

# *N'*-(2,6-Dimethylphenyl)-*N*-phenylmethanimidamide

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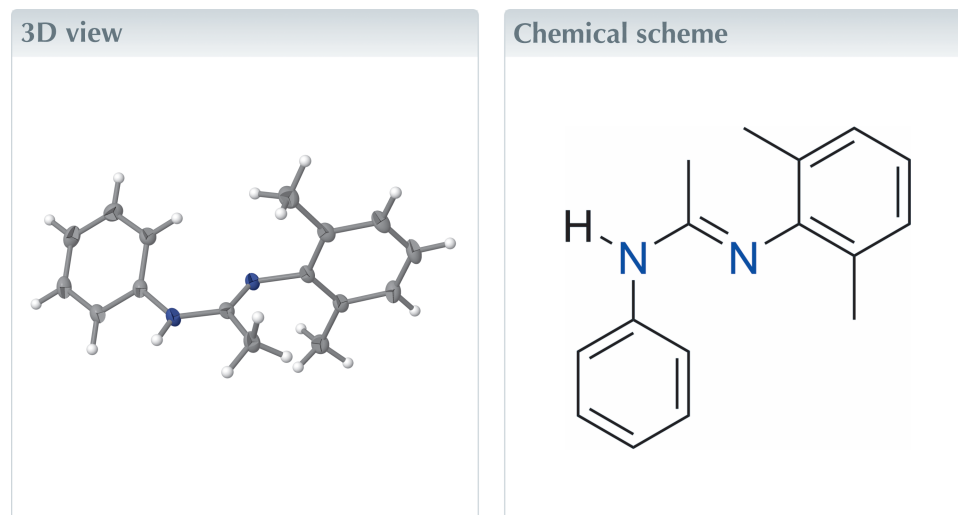
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**Keywords:** crystal structure; acetamidine; hydrogen bonding.

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

The title compound, C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>, is a non-symmetrically *N,N'*-disubstituted acetamidine having a phenyl and a bulky 2,6-dimethylphenyl as substituents on the two N atoms of the N—C—N linkage. It crystallizes in an *E-syn* configuration and its amidine C—N bonds present distinct amine [1.366 (1) Å] and imine [1.288 (1) Å] bond lengths. In the extended structure, strong N—H...N hydrogen bonds link the molecules into infinite *C*(4) chains propagating along the *c*-axis direction; weak C—H... $\pi$  interactions are also present in the crystal packing.



## Structure description

The molecular structure of the title compound, C<sub>16</sub>H<sub>18</sub>N<sub>2</sub> (**1**) (Fig. 1) was determined at 100 K. Compound **1** was obtained as a result of a test reaction for synthesizing non-symmetrical amidines under microwave activation by sequential introduction of the *N*-substituents, with the final goal to serve as precursor for the corresponding amidine-*N*-oxide/hydroxyamidine derivative (Cibian *et al.*, 2011; Saha *et al.*, 2024). Although crystallographic evidence of various non-symmetric acetamidines with *N,N'*-bisarylamidines exists (*e.g.*, Stibrany & Potenza, 2007; Peoples *et al.*, 2012), this is the first report of **1**, an acetamidine having a phenyl and a bulky 2,6-dimethylphenyl as substituents on the two N atoms of the N—C—N linkage. It crystallizes in the monoclinic *P*2<sub>1</sub>/*c* space group, in the *E-syn* configuration (Kalz *et al.*, 2016). Its amidine C—N bonds present distinct amine [1.366 (1) Å] and imine [1.288 (1) Å] bond lengths, as also found for *N,N'*-disubstituted arylamidine (Boéré *et al.*, 1998; Cottin *et al.*, 2021). The phenyl and 2,6-dimethylphenyl groups are positioned on the amine and imine N atoms, respectively.

In **1**, the bulky substituted C9—C14 aryl ring and the C3—C8 phenyl ring subtend tilt angles of 85.3 (1) and 40.4 (1)°, respectively, with the N1—C1—N2 plane; the pendant

**Table 1**

Hydrogen-bond geometry (Å, °).

