of naturally occurring compounds and have found numerous applications as active catalysts (Yang *et al.*, 2004) and intermediates (Garcia-Marco *et al.*, 2006). We report herein the crystal structure of the title compound, (I).

The asymmetric unit of (I) (Fig. 1) contains two independent molecules, in which the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings A (C2—C7), B (C10—C15), C (C18—C23) and D(C26—C31) are, of course, planar and the dihedral angles between them are A/B = 78.94 (3)° and C/D = 77.76 (3)°.

As can be seen from the packing diagram (Fig. 2), the molecules of (I) are elongated along the *b* axis and stacked along the *a* axis.

S2. Experimental

N,*N*′-di-*p*-tolyl-ethylenediimine, (II), was firstly synthesized, according to a literature method (Türkmen & Çetinkaya, 2006). For the preparation of the title compound, (I), compound (II) (2.4 g, 10 mmol) was dissolved in methanol/furanidine (40/60 ml) and mixed with $NaBH_4$ (3.8 g, 100 mmol) (Grasa *et al.*, 2001). The mixture was kept at 298 K and stirred for 30 min, and then deionized water (200 ml) was used to quench the reaction. The mixture was extracted 3 times with ether (50 ml). Ether extracts were dried over $MgSO_4$ and evaporated under reduced pressure to afford (I). The product was purified by repeated crystallization. Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of ethanol (yield; 2.0 g, m.p. 366 K).

S3. Refinement

H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*N*), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

