Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(2-Methylphenyl)-4,5-diphenyl-1*H*-imidazole

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.103
Data-to-parameter ratio = 8.7

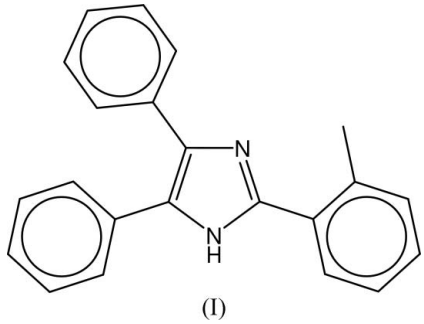
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 26 May 2006
Accepted 2 June 2006

In the title molecule, $C_{22}H_{18}N_2$, all bond lengths and angles are normal. Intermolecular N—H···N hydrogen bonds with an N···N distance of 2.933 (2) Å, link the molecules into chains running along the *c* axis. The crystal packing is further stabilized by van der Waals forces.

Comment

Several heterocyclic compounds with aryl substituents have previously been reported to exhibit anti-inflammatory activity in animals (Almirante *et al.*, 1965; Marchetti *et al.*, 1968). Of the various polyaryl heterocycles, certain 4,5-diphenyl-2-substituted imidazoles exhibited anti-inflamatory activity comparable to phenylbutazone in the carrageenan rat paw edema test (Lombardino & Wiseman, 1974). In view of this importance, we report here the crystal structure of the title compound, (I), which is a 4,5-diphenyl-2-substituted imidazole derivative.



(I)

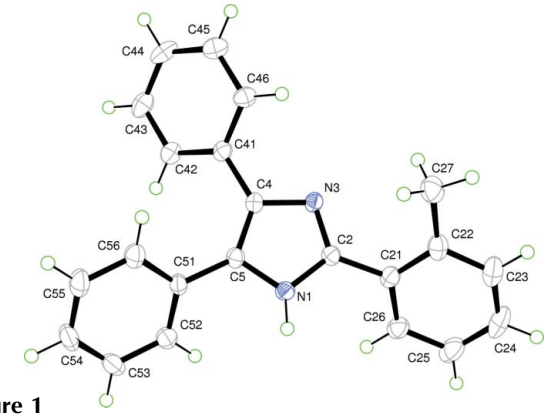


Figure 1
View of (I), showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. H atoms are represented by circles of arbitrary radii.

The bond lengths and angles in (I) (Fig. 1) are in good agreement with the literature values (Allen *et al.*, 1987). The imidazole ring makes dihedral angles of 41.2 (1), 31.5 (1) and 41.7 (1)° with the C21–C26, C41–C46 and C51–C56 aromatic rings, respectively. In the solid state, intermolecular N—H···N hydrogen bonds (Table 1) link the molecules into *C*(4) chains (Bernstein *et al.*, 1995) running along the *c* axis. The crystal packing (Fig. 2) is further stabilized by van der Waals forces.

Experimental

A mixture of benzil (5.25 g, 0.025 mol), ammonium acetate (l0 g, 0.129 mol) and 2-methylbenzaldehyde (0.018 mol) in glacial acetic acid (50 ml) was heated under reflux for 1–2 h. The product was recrystallized from aqueous ethanol (yield 80%, m.p. 484–486 K).

Crystal data

$C_{22}H_{18}N_2$
M_r = 310.38
Monoclinic, *Cc*
a = 10.7538 (5) Å
b = 19.3999 (9) Å
c = 8.7900 (3) Å
β = 112.886 (2)°
V = 1689.44 (13) Å^3
Z = 4
D_x = 1.220 Mg m^{-3}
Mo *K*α radiation
μ = 0.07 mm^{-1}
T = 120 (2) K
Rod, colourless
0.36 × 0.06 × 0.04 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.745, T_{max} = 0.927
(expected range = 0.801–0.997)
10671 measured reflections
1945 independent reflections
1744 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.103
S = 1.06
1945 reflections
223 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.7664P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0089 (16)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N3^{i}	0.88 (3)	2.07 (3)	2.933 (3)	168 (3)

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

The position of the amine H atom was determined from a difference Fourier map and refined freely along with its isotropic displacement parameter. The methyl H atoms were constrained to an ideal geometry (C—H = 0.98 Å), with U_{iso}(H) = 1.5U_{eq}(C), but were allowed to rotate freely about the C—C bond. The remaining H atoms were placed in geometrically idealized positions (C—H = 0.95 Å) and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C). Owing to the absence of any significant anomalous scatterers in the molecule, the 1433 Friedel pairs were merged before the final refinement.

