

2-(10-Bromoanthracen-9-yl)-*N*-phenylaniline

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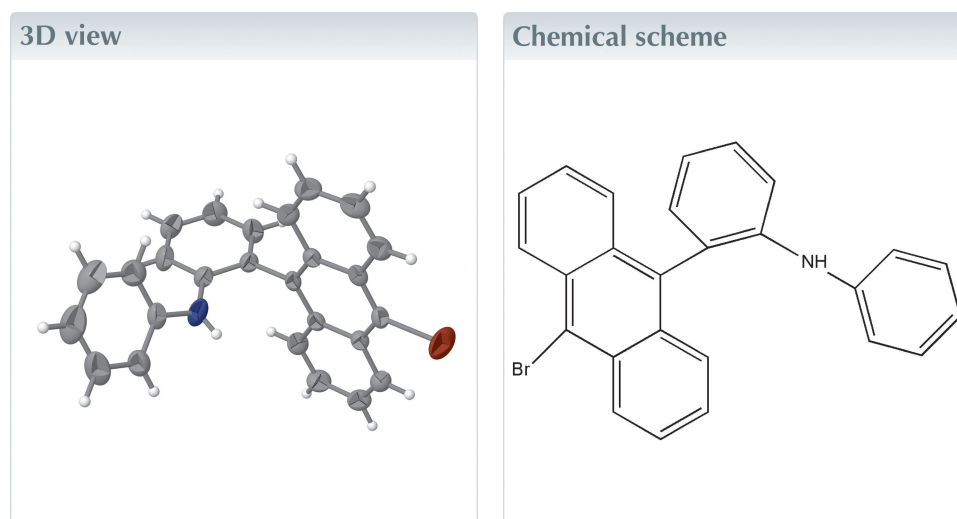
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CCDC reference: 2356945

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

In the title compound, C₂₆H₁₈BrN, the central benzene ring makes dihedral angles with its adjacent anthracene ring system and pendant benzene ring of 87.49 (13) and 62.01 (17)°, respectively. The N—H moiety is sterically blocked from forming a hydrogen bond, but weak C—H... π interactions occur in the extended structure.



Structure description

Anthracene derivatives are candidates for two-dimensional molecular crystals, which can show interesting properties with applications in electronics, biomedicine, and sensors (Yan *et al.*, 2023). As part of our studies of anthracene derivatives, we now report the synthesis and crystal structure of the title compound, C₂₆H₁₈BrN, (**I**).

The molecular structure of (**I**) is illustrated in Fig. 1. As expected, the anthracene (C1–C14) ring system is almost planar, with a maximum deviation of 0.039 (4) Å for atom C1. The central benzene (C15–C20) ring makes dihedral angles of 87.49 (13) and 62.01 (17)° with the anthracene ring system and the terminal C21–C26 phenyl ring, respectively. The dihedral angle between the phenyl ring and anthracene ring system is 87.92 (14)°.

In the extended structure, the N—H grouping in (**I**) is presumably blocked from forming a hydrogen bond due to steric reasons but two weak C—H... π interactions are observed (Table 1). The packing is illustrated in Fig. 2.

Related structures reported in the Cambridge Structural Database (CSD, Version 5.41, updated November 2019; Groom *et al.*, 2016) include {1-[2-(9-anthryl)phenyl]-3-[2-(4-isopropyl-4,5-dihydro-1,3-oxazol-2-yl)propan-2-yl]-1,3-dihydro-2*H*-benzimidazole-2-thione}dichloropalladium(II) deuteriochloroform solvate (CSD refcode BUVGEF; Gao *et al.* 2010), 10-bromo-2,7-di-*tert*-butyl-*N,N*-bis(4-methylphenyl) anthracen-9-amine (FEKTOG; Hoffend *et al.*, 2012) and 9-(10'-bromo-9'-anthryl)carbazole (PEDSUM; Boyer *et al.*, 1993).

Table 1

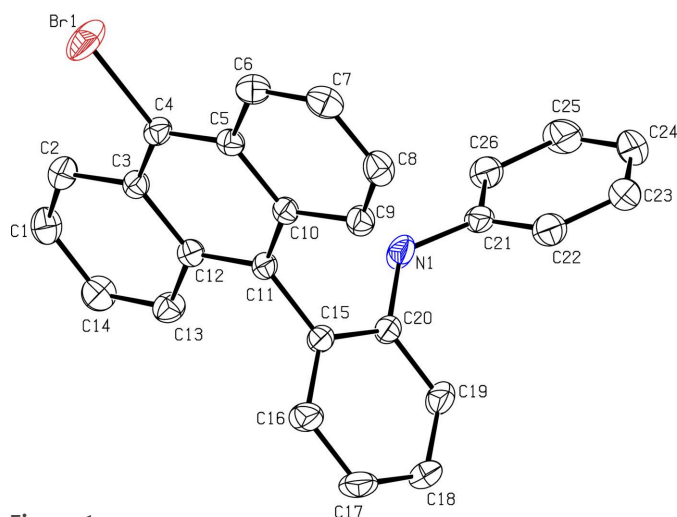
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C17–H17 \cdots Cg3 ⁱ	0.93	2.77	3.598 (4)	148
C18–H18 \cdots Cg5 ⁱ	0.93	2.85	3.661 (4)	146