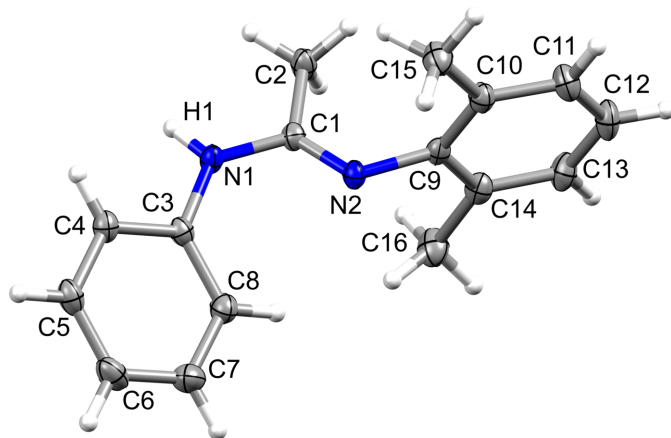
$Cg_1$  and  $Cg_2$  are the centroids of the C3–C8 phenyl and C9–C14 2,6-dimethylphenyl rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots N2^i$	0.882 (15)	2.172 (15)	3.0530 (14)	176.3 (14)
$C2-H2C\cdots Cg_1^i$	0.98	2.83	3.5601 (14)	132
$C4-H4\cdots Cg_2^i$	0.95	2.59	3.5092 (13)	162
$C15-H15A\cdots Cg_1^{ii}$	0.98	2.83	3.6346 (15)	140

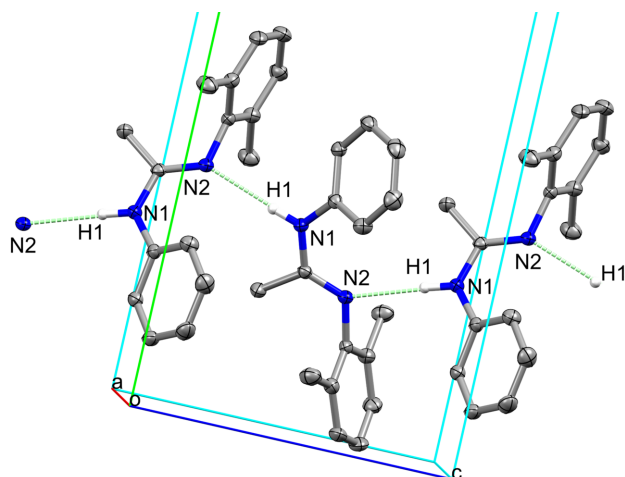
Symmetry codes: (i)  $x, -y + \frac{3}{2}, z + \frac{1}{2}$ ; (ii)  $x - 1, -y + \frac{3}{2}, z - \frac{1}{2}$ .

rings are tilted by  $64.3(1)^\circ$  with respect to each other. The C3–N1–C1–N2 and N1–C1–N2–C9 torsion angles are  $-11.33(18)$  and  $176.57(10)^\circ$ , respectively.

In the extended structure of **1** (Table 1 and Figs. 2 and 3), the molecules are linked by  $N-H\cdots N$  strong hydrogen bonds (Desiraju & Steiner, 2001) between the amidine H1 proton and the N2 atom of the amidine unit in an adjacent molecule, thereby forming infinite  $C(4)$  chains of molecules propagating along the  $c$ -axis direction. Weak  $C-H\cdots\pi$  interactions (Desiraju & Steiner, 2001) complete the crystal packing.



**Figure 1**  
The molecular structure of **1**, with displacement ellipsoids drawn at 50% probability level.



**Figure 2**  
Part of a [001] hydrogen-bonded chain in the extended structure of **1**.

**Table 2**

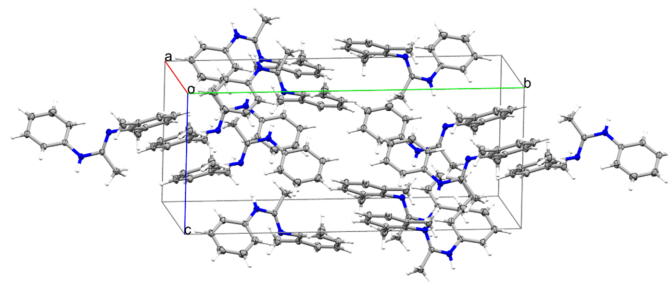
Experimental details.