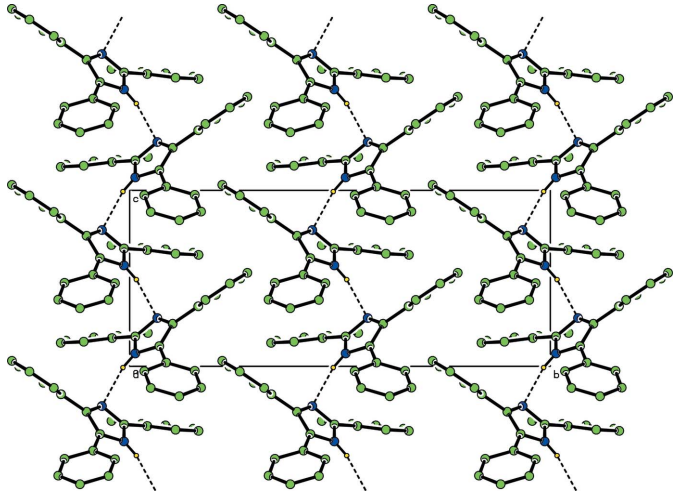


Figure 2
The crystal packing of (I), viewed along the *a* axis. The intermolecular N—H···N hydrogen bonds are shown as dashed lines. All the H atoms, except those involved in hydrogen bonding, have been omitted for clarity.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors thank the EPSRC National Crystallography Service (Southampton, England). TS thanks Professors V. Parthasarathi, School of Physics and M. Nallu, School of Chemistry, Bharathidasan University, Tiruchirappalli, for their generous help.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Almirante, L., Polo, L., Mugnaini, A., Provinciali, E., Rugarli, P., Biancotti, A., Gamba, A. & Murmann, W. (1965). *J. Med. Chem.* **8**, 305–312.
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hooft, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Lombardino, J. G. & Wiseman, E. H. (1974). *J. Med. Chem.* **17**, 1182–1188.
Marchetti, E., Mattalia, G. & Rosnati, V. (1968). *J. Med. Chem.* **11**, 1092–1093.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supporting information

Acta Cryst. (2006). E**62**, o2803–o2804 [https://doi.org/10.1107/S160053680602109X]

