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Crystal structure of 1,2-bis(2,6-dimethylphenyl)-3-phenylguanidine

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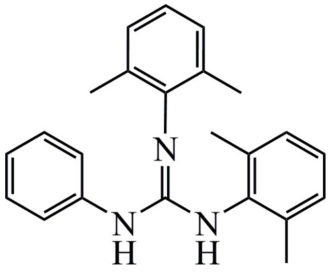
In the title compound, $C_{23}H_{25}N_3$, the dihedral angles between the planes of the benzene ring and the two substituent dimethylphenyl rings are 60.94 (7)° and 88.08 (7)°, and the dihedral angle between the planes of the two dimethylphenyl rings is 58.01 (7)°. In the crystal, weak C—H···N interactions exist between adjacent molecules. One of the dimethylphenyl rings has a small amount of π–π overlap with the phenyl ring of an adjacent molecule [centroid-to-centroid distance = 3.9631 (12) Å].

Keywords: crystal structure; guanidines; hydrogen bonding; π–π overlap.

CCDC reference: 1407910

1. Related literature

For similar structures of various related compounds, see: Boeré *et al.* (2000); Brazeau *et al.* (2012); Ghosh *et al.* (2008); Han & Huynh (2009); Chlupatý & Padělková (2014); Yıldırım *et al.* (2007); Zhang *et al.* (2009). For applications of guanidines, see: Berlinck (2002); Heys *et al.* (2000); Laeckmann *et al.* (2002); Kelley *et al.* (2001); Moroni *et al.* (2001).



2. Experimental

2.1. Crystal data

$C_{23}H_{25}N_3$
M_r = 343.46
Orthorhombic, $Pca2_1$
a = 19.003 (7) Å
b = 7.924 (3) Å
c = 13.056 (5) Å
V = 1966.0 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 194 K
0.35 × 0.33 × 0.30 mm

2.2. Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.980
10737 measured reflections
3547 independent reflections
2649 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.104
S = 1.02
3547 reflections
239 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···N2^{i}	0.95	2.61	3.457 (3)	148

Symmetry code: (i) $x+\frac{1}{2}, -y+2, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: PK2556).

References

Berlinck, R. G. S. (2002). *Nat. Prod. Rep.* **19**, 617–649.
Boeré, R. E., Boeré, R. T., Masuda, J. & Wolmershäuser, G. (2000). *Can. J. Chem.* **78**, 1613–1619.
Brazeau, A. L., Hänninen, M. M., Tuononen, H. M., Jones, N. D. & Ragogna, P. J. (2012). *J. Am. Chem. Soc.* **134**, 5398–5414.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chlupatý, T. & Padělková, Z. (2014). *Acta Cryst.* E**70**, o785.

Ghosh, H., Yella, R., Nath, J. & Patel, B. K. (2008). *Eur. J. Org. Chem.* pp, 6189–6196.
Han, Y. & Huynh, H. V. (2009). *Dalton Trans.*, pp. 2201–2209.
Heys, L., Moore, C. G. & Murphy, P. J. (2000). *Chem. Soc. Rev.* **29**, 57–67.
Kelley, M. T., Bürckstümmer, T., Wenzel-Seifert, K., Dove, S., Buschauer, A. & Seifert, R. (2001). *Mol. Pharmacol.* **60**, 1210–1225.
Laeckmann, D., Rogister, F., Dejardin, J.-V., Prosperi-Meys, C., Géczy, J., Delarge, J. & Masereel, B. (2002). *Bioorg. Med. Chem.* **10**, 1793–1804.
Moroni, M., Koksch, B., Osipov, S. N., Crucianelli, M., Frigerio, M., Bravo, P. & Burger, K. (2001). *J. Org. Chem.* **66**, 130–133.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Yıldırım, S. Ö., Akkurt, M., Servi, S., Şekerci, M. & Heinemann, F. W. (2007). *Acta Cryst.* E**63**, o2130–o2132.
Zhang, W.-X., Li, D., Wang, Z. & Xi, Z. (2009). *Organometallics*, **28**, 882–887.