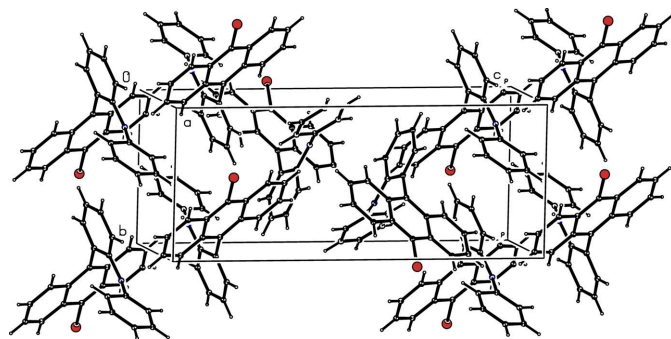
 Symmetry code: (i) $x, y + 1, z$.

Synthesis and crystallization

Following the method of Justin Thomas *et al.* (2005), a mixture of diphenylamine (1.69 g, 10.0 mmol), sodium *tert*-butoxide (1.15 g, 12.0 mmol) and Pd₂(dba)₃ (dba = dibenzylideneacetone; 23 mg, 0.10 mmol) was dissolved in dry toluene (50 ml), and 9,10-dibromoanthracene (3.33 g, 10.0 mmol) and 1,1'-ferrocenediyl-bis(diphenylphosphine) (0.277 g, 0.5 mmol) were added sequentially. The mixture was heated to reflux, stirred for 24 h and then cooled and 5 ml of water were added. The solution was extracted with dichloromethane/water. The organic layer was dried over anhydrous sodium sulfate, filtered, and dried. The residue was chromatographed through silica gel using a mixture of dichloromethane and hexane as the eluent to give the pure product as yellow crystals.


Figure 1

The molecular structure of (I) showing displacement ellipsoids at the 50% probability level (H atoms are omitted for clarity).


Figure 2

The crystal packing of (I) viewed approximately down [000].

Table 2

Experimental details.

Crystal data	
Chemical formula	C ₂₆ H ₁₈ BrN
M_r	424.32
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	13.0619 (17), 7.6891 (10), 20.475 (3)
β (°)	106.809 (14)
V (Å ³)	1968.6 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	2.10
Crystal size (mm)	0.48 × 0.39 × 0.30
Data collection	
Diffractometer	Agilent Xcalibur, Atlas, Gemini Analytical (<i>CrysAlis RED</i> ; Agilent, 2012)
Absorption correction	
T_{\min}, T_{\max}	0.432, 0.572
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12046, 3999, 3115
R_{int}	0.037
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.049, 0.129, 1.05
No. of reflections	3999
No. of parameters	257
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.81, -1.40

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXT* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b) and *PLATON* (Spek, 2020).

Refinement

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

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full crystallographic data

IUCrData (2024). **9**, x240475 [https://doi.org/10.1107/S2414314624004759]

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2-(10-Bromoanthracen-9-yl)-*N*-phenylaniline*Crystal data*

$C_{26}H_{18}BrN$

$M_r = 424.32$

Monoclinic, $P2_1/c$

$a = 13.0619$ (17) Å

$b = 7.6891$ (10) Å

$c = 20.475$ (3) Å

$\beta = 106.809$ (14)°

$V = 1968.6$ (5) Å³

$Z = 4$

$F(000) = 864$

$D_x = 1.432$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3999 reflections

$\theta = 3.4$ – 26.4 °

$\mu = 2.10$ mm⁻¹

$T = 293$ K

Plate, yellow

$0.48 \times 0.39 \times 0.30$ mm

Data collection

Agilent Xcalibur, Atlas, Gemini diffractometer

Radiation source: fine-focus sealed tube

ω scans

Absorption correction: analytical (CrysAlis RED; Agilent, 2012)

$T_{\min} = 0.432$, $T_{\max} = 0.572$

12046 measured reflections

3999 independent reflections

3115 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 26.4$ °, $\theta_{\min} = 3.4$ °

$h = -16$ → 14

$k = -9$ → 8

$l = -25$ → 25

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.129$

$S = 1.05$

3999 reflections

257 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 1.6534P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.81$ e Å⁻³