Crystal data	$C_{16}H_{18}N_2$
Chemical formula	238.32
$M_r$	Monoclinic, $P2_1/c$
Crystal system, space group	100
Temperature (K)	7.2094 (1), 21.3517 (4), 8.9033 (2)
$a, b, c$ (Å)	95.418 (1)
$\beta$ (°)	1364.39 (4)
$V$ (Å <sup>3</sup> )	4
$Z$	Cu $K\alpha$
Radiation type	0.53
$\mu$ (mm <sup>-1</sup> )	0.21 × 0.04 × 0.01 × 0.01 (radius)
Crystal size (mm)	
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	For a sphere (SADABS; Krause <i>et al.</i> , 2015)
$T_{min}, T_{max}$	0.807, 0.993
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	21279, 2595, 2160
$R_{int}$	0.030
$(\sin \theta/\lambda)_{max}$ (Å <sup>-1</sup> )	0.613
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.038, 0.113, 1.08
No. of reflections	2595
No. of parameters	170
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.28, -0.27

Computer programs: APEX2 (Bruker, 2009), SAINT (Bruker, 2020), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), OLEX2 (Dolomanov *et al.*, 2009), ORTEP-3 for Windows (Farrugia, 2012), publCIF (Westrip, 2010), POV-RAY (POVRAY, 2013), PLATON (Spek, 2020) and Mercury (Macrae *et al.*, 2020).

## Synthesis and crystallization

A microwave vial was charged with 600 mg of 4 Å molecular sieves, triethylorthoacetate (1.5 ml, 8.18 mmol, 1 equiv.), 2 drops of acetic acid, and aniline (0.75 ml, 8.18 mmol, 1 equiv.). The reaction was conducted under microwave irradiation at 90 °C for 10 min. After cooling down, 2,6-dimethylaniline (1.01 ml, 8.18 mmol, 1 equiv.) was added to the crude reaction mixture and the reaction was continued at 90 °C for another 16 h. Part of the reaction mixture was taken in hexane (the molecular sieves were removed by filtration) and the solution was placed in the freezer ( $-10^\circ\text{C}$ ). XRD-quality colorless crystals were obtained (0.50 g, 2.10 mmol, partial yield: 26% – only part of the product was purified).



**Figure 3**  
View of the crystal packing of **1** in the unit cell.

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ): 1.69 (s, 3H); 1.99 (s, 6H), 6.76 (t,  $J = 7.5$  Hz, 1H), 6.91 (t,  $J = 7.3$  Hz, 1H), 6.98 (d,  $J = 7.5$  Hz, 2H), 7.25 (t,  $J = 7.5$  Hz, 2H), 7.82 (d,  $J = 7.9$  Hz, 2H), 8.87 (s, 1H, NH).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ): 17.9, 18.0, 118.7, 121.0, 121.1, 127.0, 127.5, 128.2, 141.4, 148.5, 152.2 (N=C=N). Elemental analysis C/H/N: calculated (%) for  $\text{C}_{16}\text{H}_{18}\text{N}_2$ : C 80.63, H 7.61, N 11.75; exp.: C 80.57, H 7.56, N 11.81. HRMS (ESI, positive):  $m/z$  [ $M + \text{H}$ ] $^+$  calculated: 239.15428; exp.: 239.15398 (diff. 1.25 p.p.m.).

## Refinement

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

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## full crystallographic data

*IUCrData* (2025). **10**, x250867 [https://doi.org/10.1107/S2414314625008673]

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## Crystal data

$C_{16}H_{18}N_2$	$F(000) = 512$
$M_r = 238.32$	$D_x = 1.160 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
$a = 7.2094 (1) \text{ \AA}$	Cell parameters from 7241 reflections
$b = 21.3517 (4) \text{ \AA}$	$\theta = 4.1\text{--}70.8^\circ$
$c = 8.9033 (2) \text{ \AA}$	$\mu = 0.53 \text{ mm}^{-1}$
$\beta = 95.418 (1)^\circ$	$T = 100 \text{ K}$
$V = 1364.39 (4) \text{ \AA}^3$	Needle, colourless
$Z = 4$	$0.21 \times 0.04 \times 0.01 \times 0.01$ (radius) mm