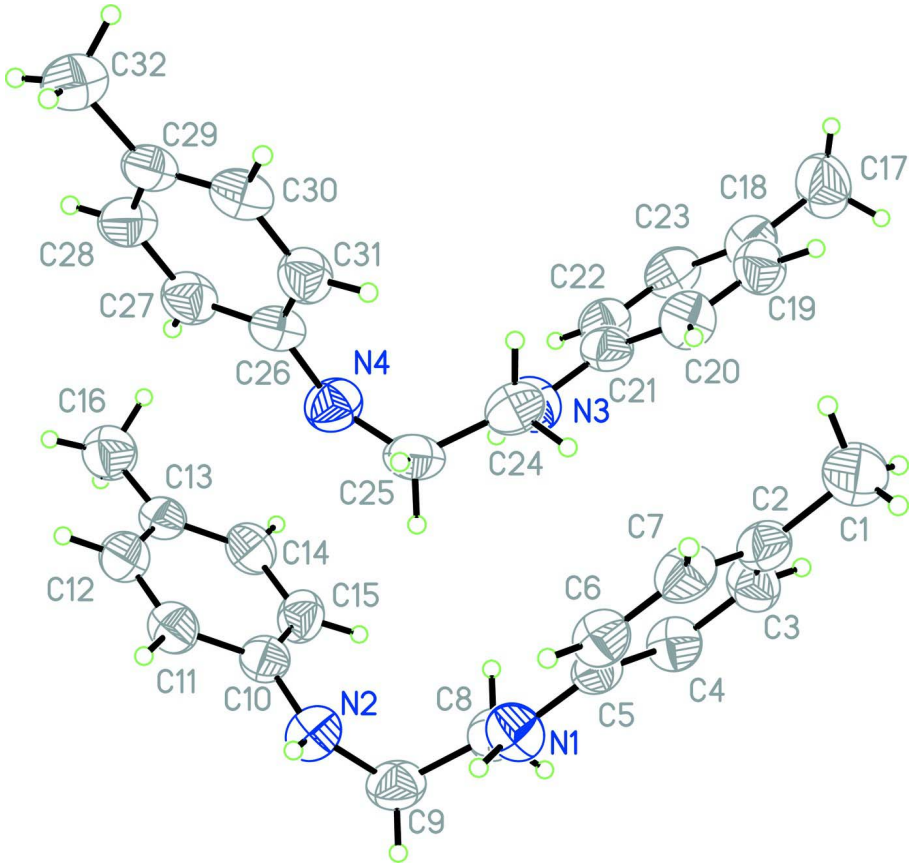

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

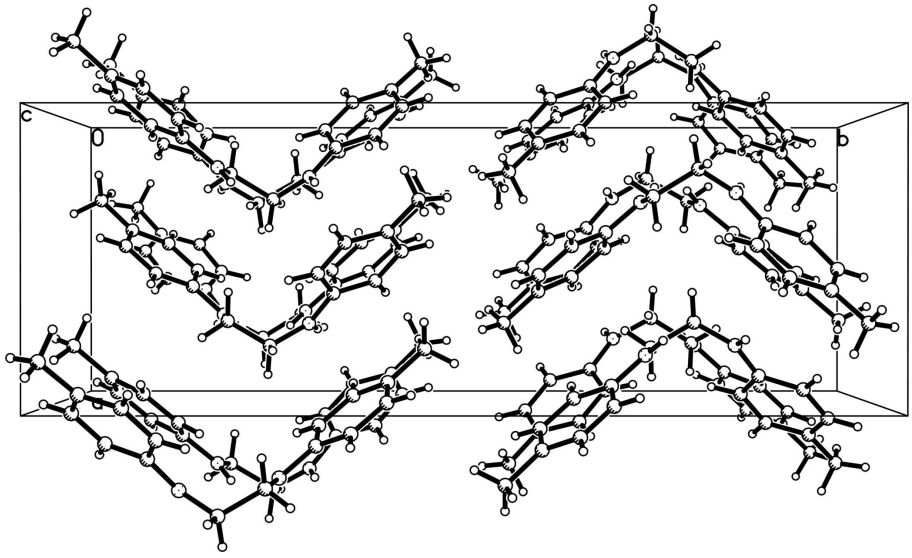

Figure 2

A packing diagram of (I).

N,*N*′-Di-*p*-tolylethylenediamine

Crystal data

$C_{16}H_{20}N_2$
$M_r = 240.34$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.9070$ (18) Å
$b = 25.252$ (5) Å
$c = 12.287$ (3) Å
$\beta = 90.30$ (3)°
$V = 2763.5$ (10) Å^3
$Z = 8$
$F(000) = 1040$
$D_x = 1.155$ Mg m^{-3}
Melting point: 366 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–13°
$\mu = 0.07$ mm^{-1}
$T = 298$ K
Block, yellow
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.963$, $T_{max} = 0.987$
5764 measured reflections
5408 independent reflections
2777 reflections with $I > 2\sigma(I)$
$R_{int} = 0.073$
$\theta_{max} = 26.1°$, $\theta_{min} = 1.6°$
$h = -10 \rightarrow 10$
$k = 0 \rightarrow 31$
$l = 0 \rightarrow 15$
3 standard reflections every 120 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.090$
$wR(F^2) = 0.205$
$S = 1.01$
5408 reflections
325 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.030P)^2 + 5.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
N1	0.6890 (4)	0.29404 (14)	0.1934 (3)	0.0578 (10)
H1A	0.7405	0.2759	0.2396	0.069*
N2	0.7171 (4)	0.18725 (14)	0.1110 (3)	0.0583 (9)