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Crystal data

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Monoclinic, *Cc*
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$a = 10.7538$ (5) Å
$b = 19.3999$ (9) Å
$c = 8.7900$ (3) Å
$\beta = 112.886$ (2)°
$V = 1689.44$ (13) Å^3
$Z = 4$
$F(000) = 656$
$D_x = 1.220$ Mg m^{-3}
Melting point: 484 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1980 reflections
$\theta = 2.9$–27.5°
$\mu = 0.07$ mm^{-1}
$T = 120$ K
Rod, colourless
0.36 × 0.06 × 0.04 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker Nonius FR591 rotating anode
10 cm confocal mirrors monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.745$, $T_{max} = 0.927$
10671 measured reflections
1945 independent reflections
1744 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -11 \rightarrow 13$
$k = -25 \rightarrow 25$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.103$
$S = 1.06$
1945 reflections
223 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.7664P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0089 (16)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.7086 (2)	0.01344 (11)	0.0732 (2)	0.0210 (4)
H1	0.698 (3)	−0.0160 (15)	−0.007 (4)	0.019 (7)*
N3	0.6705 (2)	0.06587 (10)	0.2743 (2)	0.0211 (4)
C2	0.6360 (2)	0.01323 (12)	0.1697 (3)	0.0204 (5)
C4	0.7688 (2)	0.10230 (12)	0.2418 (3)	0.0204 (5)
C5	0.7926 (3)	0.07057 (12)	0.1148 (3)	0.0215 (5)
C21	0.5397 (3)	−0.04191 (13)	0.1607 (3)	0.0241 (5)
C22	0.4158 (3)	−0.02859 (15)	0.1729 (3)	0.0292 (6)
C23	0.3333 (3)	−0.08493 (16)	0.1644 (4)	0.0398 (7)
H23	0.2486	−0.0772	0.1719	0.048*
C24	0.3697 (4)	−0.15116 (17)	0.1458 (4)	0.0455 (8)
H24	0.3110	−0.1884	0.1415	0.055*
C25	0.4917 (4)	−0.16377 (14)	0.1332 (4)	0.0393 (7)
H25	0.5173	−0.2096	0.1201	0.047*
C26	0.5763 (3)	−0.10916 (14)	0.1399 (3)	0.0292 (6)
H26	0.6600	−0.1175	0.1302	0.035*
C27	0.3689 (3)	0.04324 (16)	0.1896 (4)	0.0361 (7)
H271	0.2753	0.0415	0.1807	0.054*
H272	0.3745	0.0725	0.1016	0.054*
H273	0.4265	0.0623	0.2973	0.054*
C41	0.8327 (3)	0.16304 (12)	0.3411 (3)	0.0220 (5)
C42	0.9678 (3)	0.18026 (13)	0.3771 (3)	0.0261 (5)
H42	1.0207	0.1520	0.3372	0.031*
C43	1.0247 (3)	0.23823 (14)	0.4704 (3)	0.0320 (6)
H43	1.1161	0.2496	0.4930	0.038*
C44	0.9492 (3)	0.27985 (13)	0.5311 (3)	0.0329 (6)
H44	0.9885	0.3197	0.5944	0.039*
C45	0.8167 (3)	0.26271 (14)	0.4986 (3)	0.0312 (6)
H45	0.7646	0.2909	0.5399	0.037*
C46	0.7595 (3)	0.20471 (13)	0.4064 (3)	0.0260 (6)
H46	0.6688	0.1930	0.3870	0.031*
C51	0.8762 (2)	0.08675 (13)	0.0212 (3)	0.0230 (5)
C52	0.9424 (3)	0.03489 (15)	−0.0275 (3)	0.0277 (6)
H52	0.9372	−0.0114	0.0048	0.033*
C53	1.0161 (3)	0.05019 (16)	−0.1228 (3)	0.0325 (6)

H53	1.0609	0.0145	−0.1556	0.039*
C54	1.0237 (3)	0.11818 (17)	−0.1700 (4)	0.0379 (7)
H54	1.0732	0.1289	−0.2360	0.045*
C55	0.9597 (3)	0.16969 (15)	−0.1210 (3)	0.0345 (7)
H55	0.9658	0.2160	−0.1528	0.041*
C56	0.8860 (3)	0.15480 (14)	−0.0255 (3)	0.0288 (6)
H56	0.8425	0.1908	0.0081	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0242 (11)	0.0209 (10)	0.0183 (10)	−0.0017 (8)	0.0088 (9)	−0.0005 (8)
N3	0.0226 (10)	0.0208 (9)	0.0197 (9)	−0.0028 (8)	0.0082 (8)	0.0007 (8)
C2	0.0231 (13)	0.0205 (11)	0.0174 (11)	0.0003 (10)	0.0079 (10)	0.0029 (9)
C4	0.0187 (12)	0.0208 (11)	0.0211 (11)	−0.0001 (9)	0.0072 (9)	0.0024 (9)
C5	0.0242 (13)	0.0202 (11)	0.0209 (11)	−0.0007 (10)	0.0096 (10)	0.0035 (9)
C21	0.0281 (14)	0.0246 (12)	0.0186 (11)	−0.0051 (10)	0.0081 (10)	0.0013 (10)
C22	0.0258 (14)	0.0348 (15)	0.0256 (12)	−0.0046 (11)	0.0086 (11)	0.0047 (11)
C23	0.0326 (17)	0.0443 (17)	0.0429 (17)	−0.0126 (14)	0.0152 (14)	0.0029 (14)
C24	0.045 (2)	0.0362 (16)	0.0511 (19)	−0.0205 (14)	0.0139 (16)	0.0030 (14)
C25	0.051 (2)	0.0252 (14)	0.0413 (16)	−0.0104 (13)	0.0182 (15)	−0.0013 (12)
C26	0.0356 (16)	0.0253 (13)	0.0271 (13)	−0.0044 (11)	0.0128 (12)	−0.0005 (10)
C27	0.0258 (14)	0.0404 (16)	0.0416 (16)	0.0003 (13)	0.0127 (13)	0.0006 (13)
C41	0.0257 (13)	0.0193 (11)	0.0203 (10)	−0.0003 (10)	0.0083 (10)	0.0040 (9)
C42	0.0225 (13)	0.0246 (12)	0.0282 (13)	−0.0004 (10)	0.0064 (11)	0.0020 (10)
C43	0.0265 (15)	0.0277 (14)	0.0343 (14)	−0.0045 (11)	0.0037 (12)	0.0024 (11)
C44	0.0367 (17)	0.0187 (12)	0.0320 (14)	−0.0042 (11)	0.0011 (12)	−0.0036 (11)
C45	0.0353 (16)	0.0260 (13)	0.0292 (13)	0.0028 (12)	0.0090 (12)	−0.0010 (11)
C46	0.0254 (14)	0.0252 (13)	0.0243 (11)	0.0002 (11)	0.0061 (10)	−0.0017 (10)
C51	0.0210 (13)	0.0287 (13)	0.0200 (11)	−0.0061 (11)	0.0089 (10)	−0.0013 (10)
C52	0.0237 (13)	0.0346 (14)	0.0238 (12)	−0.0061 (11)	0.0081 (10)	−0.0051 (11)
C53	0.0267 (15)	0.0464 (17)	0.0285 (13)	−0.0046 (13)	0.0150 (12)	−0.0101 (12)
C54	0.0345 (17)	0.0562 (19)	0.0308 (14)	−0.0161 (14)	0.0212 (13)	−0.0070 (14)
C55	0.0372 (16)	0.0388 (16)	0.0282 (13)	−0.0114 (13)	0.0136 (12)	0.0046 (12)
C56	0.0297 (15)	0.0290 (13)	0.0286 (13)	−0.0034 (11)	0.0123 (12)	0.0038 (11)