## Data collection

Bruker SMART APEXII CCD diffractometer	$T_{\min} = 0.807, T_{\max} = 0.993$
Radiation source: microfocus sealed X-ray tube, Incoatec $I\mu\text{s}$	21279 measured reflections
Mirror optics monochromator	2595 independent reflections
Detector resolution: $7.9 \text{ pixels mm}^{-1}$	2160 reflections with $I > 2\sigma(I)$
$\omega$ and $\phi$ scans	$R_{\text{int}} = 0.030$
Absorption correction: for a sphere (SADABS; Krause <i>et al.</i> , 2015)	$\theta_{\max} = 71.0^\circ, \theta_{\min} = 4.1^\circ$
	$h = -8 \rightarrow 8$
	$k = -26 \rightarrow 26$
	$l = -10 \rightarrow 10$

## Refinement

Refinement on $F^2$	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.0716P)^2 + 0.0724P]$
$wR(F^2) = 0.113$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{\max} < 0.001$
2595 reflections	$\Delta\rho_{\max} = 0.28 \text{ e \AA}^{-3}$
170 parameters	$\Delta\rho_{\min} = -0.27 \text{ e \AA}^{-3}$
0 restraints	
Primary atom site location: dual	

## 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.** H atoms were included in calculated positions ( $C-H = 0.95\text{--}0.98 \text{ \AA}$ ) and treated as riding atoms with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ . The NH proton (H1) was located in the difference-Fourier map and refined freely.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.67938 (14)	0.76538 (4)	1.09532 (11)	0.0191 (2)
H1	0.660 (2)	0.7773 (7)	1.1875 (16)	0.030 (4)*
N2	0.62606 (14)	0.68830 (4)	0.91279 (11)	0.0180 (2)
C1	0.61447 (16)	0.70782 (5)	1.04845 (12)	0.0174 (3)
C2	0.52870 (19)	0.67095 (6)	1.16869 (13)	0.0233 (3)
H2A	0.417882	0.648897	1.123623	0.035*
H2B	0.493168	0.699538	1.247175	0.035*
H2C	0.619298	0.640440	1.213416	0.035*
C3	0.79195 (17)	0.80654 (5)	1.01846 (12)	0.0185 (3)
C4	0.77137 (17)	0.87086 (5)	1.04025 (13)	0.0209 (3)
H4	0.677614	0.885791	1.099341	0.025*
C5	0.88698 (18)	0.91300 (6)	0.97613 (14)	0.0252 (3)
H5	0.873702	0.956622	0.993177	0.030*
C6	1.02225 (19)	0.89181 (6)	0.88702 (14)	0.0295 (3)
H6	1.101809	0.920649	0.843217	0.035*
C7	1.03948 (19)	0.82817 (7)	0.86297 (15)	0.0298 (3)
H7	1.130352	0.813541	0.800713	0.036*
C8	0.92670 (17)	0.78530 (6)	0.92795 (14)	0.0237 (3)
H8	0.941096	0.741724	0.910947	0.028*
C9	0.56482 (17)	0.62633 (5)	0.87387 (12)	0.0184 (3)
C10	0.38863 (17)	0.61776 (6)	0.79602 (13)	0.0218 (3)
C11	0.33856 (19)	0.55810 (6)	0.74243 (14)	0.0274 (3)
H11	0.219225	0.551720	0.689757	0.033*
C12	0.4601 (2)	0.50815 (6)	0.76486 (15)	0.0299 (3)
H12	0.424966	0.467915	0.726479	0.036*
C13	0.6326 (2)	0.51699 (6)	0.84329 (14)	0.0267 (3)
H13	0.714719	0.482358	0.859959	0.032*
C14	0.68861 (17)	0.57583 (6)	0.89848 (13)	0.0220 (3)
C15	0.25781 (19)	0.67238 (6)	0.76836 (16)	0.0292 (3)
H15A	0.134837	0.657116	0.728148	0.044*
H15B	0.306460	0.700987	0.695456	0.044*
H15C	0.246968	0.694588	0.863457	0.044*
C16	0.87995 (19)	0.58474 (6)	0.97859 (16)	0.0314 (3)
H16A	0.963149	0.551898	0.947325	0.047*
H16B	0.873019	0.582271	1.087825	0.047*
H16C	0.928376	0.625855	0.952801	0.047*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0265 (5)	0.0145 (5)	0.0167 (5)	−0.0016 (4)	0.0034 (4)	−0.0011 (4)
N2	0.0220 (5)	0.0134 (5)	0.0184 (5)	−0.0002 (4)	0.0011 (4)	0.0001 (4)
C1	0.0194 (6)	0.0135 (6)	0.0189 (6)	0.0017 (4)	0.0004 (4)	0.0014 (4)
C2	0.0329 (7)	0.0174 (6)	0.0201 (6)	−0.0040 (5)	0.0052 (5)	−0.0003 (4)
C3	0.0209 (6)	0.0173 (6)	0.0166 (6)	−0.0025 (4)	−0.0019 (5)	0.0011 (4)