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Crystal structure of 1,2-bis(2,6-dimethylphenyl)-3-phenylguanidine

Hongfei Han, Zhiqiang Guo and Xuehong Wei

S1. Structural commentary

Guanidines are important compounds due to their possible application in medicine, biology and chemistry (Berlinck *et al.*, 2002; Heys *et al.*, 2000). In particular, they have received increasing interest as medicinal agents with antitumour, anti-hypertensive, antiglaucoma and cardiotonic activities (Laeckmann *et al.*, 2002; Kelley *et al.*, 2001; Moroni *et al.*, 2001). In search of guanidinato metal complexes and their catalytic behaviors, we synthesized a new substituted guanidine by insertion of phenylamine with a symmetric carbodiimine, the crystal structure of which is presented here. In addition to two examples of phenyl-substituted benzimidazol amines (Ghosh *et al.*, 2008; Yildirim *et al.*, 2007), the title compound is structurally similar to the known compounds, 1-cyclohexyl-2,3-diphenylguanidine (Zhang *et al.*, 2009), 1-(2,6-diisopropylphenyl)-2,3-dimesitylguanidine (Brazeau *et al.*, 2012), N,N′,N″-tris(2,6-dimethylphenyl)guanidine (Han & Huynh, 2009), 2-[2,6-Bis(propan-2-yl)phenyl]-1,3-dicyclohexylguanidine (Chlupatý & Padělková, 2014) and N,N′,N″-tris(2,6-di-isopropylphenyl)guanidine (Boere *et al.*, 2000).

The molecular structure of the title compound is illustrated in Fig. 1. The C9—N2 bond in the guanidine unit is 1.266 (2) Å, and is characteristic for a C═N imine double bond. The bond lengths of C9—N1 and C9—N3 are 1.365 (2) and 1.376 (2) Å, showing single bond character (Allen *et al.*, 1987). The N—C9—N angles are 124.15 (18)° (N1—C9—N2), 121.58 (17)° (N2—C9—N3) and 114.26 (17)° (N1—C9—N3), indicating a deviation of the CN_3 plane from an ideal trigonal planar geometry. The dihedral angles between the planes of the benzene ring and the two substituent dimethylphenyl rings are 60.94 (7) and 88.08 (7)°, and the dihedral angle between the planes of the two dimethylphenyl rings is 58.01 (7)°. In the crystal, in addition to van der Waals interactions, weak C—H···N and N—H···C interactions exist between adjacent molecules. One of the dimethylphenyl rings has a small amount of $\pi\cdots\pi$ overlap with the phenyl ring of an adjacent (1-x, 2-y, 0.5+z) molecule [centroid-to-centroid distance = 3.9631 (12) Å].

S2. Synthesis and crystallization

To a stirred solution of phenylamine (1.863 g, 20 mmol) in hexane was added N,N′-dimethylphenyl carbodiimine (5.007 g, 20 mmol), followed by the addition of the trimethylaluminum (2.5 M, 0.40 mL, 1 mmol). After stirring for 2 h, the white precipitate was collected by suction filtration and recrystallized from hexane-diethylether (1:1) solution to obtain colorless crystals of 1,2-bis(2,6-dimethylphenyl)-3-phenylguanidine (yield: 90%). Anal. Calc. for $C_{23}H_{25}N_3$: C, 80.43; H, 7.34; N, 12.23. Found: C, 80.32; H, 7.25; N, 12.31%. ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C) δ p.p.m. 2.35 (*d*, 12H, CH_3), 5.06 (*s*, 1H, NH), 5.56 (*s*, 1H, NH), 6.91 (*s*, 2H, PhH), 7.00 (*s*, 2H, PhH), 7.14 (*s*, 4H, PhH), 7.28 (*s*, 1H, PhH) , 7.58 (*s*, 2H, PhH).

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The N—H hydrogen atoms were located in a difference Fourier map and constrained (N—H = 0.87 Å). The C-bound H-atoms were included in calculated

positions and treated as riding atoms: C—H = 0.95 - 0.98 Å with U_{iso} (H) = 1.2 or 1.5U_{eq} (C_{Me}).