Geometric parameters (Å, º)

N1—C2	1.358 (3)	C41—C46	1.398 (4)
N1—C5	1.386 (3)	C41—C42	1.401 (4)
N1—H1	0.88 (3)	C42—C43	1.386 (4)
N3—C2	1.327 (3)	C42—H42	0.9500
N3—C4	1.390 (3)	C43—C44	1.390 (4)
C2—C21	1.470 (3)	C43—H43	0.9500
C4—C5	1.383 (3)	C44—C45	1.381 (4)
C4—C41	1.468 (3)	C44—H44	0.9500
C5—C51	1.469 (3)	C45—C46	1.384 (4)
C21—C26	1.395 (4)	C45—H45	0.9500

C21—C22	1.401 (4)	C46—H46	0.9500
C22—C23	1.391 (4)	C51—C52	1.393 (4)
C22—C27	1.508 (4)	C51—C56	1.399 (3)
C23—C24	1.372 (5)	C52—C53	1.391 (4)
C23—H23	0.9500	C52—H52	0.9500
C24—C25	1.380 (5)	C53—C54	1.395 (4)
C24—H24	0.9500	C53—H53	0.9500
C25—C26	1.383 (4)	C54—C55	1.374 (4)
C25—H25	0.9500	C54—H54	0.9500
C26—H26	0.9500	C55—C56	1.391 (4)
C27—H271	0.9800	C55—H55	0.9500
C27—H272	0.9800	C56—H56	0.9500
C27—H273	0.9800		