C4	0.0260 (6)	0.0174 (6)	0.0187 (6)	-0.0006 (5)	-0.0007 (5)	-0.0001 (4)
C5	0.0333 (7)	0.0177 (6)	0.0236 (6)	-0.0055 (5)	-0.0027 (5)	0.0023 (4)
C6	0.0324 (7)	0.0292 (7)	0.0269 (7)	-0.0119 (6)	0.0027 (6)	0.0040 (5)
C7	0.0263 (7)	0.0335 (8)	0.0307 (7)	-0.0045 (6)	0.0081 (6)	-0.0017 (5)
C8	0.0237 (6)	0.0200 (6)	0.0275 (6)	0.0004 (5)	0.0027 (5)	-0.0014 (5)
C9	0.0261 (6)	0.0148 (6)	0.0148 (6)	-0.0012 (5)	0.0044 (5)	0.0005 (4)
C10	0.0262 (6)	0.0171 (6)	0.0223 (6)	-0.0005 (5)	0.0026 (5)	-0.0002 (4)
C11	0.0314 (7)	0.0216 (7)	0.0278 (7)	-0.0049 (5)	-0.0041 (5)	-0.0020 (5)
C12	0.0444 (8)	0.0156 (6)	0.0287 (7)	-0.0032 (6)	-0.0006 (6)	-0.0034 (5)
C13	0.0396 (8)	0.0150 (6)	0.0251 (6)	0.0051 (5)	0.0007 (6)	0.0007 (5)
C14	0.0292 (7)	0.0184 (6)	0.0184 (6)	0.0016 (5)	0.0022 (5)	0.0019 (4)
C15	0.0257 (7)	0.0249 (7)	0.0361 (8)	0.0019 (5)	-0.0023 (6)	-0.0032 (5)
C16	0.0322 (7)	0.0240 (7)	0.0368 (8)	0.0059 (5)	-0.0036 (6)	-0.0018 (5)

*Geometric parameters (Å, °)*

N1—H1	0.882 (15)	C8—H8	0.9500
N1—C1	1.3663 (15)	C9—C10	1.4004 (17)
N1—C3	1.4157 (15)	C9—C14	1.4036 (16)
N2—C1	1.2879 (14)	C10—C11	1.3957 (17)
N2—C9	1.4272 (14)	C10—C15	1.5055 (17)
C1—C2	1.5078 (15)	C11—H11	0.9500
C2—H2A	0.9800	C11—C12	1.3826 (19)
C2—H2B	0.9800	C12—H12	0.9500
C2—H2C	0.9800	C12—C13	1.3810 (19)
C3—C4	1.3967 (16)	C13—H13	0.9500
C3—C8	1.3952 (17)	C13—C14	1.3946 (17)
C4—H4	0.9500	C14—C16	1.5040 (18)
C4—C5	1.3857 (17)	C15—H15A	0.9800
C5—H5	0.9500	C15—H15B	0.9800
C5—C6	1.3897 (19)	C15—H15C	0.9800
C6—H6	0.9500	C16—H16A	0.9800
C6—C7	1.3830 (19)	C16—H16B	0.9800
C7—H7	0.9500	C16—H16C	0.9800
C7—C8	1.3865 (18)		
C1—N1—H1	117.7 (10)	C10—C9—N2	119.12 (10)
C1—N1—C3	127.32 (10)	C10—C9—C14	120.70 (11)
C3—N1—H1	114.6 (10)	C14—C9—N2	119.79 (11)
C1—N2—C9	118.81 (9)	C9—C10—C15	120.32 (11)
N1—C1—C2	113.86 (10)	C11—C10—C9	118.79 (11)
N2—C1—N1	121.80 (10)	C11—C10—C15	120.88 (12)
N2—C1—C2	124.34 (10)	C10—C11—H11	119.5
C1—C2—H2A	109.5	C12—C11—C10	120.98 (12)
C1—C2—H2B	109.5	C12—C11—H11	119.5
C1—C2—H2C	109.5	C11—C12—H12	120.1
H2A—C2—H2B	109.5	C13—C12—C11	119.72 (12)
H2A—C2—H2C	109.5	C13—C12—H12	120.1