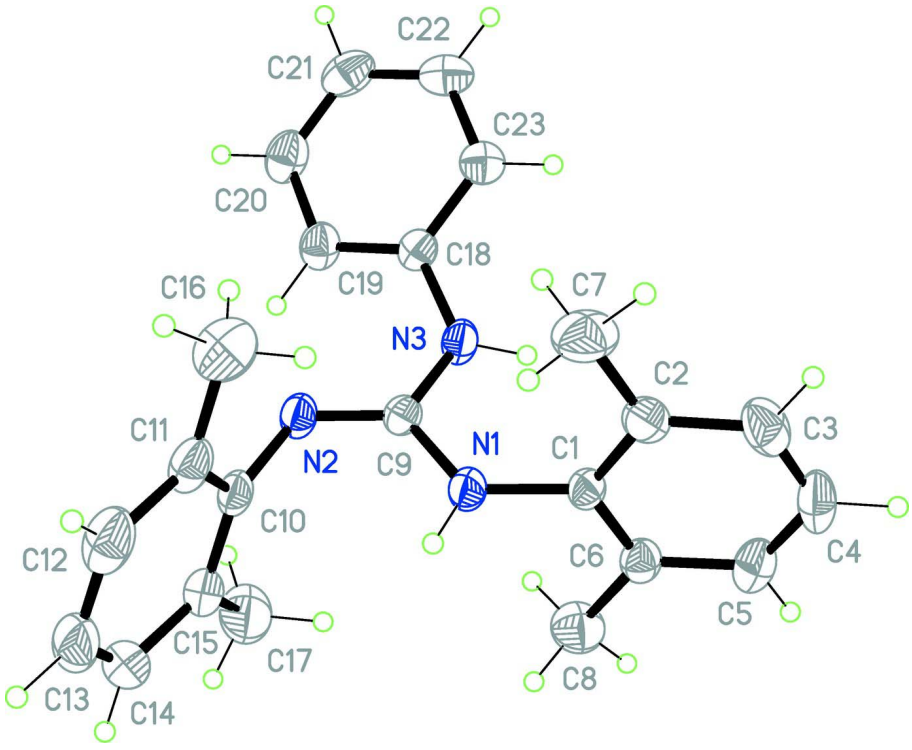

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

1,2-Bis(2,6-dimethylphenyl)-3-phenylguanidine

Crystal data

$C_{23}H_{25}N_3$
M_r = 343.46
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
a = 19.003 (7) Å
b = 7.924 (3) Å
c = 13.056 (5) Å
V = 1966.0 (13) Å^3
Z = 4
$F(000)$ = 736
D_x = 1.160 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2316 reflections
θ = 2.8–23.5°
μ = 0.07 mm^{-1}
T = 194 K
Block, colourless
0.35 × 0.33 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.980
10737 measured reflections
3547 independent reflections
2649 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 25.5°, θ_{min} = 2.7°
h = −23→23
k = −9→5
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.104$
$S = 1.01$
3547 reflections
239 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ 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.

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 $F^2 > 2$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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.51390 (8)	0.8726 (2)	0.22933 (14)	0.0499 (4)
H1	0.5001	0.8129	0.2815	0.060*
N2	0.39761 (8)	0.9417 (2)	0.19326 (13)	0.0470 (4)
N3	0.48706 (8)	1.0319 (2)	0.08715 (13)	0.0494 (5)
H3	0.5300	1.0109	0.0680	0.059*
C1	0.58760 (9)	0.8820 (3)	0.21187 (15)	0.0414 (5)
C2	0.62483 (11)	1.0196 (3)	0.24776 (18)	0.0535 (6)
C3	0.69708 (12)	1.0198 (4)	0.2354 (2)	0.0693 (7)
H3A	0.7238	1.1136	0.2586	0.083*
C4	0.73035 (12)	0.8867 (4)	0.1904 (2)	0.0695 (7)
H4	0.7801	0.8879	0.1840	0.083*
C5	0.69327 (12)	0.7521 (4)	0.15447 (18)	0.0612 (6)
H5	0.7173	0.6614	0.1223	0.073*
C6	0.62094 (10)	0.7464 (3)	0.16442 (17)	0.0482 (5)
C7	0.58943 (16)	1.1640 (3)	0.3014 (2)	0.0825 (8)
H7A	0.5631	1.1213	0.3605	0.124*
H7B	0.5570	1.2202	0.2539	0.124*
H7C	0.6250	1.2448	0.3247	0.124*
C8	0.57928 (15)	0.5980 (3)	0.1261 (2)	0.0732 (7)
H8A	0.5423	0.6375	0.0796	0.110*
H8B	0.5578	0.5392	0.1843	0.110*
H8C	0.6106	0.5204	0.0894	0.110*
C9	0.46259 (9)	0.9480 (3)	0.17228 (15)	0.0392 (4)
C10	0.37336 (10)	0.8594 (3)	0.28195 (16)	0.0470 (5)
C11	0.36221 (11)	0.9503 (4)	0.37126 (18)	0.0592 (7)