H2A	0.7386	0.1788	0.1770	0.070*
N3	0.1908 (4)	0.29364 (15)	0.0572 (3)	0.0604 (10)
H3B	0.2402	0.2755	0.0102	0.072*
N4	0.2184 (4)	0.18680 (14)	0.1392 (3)	0.0589 (10)
H4B	0.2398	0.1786	0.0732	0.071*
C1	0.2841 (5)	0.4526 (2)	0.3496 (4)	0.0787 (15)
H1B	0.2637	0.4781	0.2936	0.118*
H1C	0.3271	0.4701	0.4117	0.118*
H1D	0.1922	0.4355	0.3703	0.118*
C2	0.3925 (4)	0.41180 (17)	0.3077 (3)	0.0505 (10)
C3	0.4474 (5)	0.41291 (17)	0.2034 (3)	0.0546 (11)
H3A	0.4176	0.4403	0.1576	0.065*
C4	0.5447 (5)	0.37524 (17)	0.1638 (3)	0.0519 (10)
H4A	0.5800	0.3778	0.0929	0.062*
C5	0.5898 (4)	0.33369 (16)	0.2295 (3)	0.0438 (9)
C6	0.5381 (5)	0.33210 (17)	0.3359 (3)	0.0524 (10)
H6A	0.5695	0.3052	0.3824	0.063*
C7	0.4398 (5)	0.37049 (18)	0.3731 (3)	0.0547 (11)
H7A	0.4047	0.3684	0.4442	0.066*
C8	0.7036 (5)	0.28406 (17)	0.0793 (3)	0.0539 (11)
H8A	0.7553	0.3134	0.0449	0.065*
H8B	0.6049	0.2808	0.0462	0.065*
C9	0.7923 (5)	0.23291 (18)	0.0624 (4)	0.0621 (12)
H9A	0.8048	0.2268	−0.0149	0.075*
H9B	0.8913	0.2367	0.0947	0.075*
C10	0.6120 (4)	0.15681 (16)	0.0544 (3)	0.0472 (10)
C11	0.5711 (4)	0.10780 (17)	0.0971 (3)	0.0505 (10)
H11A	0.6138	0.0964	0.1623	0.061*
C12	0.4682 (5)	0.07583 (18)	0.0440 (3)	0.0552 (11)
H12A	0.4420	0.0436	0.0751	0.066*
C13	0.4026 (4)	0.09042 (17)	−0.0545 (3)	0.0491 (10)
C14	0.4421 (5)	0.13987 (17)	−0.0947 (3)	0.0541 (11)
H14A	0.3987	0.1516	−0.1593	0.065*
C15	0.5450 (5)	0.17251 (17)	−0.0407 (3)	0.0534 (11)
H15A	0.5684	0.2054	−0.0700	0.064*
C16	0.3006 (5)	0.05418 (19)	−0.1158 (4)	0.0711 (13)
H16A	0.2869	0.0221	−0.0751	0.107*
H16B	0.3440	0.0460	−0.1852	0.107*
H16C	0.2052	0.0711	−0.1267	0.107*
C17	−0.2095 (6)	0.4545 (2)	−0.0923 (4)	0.0838 (16)
H17A	−0.2377	0.4474	−0.1664	0.126*
H17B	−0.1620	0.4886	−0.0881	0.126*
H17C	−0.2974	0.4543	−0.0475	0.126*
C18	−0.1028 (5)	0.41301 (19)	−0.0536 (4)	0.0593 (12)
C19	−0.0466 (5)	0.41364 (19)	0.0526 (4)	0.0604 (12)
H19A	−0.0737	0.4410	0.0991	0.073*
C20	0.0485 (5)	0.37439 (18)	0.0901 (3)	0.0581 (11)
H20A	0.0829	0.3756	0.1617	0.070*