H2B—C2—H2C	109.5	C12—C13—H13	119.4
C4—C3—N1	118.03 (11)	C12—C13—C14	121.21 (12)
C8—C3—N1	122.65 (11)	C14—C13—H13	119.4
C8—C3—C4	119.25 (11)	C9—C14—C16	121.20 (11)
C3—C4—H4	119.8	C13—C14—C9	118.58 (12)
C5—C4—C3	120.35 (12)	C13—C14—C16	120.20 (11)
C5—C4—H4	119.8	C10—C15—H15A	109.5
C4—C5—H5	119.8	C10—C15—H15B	109.5
C4—C5—C6	120.37 (12)	C10—C15—H15C	109.5
C6—C5—H5	119.8	H15A—C15—H15B	109.5
C5—C6—H6	120.4	H15A—C15—H15C	109.5
C7—C6—C5	119.10 (12)	H15B—C15—H15C	109.5
C7—C6—H6	120.4	C14—C16—H16A	109.5
C6—C7—H7	119.4	C14—C16—H16B	109.5
C6—C7—C8	121.28 (12)	C14—C16—H16C	109.5
C8—C7—H7	119.4	H16A—C16—H16B	109.5
C3—C8—H8	120.2	H16A—C16—H16C	109.5
C7—C8—C3	119.62 (12)	H16B—C16—H16C	109.5
C7—C8—H8	120.2		
N1—C3—C4—C5	175.50 (11)	C5—C6—C7—C8	-1.1 (2)
N1—C3—C8—C7	-176.26 (11)	C6—C7—C8—C3	0.5 (2)
N2—C9—C10—C11	172.39 (10)	C8—C3—C4—C5	-1.79 (17)
N2—C9—C10—C15	-6.41 (17)	C9—N2—C1—N1	176.57 (10)
N2—C9—C14—C13	-172.50 (10)	C9—N2—C1—C2	-4.01 (17)
N2—C9—C14—C16	5.76 (17)	C9—C10—C11—C12	-0.21 (19)
C1—N1—C3—C4	149.38 (11)	C10—C9—C14—C13	0.23 (18)
C1—N1—C3—C8	-33.43 (18)	C10—C9—C14—C16	178.49 (11)
C1—N2—C9—C10	100.22 (13)	C10—C11—C12—C13	1.0 (2)
C1—N2—C9—C14	-86.95 (14)	C11—C12—C13—C14	-1.1 (2)
C3—N1—C1—N2	-11.33 (18)	C12—C13—C14—C9	0.53 (19)
C3—N1—C1—C2	169.20 (11)	C12—C13—C14—C16	-177.75 (12)
C3—C4—C5—C6	1.26 (18)	C14—C9—C10—C11	-0.38 (18)
C4—C3—C8—C7	0.89 (18)	C14—C9—C10—C15	-179.18 (11)
C4—C5—C6—C7	0.17 (19)	C15—C10—C11—C12	178.58 (12)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$Cg1$  and  $Cg2$  are the centroids of the C3–C8 phenyl and C9–C14 2,6-dimethylphenyl rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 $\cdots$ N2 <sup>i</sup>	0.882 (15)	2.172 (15)	3.0530 (14)	176.3 (14)
C2—H2C $\cdots$ Cg1 <sup>i</sup>	0.98	2.83	3.5601 (14)	132
C4—H4 $\cdots$ Cg2 <sup>i</sup>	0.95	2.59	3.5092 (13)	162
C15—H15A $\cdots$ Cg1 <sup>ii</sup>	0.98	2.83	3.6346 (15)	140

Symmetry codes: (i)  $x, -y+3/2, z+1/2$ ; (ii)  $x-1, -y+3/2, z-1/2$ .