C12	0.32944 (14)	0.8739 (5)	0.4525 (2)	0.0830 (9)
H12	0.3214	0.9366	0.5133	0.100*
C13	0.30812 (15)	0.7093 (6)	0.4476 (3)	0.0950 (12)
H13	0.2852	0.6584	0.5044	0.114*
C14	0.32015 (14)	0.6189 (4)	0.3606 (3)	0.0918 (11)
H14	0.3059	0.5041	0.3580	0.110*
C15	0.35250 (11)	0.6897 (3)	0.2757 (2)	0.0628 (7)
C16	0.38379 (16)	1.1319 (4)	0.3781 (2)	0.0814 (9)
H16A	0.3731	1.1888	0.3133	0.122*
H16B	0.4344	1.1389	0.3916	0.122*
H16C	0.3580	1.1868	0.4338	0.122*
C17	0.36204 (16)	0.5931 (4)	0.1775 (3)	0.0942 (10)
H17A	0.3381	0.6526	0.1217	0.141*
H17B	0.3419	0.4799	0.1850	0.141*
H17C	0.4123	0.5839	0.1619	0.141*
C18	0.44829 (10)	1.1495 (3)	0.02788 (14)	0.0437 (5)
C19	0.37790 (11)	1.1326 (3)	0.00775 (16)	0.0546 (6)
H19	0.3529	1.0372	0.0326	0.065*
C20	0.34337 (13)	1.2550 (3)	−0.04892 (17)	0.0641 (7)
H20	0.2943	1.2446	−0.0611	0.077*
C21	0.37888 (15)	1.3896 (3)	−0.0873 (2)	0.0685 (7)
H21	0.3546	1.4731	−0.1258	0.082*
C22	0.44980 (15)	1.4048 (3)	−0.07045 (19)	0.0666 (7)
H22	0.4749	1.4976	−0.0985	0.080*
C23	0.48466 (11)	1.2853 (3)	−0.01269 (16)	0.0533 (5)
H23	0.5338	1.2964	−0.0007	0.064*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0348 (8)	0.0591 (10)	0.0557 (10)	0.0034 (8)	0.0009 (8)	0.0171 (9)
N2	0.0339 (9)	0.0611 (11)	0.0460 (10)	0.0061 (8)	0.0012 (7)	0.0097 (9)
N3	0.0358 (9)	0.0664 (12)	0.0461 (9)	0.0083 (8)	0.0054 (7)	0.0140 (10)
C1	0.0336 (10)	0.0483 (11)	0.0424 (11)	−0.0002 (9)	−0.0060 (8)	0.0072 (10)
C2	0.0533 (12)	0.0528 (13)	0.0543 (13)	−0.0053 (11)	−0.0068 (11)	0.0059 (11)
C3	0.0564 (14)	0.0834 (19)	0.0682 (15)	−0.0248 (14)	−0.0165 (13)	0.0080 (15)
C4	0.0356 (11)	0.111 (2)	0.0622 (15)	−0.0066 (13)	−0.0028 (11)	0.0113 (17)
C5	0.0477 (13)	0.0820 (18)	0.0540 (13)	0.0115 (12)	0.0023 (10)	−0.0007 (13)
C6	0.0432 (11)	0.0551 (13)	0.0461 (11)	0.0001 (10)	−0.0039 (10)	0.0016 (11)
C7	0.0967 (19)	0.0517 (14)	0.099 (2)	0.0000 (14)	−0.0121 (17)	−0.0118 (17)
C8	0.0800 (18)	0.0600 (17)	0.0795 (17)	−0.0056 (14)	−0.0001 (14)	−0.0135 (14)
C9	0.0368 (10)	0.0428 (11)	0.0379 (10)	0.0029 (9)	−0.0032 (9)	−0.0003 (9)
C10	0.0295 (9)	0.0615 (14)	0.0498 (12)	0.0091 (10)	0.0007 (9)	0.0086 (11)
C11	0.0449 (13)	0.0842 (18)	0.0483 (13)	0.0202 (13)	0.0008 (10)	0.0096 (13)
C12	0.0684 (18)	0.127 (3)	0.0534 (15)	0.0326 (18)	0.0107 (13)	0.0181 (18)
C13	0.0656 (17)	0.129 (3)	0.091 (2)	0.0279 (19)	0.0308 (16)	0.058 (2)
C14	0.0606 (16)	0.078 (2)	0.137 (3)	0.0074 (15)	0.0213 (18)	0.044 (2)
C15	0.0420 (12)	0.0628 (15)	0.0837 (17)	0.0046 (11)	0.0078 (12)	0.0096 (15)