C21	0.0935 (4)	0.33335 (18)	0.0231 (3)	0.0496 (10)
C22	0.0385 (5)	0.33360 (18)	−0.0840 (3)	0.0530 (11)
H22A	0.0676	0.3070	−0.1318	0.064*
C23	−0.0559 (5)	0.37197 (19)	−0.1190 (3)	0.0582 (11)
H23A	−0.0909	0.3706	−0.1904	0.070*
C24	0.2085 (5)	0.28304 (18)	0.1726 (3)	0.0576 (11)
H24A	0.1106	0.2807	0.2065	0.069*
H24B	0.2636	0.3117	0.2068	0.069*
C25	0.2919 (5)	0.23195 (18)	0.1878 (4)	0.0612 (12)
H25A	0.3911	0.2355	0.1565	0.073*
H25B	0.3044	0.2255	0.2652	0.073*
C26	0.1144 (4)	0.15593 (17)	0.1944 (3)	0.0494 (10)
C27	0.0724 (5)	0.10681 (17)	0.1522 (3)	0.0554 (11)
H27A	0.1130	0.0957	0.0864	0.067*
C28	−0.0276 (4)	0.07439 (19)	0.2054 (3)	0.0563 (11)
H28A	−0.0522	0.0417	0.1754	0.068*
C29	−0.0921 (4)	0.08947 (18)	0.3025 (4)	0.0528 (11)
C30	−0.0557 (4)	0.13840 (18)	0.3422 (3)	0.0543 (11)
H30A	−0.1002	0.1500	0.4062	0.065*
C31	0.0463 (5)	0.17143 (17)	0.2895 (3)	0.0532 (11)
H31A	0.0686	0.2044	0.3190	0.064*
C32	−0.1948 (5)	0.0527 (2)	0.3631 (4)	0.0749 (14)
H32A	−0.2045	0.0201	0.3236	0.112*
H32B	−0.2918	0.0689	0.3704	0.112*
H32C	−0.1536	0.0456	0.4340	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.061 (2)	0.063 (2)	0.049 (2)	0.0077 (19)	−0.0055 (17)	−0.0029 (18)
N2	0.060 (2)	0.058 (2)	0.057 (2)	−0.0088 (19)	−0.0006 (17)	−0.0001 (18)
N3	0.062 (2)	0.067 (3)	0.053 (2)	0.006 (2)	0.0096 (18)	−0.0017 (18)
N4	0.056 (2)	0.063 (2)	0.058 (2)	−0.0058 (19)	0.0077 (17)	−0.0012 (19)
C1	0.068 (3)	0.073 (4)	0.096 (4)	−0.001 (3)	0.024 (3)	−0.004 (3)
C2	0.044 (2)	0.050 (3)	0.057 (3)	−0.008 (2)	0.0098 (19)	0.000 (2)
C3	0.055 (3)	0.050 (3)	0.058 (3)	0.007 (2)	0.002 (2)	0.011 (2)
C4	0.055 (3)	0.055 (3)	0.045 (2)	−0.002 (2)	0.0029 (19)	0.006 (2)
C5	0.037 (2)	0.047 (2)	0.047 (2)	−0.0055 (18)	−0.0002 (16)	−0.0055 (19)
C6	0.056 (3)	0.055 (3)	0.047 (2)	−0.005 (2)	−0.0011 (19)	0.006 (2)
C7	0.057 (3)	0.061 (3)	0.046 (2)	−0.013 (2)	0.014 (2)	0.001 (2)
C8	0.054 (3)	0.054 (3)	0.054 (3)	−0.003 (2)	0.013 (2)	0.001 (2)
C9	0.047 (3)	0.070 (3)	0.069 (3)	−0.004 (2)	0.012 (2)	−0.008 (2)
C10	0.043 (2)	0.050 (3)	0.048 (2)	0.0009 (19)	0.0076 (18)	−0.0017 (19)
C11	0.051 (3)	0.053 (3)	0.047 (2)	0.005 (2)	0.0049 (19)	0.007 (2)
C12	0.051 (3)	0.053 (3)	0.061 (3)	0.002 (2)	0.004 (2)	0.007 (2)
C13	0.039 (2)	0.048 (3)	0.061 (3)	0.0031 (19)	0.0045 (19)	−0.005 (2)
C14	0.057 (3)	0.057 (3)	0.048 (2)	0.009 (2)	−0.003 (2)	0.000 (2)
C15	0.060 (3)	0.046 (3)	0.055 (3)	−0.003 (2)	0.008 (2)	0.007 (2)