C2—N1—C5	108.2 (2)	C46—C41—C42	118.0 (2)
C2—N1—H1	124.7 (18)	C46—C41—C4	120.0 (2)
C5—N1—H1	126.9 (18)	C42—C41—C4	122.0 (2)
C2—N3—C4	106.22 (19)	C43—C42—C41	120.5 (2)
N3—C2—N1	110.9 (2)	C43—C42—H42	119.7
N3—C2—C21	126.8 (2)	C41—C42—H42	119.7
N1—C2—C21	122.2 (2)	C42—C43—C44	120.6 (3)
C5—C4—N3	109.5 (2)	C42—C43—H43	119.7
C5—C4—C41	130.3 (2)	C44—C43—H43	119.7
N3—C4—C41	120.2 (2)	C45—C44—C43	119.4 (2)
C4—C5—N1	105.3 (2)	C45—C44—H44	120.3
C4—C5—C51	134.6 (2)	C43—C44—H44	120.3
N1—C5—C51	120.0 (2)	C44—C45—C46	120.3 (3)
C26—C21—C22	120.5 (2)	C44—C45—H45	119.8
C26—C21—C2	117.3 (2)	C46—C45—H45	119.8
C22—C21—C2	122.2 (2)	C45—C46—C41	121.2 (3)
C23—C22—C21	117.2 (3)	C45—C46—H46	119.4
C23—C22—C27	120.0 (3)	C41—C46—H46	119.4
C21—C22—C27	122.8 (2)	C52—C51—C56	119.1 (2)
C24—C23—C22	122.5 (3)	C52—C51—C5	121.0 (2)
C24—C23—H23	118.8	C56—C51—C5	119.9 (2)
C22—C23—H23	118.8	C53—C52—C51	120.7 (3)
C23—C24—C25	120.0 (3)	C53—C52—H52	119.7
C23—C24—H24	120.0	C51—C52—H52	119.7
C25—C24—H24	120.0	C52—C53—C54	119.6 (3)
C24—C25—C26	119.4 (3)	C52—C53—H53	120.2
C24—C25—H25	120.3	C54—C53—H53	120.2
C26—C25—H25	120.3	C55—C54—C53	120.0 (2)
C25—C26—C21	120.5 (3)	C55—C54—H54	120.0
C25—C26—H26	119.8	C53—C54—H54	120.0
C21—C26—H26	119.8	C54—C55—C56	120.7 (3)
C22—C27—H271	109.5	C54—C55—H55	119.7
C22—C27—H272	109.5	C56—C55—H55	119.7
H271—C27—H272	109.5	C55—C56—C51	119.9 (3)

C22—C27—H273	109.5	C55—C56—H56	120.0
H271—C27—H273	109.5	C51—C56—H56	120.0
H272—C27—H273	109.5		

C4—N3—C2—N1	0.9 (3)	C2—C21—C26—C25	178.9 (2)
C4—N3—C2—C21	177.1 (2)	C5—C4—C41—C46	150.7 (3)
C5—N1—C2—N3	−1.7 (3)	N3—C4—C41—C46	−31.7 (3)
C5—N1—C2—C21	−178.1 (2)	C5—C4—C41—C42	−31.0 (4)
C2—N3—C4—C5	0.2 (3)	N3—C4—C41—C42	146.6 (2)
C2—N3—C4—C41	−177.9 (2)	C46—C41—C42—C43	−2.0 (4)
N3—C4—C5—N1	−1.1 (3)	C4—C41—C42—C43	179.6 (2)
C41—C4—C5—N1	176.7 (2)	C41—C42—C43—C44	0.6 (4)
N3—C4—C5—C51	175.4 (3)	C42—C43—C44—C45	0.4 (4)
C41—C4—C5—C51	−6.8 (5)	C43—C44—C45—C46	−0.1 (4)
C2—N1—C5—C4	1.7 (3)	C44—C45—C46—C41	−1.4 (4)
C2—N1—C5—C51	−175.5 (2)	C42—C41—C46—C45	2.4 (4)
N3—C2—C21—C26	−136.8 (3)	C4—C41—C46—C45	−179.2 (2)
N1—C2—C21—C26	39.0 (3)	C4—C5—C51—C52	142.6 (3)
N3—C2—C21—C22	43.0 (4)	N1—C5—C51—C52	−41.2 (3)
N1—C2—C21—C22	−141.2 (2)	C4—C5—C51—C56	−39.7 (4)
C26—C21—C22—C23	0.4 (4)	N1—C5—C51—C56	136.4 (3)
C2—C21—C22—C23	−179.3 (2)	C56—C51—C52—C53	−0.8 (4)
C26—C21—C22—C27	−177.8 (2)	C5—C51—C52—C53	176.9 (3)
C2—C21—C22—C27	2.4 (4)	C51—C52—C53—C54	0.1 (4)
C21—C22—C23—C24	0.3 (4)	C52—C53—C54—C55	0.6 (4)
C27—C22—C23—C24	178.6 (3)	C53—C54—C55—C56	−0.5 (5)
C22—C23—C24—C25	−0.6 (5)	C54—C55—C56—C51	−0.3 (4)
C23—C24—C25—C26	0.1 (5)	C52—C51—C56—C55	0.9 (4)
C24—C25—C26—C21	0.6 (4)	C5—C51—C56—C55	−176.8 (3)
C22—C21—C26—C25	−0.9 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N3^{i}	0.88 (3)	2.07 (3)	2.933 (3)	168 (3)

Symmetry code: (i) $x, -y, z-1/2$.