C16	0.088 (2)	0.085 (2)	0.0710 (17)	0.0123 (17)	−0.0064 (15)	−0.0176 (17)
C17	0.0784 (18)	0.0710 (18)	0.133 (3)	−0.0084 (15)	0.015 (2)	−0.023 (2)
C18	0.0450 (11)	0.0506 (13)	0.0355 (10)	0.0058 (9)	0.0019 (9)	0.0008 (10)
C19	0.0453 (12)	0.0729 (17)	0.0455 (12)	0.0040 (11)	−0.0026 (9)	0.0083 (12)
C20	0.0533 (13)	0.0902 (19)	0.0487 (12)	0.0137 (13)	−0.0040 (11)	0.0067 (14)
C21	0.0819 (18)	0.0696 (18)	0.0541 (14)	0.0251 (15)	−0.0055 (13)	0.0062 (14)
C22	0.090 (2)	0.0497 (15)	0.0606 (15)	0.0046 (13)	−0.0032 (13)	0.0051 (13)
C23	0.0574 (13)	0.0517 (13)	0.0509 (12)	−0.0007 (11)	−0.0028 (11)	−0.0014 (12)

Geometric parameters (Å, º)

N1—C9	1.365 (2)	C11—C12	1.370 (4)
N1—C1	1.421 (2)	C11—C16	1.499 (4)
N1—H1	0.8700	C12—C13	1.368 (5)
N2—C9	1.266 (2)	C12—H12	0.9500
N2—C10	1.407 (3)	C13—C14	1.363 (5)
N3—C9	1.376 (2)	C13—H13	0.9500
N3—C18	1.418 (3)	C14—C15	1.386 (4)
N3—H3	0.8699	C14—H14	0.9500
C1—C2	1.381 (3)	C15—C17	1.503 (4)
C1—C6	1.393 (3)	C16—H16A	0.9800
C2—C3	1.382 (3)	C16—H16B	0.9800
C2—C7	1.501 (4)	C16—H16C	0.9800
C3—C4	1.363 (4)	C17—H17A	0.9800
C3—H3A	0.9500	C17—H17B	0.9800
C4—C5	1.362 (3)	C17—H17C	0.9800
C4—H4	0.9500	C18—C19	1.370 (3)
C5—C6	1.381 (3)	C18—C23	1.385 (3)
C5—H5	0.9500	C19—C20	1.385 (3)
C6—C8	1.503 (3)	C19—H19	0.9500
C7—H7A	0.9800	C20—C21	1.358 (3)
C7—H7B	0.9800	C20—H20	0.9500
C7—H7C	0.9800	C21—C22	1.371 (4)
C8—H8A	0.9800	C21—H21	0.9500
C8—H8B	0.9800	C22—C23	1.380 (3)
C8—H8C	0.9800	C22—H22	0.9500
C10—C11	1.387 (3)	C23—H23	0.9500
C10—C15	1.405 (3)		
C9—N1—C1	126.42 (17)	C12—C11—C16	120.2 (3)
C9—N1—H1	116.8	C10—C11—C16	120.5 (2)
C1—N1—H1	116.8	C13—C12—C11	121.3 (3)
C9—N2—C10	121.07 (16)	C13—C12—H12	119.3
C9—N3—C18	125.64 (16)	C11—C12—H12	119.3
C9—N3—H3	117.2	C14—C13—C12	119.3 (3)
C18—N3—H3	117.2	C14—C13—H13	120.3
C2—C1—C6	121.78 (17)	C12—C13—H13	120.3
C2—C1—N1	119.46 (19)	C13—C14—C15	121.9 (3)