C16	0.065 (3)	0.066 (3)	0.083 (3)	0.002 (3)	−0.008 (3)	−0.006 (3)
C17	0.082 (4)	0.068 (3)	0.101 (4)	0.012 (3)	−0.029 (3)	−0.003 (3)
C18	0.062 (3)	0.058 (3)	0.058 (3)	−0.007 (2)	−0.003 (2)	0.001 (2)
C19	0.059 (3)	0.058 (3)	0.064 (3)	0.003 (2)	−0.002 (2)	−0.013 (2)
C20	0.067 (3)	0.064 (3)	0.043 (2)	−0.002 (2)	−0.005 (2)	−0.006 (2)
C21	0.041 (2)	0.057 (3)	0.051 (2)	−0.002 (2)	0.0087 (18)	0.002 (2)
C22	0.053 (3)	0.059 (3)	0.047 (2)	−0.008 (2)	0.0018 (19)	−0.007 (2)
C23	0.058 (3)	0.068 (3)	0.048 (2)	−0.011 (2)	−0.003 (2)	0.001 (2)
C24	0.052 (3)	0.064 (3)	0.057 (3)	−0.010 (2)	−0.006 (2)	−0.003 (2)
C25	0.037 (2)	0.071 (3)	0.075 (3)	0.001 (2)	−0.001 (2)	0.005 (3)
C26	0.037 (2)	0.060 (3)	0.052 (2)	0.004 (2)	0.0011 (18)	−0.003 (2)
C27	0.053 (3)	0.059 (3)	0.054 (3)	0.006 (2)	0.007 (2)	−0.010 (2)
C28	0.044 (2)	0.064 (3)	0.061 (3)	−0.002 (2)	0.001 (2)	−0.006 (2)
C29	0.037 (2)	0.057 (3)	0.064 (3)	0.006 (2)	0.0062 (19)	0.005 (2)
C30	0.044 (2)	0.069 (3)	0.050 (2)	0.008 (2)	0.0035 (19)	−0.005 (2)
C31	0.054 (3)	0.051 (3)	0.054 (2)	0.003 (2)	0.001 (2)	−0.008 (2)
C32	0.055 (3)	0.078 (4)	0.092 (4)	−0.004 (3)	0.011 (3)	0.012 (3)

Geometric parameters (Å, º)

N1—C5	1.409 (5)	N3—C21	1.389 (5)
N1—C8	1.430 (5)	N3—C24	1.451 (5)
N1—H1A	0.8600	N3—H3B	0.8600
N2—C10	1.394 (5)	N4—C26	1.389 (5)
N2—C9	1.462 (5)	N4—C25	1.443 (5)
N2—H2A	0.8600	N4—H4B	0.8600
C1—C2	1.504 (6)	C17—C18	1.491 (6)
C1—H1B	0.9600	C17—H17A	0.9600
C1—H1C	0.9600	C17—H17B	0.9600
C1—H1D	0.9600	C17—H17C	0.9600
C2—C3	1.374 (5)	C18—C23	1.377 (6)
C2—C7	1.381 (6)	C18—C19	1.396 (6)
C3—C4	1.378 (6)	C19—C20	1.381 (6)
C3—H3A	0.9300	C19—H19A	0.9300
C4—C5	1.383 (5)	C20—C21	1.384 (6)
C4—H4A	0.9300	C20—H20A	0.9300
C5—C6	1.389 (5)	C21—C22	1.402 (5)
C6—C7	1.385 (6)	C22—C23	1.352 (6)
C6—H6A	0.9300	C22—H22A	0.9300
C7—H7A	0.9300	C23—H23A	0.9300
C8—C9	1.529 (6)	C24—C25	1.500 (6)
C8—H8A	0.9700	C24—H24A	0.9700
C8—H8B	0.9700	C24—H24B	0.9700
C9—H9A	0.9700	C25—H25A	0.9700
C9—H9B	0.9700	C25—H25B	0.9700
C10—C15	1.368 (5)	C26—C31	1.376 (5)
C10—C11	1.393 (5)	C26—C27	1.395 (6)
C11—C12	1.383 (6)	C27—C28	1.378 (6)

C11—H11A	0.9300	C27—H27A	0.9300
C12—C13	1.391 (6)	C28—C29	1.380 (6)
C12—H12A	0.9300	C28—H28A	0.9300
C13—C14	1.389 (6)	C29—C30	1.367 (6)
C13—C16	1.491 (6)	C29—C32	1.504 (6)
C14—C15	1.398 (6)	C30—C31	1.396 (6)
C14—H14A	0.9300	C30—H30A	0.9300
C15—H15A	0.9300	C31—H31A	0.9300
C16—H16A	0.9600	C32—H32A	0.9600
C16—H16B	0.9600	C32—H32B	0.9600
C16—H16C	0.9600	C32—H32C	0.9600

C5—N1—C8	119.7 (3)	C21—N3—C24	119.5 (4)
C5—N1—H1A	120.2	C21—N3—H3B	120.3
C8—N1—H1A	120.2	C24—N3—H3B	120.3
C10—N2—C9	122.6 (4)	C26—N4—C25	122.9 (4)
C10—N2—H2A	118.7	C26—N4—H4B	118.5
C9—N2—H2A	118.7	C25—N4—H4B	118.5
C2—C1—H1B	109.5	C18—C17—H17A	109.5
C2—C1—H1C	109.5	C18—C17—H17B	109.5
H1B—C1—H1C	109.5	H17A—C17—H17B	109.5
C2—C1—H1D	109.5	C18—C17—H17C	109.5
H1B—C1—H1D	109.5	H17A—C17—H17C	109.5
H1C—C1—H1D	109.5	H17B—C17—H17C	109.5
C3—C2—C7	116.7 (4)	C23—C18—C19	116.4 (4)
C3—C2—C1	122.5 (4)	C23—C18—C17	122.6 (4)
C7—C2—C1	120.8 (4)	C19—C18—C17	121.0 (4)
C2—C3—C4	122.9 (4)	C20—C19—C18	121.4 (4)
C2—C3—H3A	118.5	C20—C19—H19A	119.3
C4—C3—H3A	118.5	C18—C19—H19A	119.3
C3—C4—C5	119.9 (4)	C19—C20—C21	121.2 (4)
C3—C4—H4A	120.1	C19—C20—H20A	119.4
C5—C4—H4A	120.1	C21—C20—H20A	119.4
C4—C5—C6	118.4 (4)	C20—C21—N3	122.9 (4)
C4—C5—N1	122.4 (4)	C20—C21—C22	117.0 (4)
C6—C5—N1	119.2 (4)	N3—C21—C22	120.0 (4)
C7—C6—C5	120.2 (4)	C23—C22—C21	121.0 (4)
C7—C6—H6A	119.9	C23—C22—H22A	119.5
C5—C6—H6A	119.9	C21—C22—H22A	119.5
C2—C7—C6	121.8 (4)	C22—C23—C18	123.0 (4)
C2—C7—H7A	119.1	C22—C23—H23A	118.5
C6—C7—H7A	119.1	C18—C23—H23A	118.5
N1—C8—C9	109.4 (4)	N3—C24—C25	109.4 (4)
N1—C8—H8A	109.8	N3—C24—H24A	109.8
C9—C8—H8A	109.8	C25—C24—H24A	109.8
N1—C8—H8B	109.8	N3—C24—H24B	109.8
C9—C8—H8B	109.8	C25—C24—H24B	109.8
H8A—C8—H8B	108.2	H24A—C24—H24B	108.2