C6—C1—N1	118.63 (17)	C13—C14—H14	119.0
C1—C2—C3	118.0 (2)	C15—C14—H14	119.0
C1—C2—C7	122.0 (2)	C14—C15—C10	117.8 (3)
C3—C2—C7	119.9 (2)	C14—C15—C17	122.0 (3)
C4—C3—C2	120.7 (2)	C10—C15—C17	120.2 (2)
C4—C3—H3A	119.7	C11—C16—H16A	109.5
C2—C3—H3A	119.7	C11—C16—H16B	109.5
C5—C4—C3	121.0 (2)	H16A—C16—H16B	109.5
C5—C4—H4	119.5	C11—C16—H16C	109.5
C3—C4—H4	119.5	H16A—C16—H16C	109.5
C4—C5—C6	120.5 (2)	H16B—C16—H16C	109.5
C4—C5—H5	119.7	C15—C17—H17A	109.5
C6—C5—H5	119.7	C15—C17—H17B	109.5
C5—C6—C1	118.0 (2)	H17A—C17—H17B	109.5
C5—C6—C8	121.2 (2)	C15—C17—H17C	109.5
C1—C6—C8	120.80 (18)	H17A—C17—H17C	109.5
C2—C7—H7A	109.5	H17B—C17—H17C	109.5
C2—C7—H7B	109.5	C19—C18—C23	119.3 (2)
H7A—C7—H7B	109.5	C19—C18—N3	123.2 (2)
C2—C7—H7C	109.5	C23—C18—N3	117.43 (18)
H7A—C7—H7C	109.5	C18—C19—C20	119.8 (2)
H7B—C7—H7C	109.5	C18—C19—H19	120.1
C6—C8—H8A	109.5	C20—C19—H19	120.1
C6—C8—H8B	109.5	C21—C20—C19	120.8 (2)
H8A—C8—H8B	109.5	C21—C20—H20	119.6
C6—C8—H8C	109.5	C19—C20—H20	119.6
H8A—C8—H8C	109.5	C20—C21—C22	119.9 (2)
H8B—C8—H8C	109.5	C20—C21—H21	120.1
N2—C9—N1	124.15 (18)	C22—C21—H21	120.1
N2—C9—N3	121.58 (17)	C21—C22—C23	120.0 (2)
N1—C9—N3	114.26 (16)	C21—C22—H22	120.0
C11—C10—C15	120.2 (2)	C23—C22—H22	120.0
C11—C10—N2	120.1 (2)	C22—C23—C18	120.2 (2)
C15—C10—N2	119.2 (2)	C22—C23—H23	119.9
C12—C11—C10	119.4 (3)	C18—C23—H23	119.9

C9—N1—C1—C2	82.9 (3)	C15—C10—C11—C12	−1.3 (3)
C9—N1—C1—C6	−101.1 (2)	N2—C10—C11—C12	170.91 (19)
C6—C1—C2—C3	0.0 (3)	C15—C10—C11—C16	−179.4 (2)
N1—C1—C2—C3	175.9 (2)	N2—C10—C11—C16	−7.3 (3)
C6—C1—C2—C7	−178.4 (2)	C10—C11—C12—C13	0.7 (4)
N1—C1—C2—C7	−2.5 (3)	C16—C11—C12—C13	178.9 (3)
C1—C2—C3—C4	−0.9 (4)	C11—C12—C13—C14	0.5 (4)
C7—C2—C3—C4	177.5 (2)	C12—C13—C14—C15	−1.0 (5)
C2—C3—C4—C5	1.4 (4)	C13—C14—C15—C10	0.4 (4)
C3—C4—C5—C6	−1.0 (4)	C13—C14—C15—C17	−176.4 (3)
C4—C5—C6—C1	0.1 (3)	C11—C10—C15—C14	0.7 (3)
C4—C5—C6—C8	−179.4 (2)	N2—C10—C15—C14	−171.5 (2)

C2—C1—C6—C5	0.4 (3)	C11—C10—C15—C17	177.6 (2)
N1—C1—C6—C5	−175.5 (2)	N2—C10—C15—C17	5.4 (3)
C2—C1—C6—C8	179.9 (2)	C9—N3—C18—C19	−37.2 (3)
N1—C1—C6—C8	4.0 (3)	C9—N3—C18—C23	144.1 (2)
C10—N2—C9—N1	2.6 (3)	C23—C18—C19—C20	−2.8 (3)
C10—N2—C9—N3	−178.32 (19)	N3—C18—C19—C20	178.5 (2)
C1—N1—C9—N2	−177.0 (2)	C18—C19—C20—C21	1.8 (3)
C1—N1—C9—N3	3.9 (3)	C19—C20—C21—C22	0.3 (4)
C18—N3—C9—N2	15.3 (3)	C20—C21—C22—C23	−1.4 (4)
C18—N3—C9—N1	−165.6 (2)	C21—C22—C23—C18	0.4 (4)
C9—N2—C10—C11	94.0 (2)	C19—C18—C23—C22	1.8 (3)
C9—N2—C10—C15	−93.7 (2)	N3—C18—C23—C22	−179.54 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···N2^{i}	0.95	2.61	3.457 (3)	148

Symmetry code: (i) *x*+1/2, −*y*+2, *z*.