N2—C9—C8	111.9 (3)	N4—C25—C24	113.9 (3)
N2—C9—H9A	109.2	N4—C25—H25A	108.8
C8—C9—H9A	109.2	C24—C25—H25A	108.8
N2—C9—H9B	109.2	N4—C25—H25B	108.8
C8—C9—H9B	109.2	C24—C25—H25B	108.8
H9A—C9—H9B	107.9	H25A—C25—H25B	107.7
C15—C10—C11	117.8 (4)	C31—C26—N4	123.5 (4)
C15—C10—N2	123.7 (4)	C31—C26—C27	116.8 (4)
C11—C10—N2	118.5 (4)	N4—C26—C27	119.7 (4)
C12—C11—C10	121.0 (4)	C28—C27—C26	121.6 (4)
C12—C11—H11A	119.5	C28—C27—H27A	119.2
C10—C11—H11A	119.5	C26—C27—H27A	119.2
C11—C12—C13	122.0 (4)	C27—C28—C29	121.3 (4)
C11—C12—H12A	119.0	C27—C28—H28A	119.3
C13—C12—H12A	119.0	C29—C28—H28A	119.3
C14—C13—C12	116.2 (4)	C30—C29—C28	117.3 (4)
C14—C13—C16	121.8 (4)	C30—C29—C32	121.7 (4)
C12—C13—C16	122.0 (4)	C28—C29—C32	121.0 (4)
C13—C14—C15	121.9 (4)	C29—C30—C31	121.9 (4)
C13—C14—H14A	119.1	C29—C30—H30A	119.0
C15—C14—H14A	119.1	C31—C30—H30A	119.0
C10—C15—C14	121.1 (4)	C26—C31—C30	121.0 (4)
C10—C15—H15A	119.5	C26—C31—H31A	119.5
C14—C15—H15A	119.5	C30—C31—H31A	119.5
C13—C16—H16A	109.5	C29—C32—H32A	109.5
C13—C16—H16B	109.5	C29—C32—H32B	109.5
H16A—C16—H16B	109.5	H32A—C32—H32B	109.5
C13—C16—H16C	109.5	C29—C32—H32C	109.5
H16A—C16—H16C	109.5	H32A—C32—H32C	109.5
H16B—C16—H16C	109.5	H32B—C32—H32C	109.5

C7—C2—C3—C4	0.1 (6)	C23—C18—C19—C20	−1.3 (7)
C1—C2—C3—C4	−178.9 (4)	C17—C18—C19—C20	177.9 (5)
C2—C3—C4—C5	0.7 (6)	C18—C19—C20—C21	1.0 (7)
C3—C4—C5—C6	−1.8 (6)	C19—C20—C21—N3	178.9 (4)
C3—C4—C5—N1	180.0 (4)	C19—C20—C21—C22	0.2 (6)
C8—N1—C5—C4	−22.9 (6)	C24—N3—C21—C20	21.4 (6)
C8—N1—C5—C6	158.9 (4)	C24—N3—C21—C22	−159.9 (4)
C4—C5—C6—C7	2.1 (6)	C20—C21—C22—C23	−1.0 (6)
N1—C5—C6—C7	−179.6 (4)	N3—C21—C22—C23	−179.8 (4)
C3—C2—C7—C6	0.2 (6)	C21—C22—C23—C18	0.7 (7)
C1—C2—C7—C6	179.2 (4)	C19—C18—C23—C22	0.4 (7)
C5—C6—C7—C2	−1.3 (6)	C17—C18—C23—C22	−178.7 (4)
C5—N1—C8—C9	−168.9 (3)	C21—N3—C24—C25	168.1 (4)
C10—N2—C9—C8	89.0 (5)	C26—N4—C25—C24	−89.5 (5)
N1—C8—C9—N2	60.7 (5)	N3—C24—C25—N4	−59.3 (5)
C9—N2—C10—C15	−14.7 (6)	C25—N4—C26—C31	15.1 (6)
C9—N2—C10—C11	165.9 (4)	C25—N4—C26—C27	−166.1 (4)

C15—C10—C11—C12	1.0 (6)	C31—C26—C27—C28	−2.6 (6)
N2—C10—C11—C12	−179.5 (4)	N4—C26—C27—C28	178.5 (4)
C10—C11—C12—C13	1.0 (6)	C26—C27—C28—C29	0.7 (6)
C11—C12—C13—C14	−2.3 (6)	C27—C28—C29—C30	1.7 (6)
C11—C12—C13—C16	175.2 (4)	C27—C28—C29—C32	−176.7 (4)
C12—C13—C14—C15	1.7 (6)	C28—C29—C30—C31	−2.2 (6)
C16—C13—C14—C15	−175.9 (4)	C32—C29—C30—C31	176.2 (4)
C11—C10—C15—C14	−1.6 (6)	N4—C26—C31—C30	−179.0 (4)
N2—C10—C15—C14	179.0 (4)	C27—C26—C31—C30	2.2 (6)
C13—C14—C15—C10	0.2 (6)	C29—C30—C31—C26	0.2 (6)