$\Delta\rho_{\min} = -1.40$ 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. The N-bound hydrogen atom was located in a difference map and its position was freely refined. The remaining hydrogen atoms were positioned geometrically [C—H = 0.93 Å] and were refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	−0.02528 (3)	−0.04566 (6)	0.34351 (2)	0.0715 (2)
N1	0.4598 (2)	0.3135 (4)	0.41519 (18)	0.0577 (9)
C3	0.1079 (2)	0.2407 (4)	0.40118 (14)	0.0324 (6)
C12	0.1886 (2)	0.3680 (4)	0.40287 (14)	0.0315 (6)
C11	0.2396 (2)	0.3735 (4)	0.35115 (14)	0.0309 (6)
C5	0.1305 (2)	0.1255 (4)	0.29426 (14)	0.0321 (6)
C10	0.2127 (2)	0.2523 (4)	0.29757 (14)	0.0306 (6)
C4	0.0816 (2)	0.1236 (4)	0.34678 (15)	0.0346 (6)
C15	0.3228 (2)	0.5092 (4)	0.35332 (15)	0.0338 (6)
C9	0.2637 (2)	0.2517 (4)	0.24464 (15)	0.0396 (7)
H9	0.317747	0.331703	0.246104	0.048*
C20	0.4302 (2)	0.4749 (4)	0.38369 (16)	0.0374 (7)
C2	0.0601 (3)	0.2382 (4)	0.45579 (15)	0.0424 (7)
H2	0.007271	0.156905	0.455513	0.051*
C8	0.2351 (3)	0.1373 (4)	0.19247 (16)	0.0467 (8)
H8	0.269377	0.139879	0.158491	0.056*
C21	0.5558 (2)	0.2265 (4)	0.41906 (17)	0.0410 (7)
C13	0.2159 (3)	0.4878 (4)	0.45853 (16)	0.0426 (7)
H13	0.267045	0.573083	0.460148	0.051*
C6	0.1034 (3)	0.0083 (4)	0.23773 (16)	0.0426 (7)
H6	0.049834	−0.073800	0.234413	0.051*
C7	0.1544 (3)	0.0148 (4)	0.18900 (17)	0.0487 (8)
H7	0.135678	−0.063095	0.152715	0.058*
C16	0.2937 (3)	0.6726 (4)	0.32505 (18)	0.0478 (8)
H16	0.221626	0.697953	0.305740	0.057*
C26	0.6048 (3)	0.1311 (4)	0.47645 (18)	0.0482 (8)
H26	0.576252	0.129337	0.513136	0.058*
C18	0.4752 (3)	0.7621 (4)	0.35375 (18)	0.0501 (8)
H18	0.526590	0.845360	0.353300	0.060*
C1	0.0911 (3)	0.3530 (5)	0.50787 (16)	0.0484 (8)
H1	0.060381	0.347710	0.543532	0.058*
C19	0.5059 (3)	0.6027 (4)	0.38339 (19)	0.0492 (8)
H19	0.578117	0.579804	0.403488	0.059*
C22	0.6002 (3)	0.2280 (5)	0.36512 (19)	0.0512 (8)
H22	0.567577	0.291351	0.325915	0.061*
C17	0.3693 (3)	0.7984 (4)	0.32496 (19)	0.0545 (9)
H17	0.348321	0.906707	0.305481	0.065*
C14	0.1681 (3)	0.4789 (5)	0.50894 (17)	0.0497 (8)
H14	0.187045	0.558049	0.544786	0.060*
C23	0.6920 (3)	0.1364 (5)	0.3695 (2)	0.0620 (10)
H23	0.721646	0.139989	0.333358	0.074*

C25	0.6966 (3)	0.0379 (5)	0.4793 (3)	0.0678 (12)
H25	0.729331	-0.027472	0.517943	0.081*
C24	0.7402 (3)	0.0409 (5)	0.4254 (3)	0.0717 (12)
H24	0.801947	-0.021919	0.427468	0.086*
H55	0.425 (3)	0.265 (6)	0.435 (2)	0.073 (14)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0704 (3)	0.0804 (3)	0.0719 (3)	-0.0470 (2)	0.0336 (2)	-0.0247 (2)
N1	0.0311 (15)	0.0545 (18)	0.092 (2)	0.0093 (13)	0.0244 (16)	0.0365 (17)
C3	0.0271 (14)	0.0351 (15)	0.0330 (15)	0.0021 (11)	0.0057 (11)	0.0035 (12)
C12	0.0279 (14)	0.0333 (14)	0.0306 (15)	0.0019 (11)	0.0041 (11)	0.0025 (11)
C11	0.0212 (13)	0.0327 (14)	0.0357 (15)	0.0024 (11)	0.0036 (11)	0.0057 (12)
C5	0.0284 (14)	0.0309 (14)	0.0329 (15)	0.0031 (11)	0.0024 (12)	0.0014 (11)
C10	0.0255 (13)	0.0326 (14)	0.0314 (14)	0.0047 (11)	0.0047 (11)	0.0053 (11)
C4	0.0260 (14)	0.0365 (15)	0.0378 (16)	-0.0035 (12)	0.0039 (12)	0.0021 (12)
C15	0.0315 (15)	0.0330 (14)	0.0371 (16)	-0.0015 (12)	0.0103 (13)	0.0024 (12)
C9	0.0374 (16)	0.0413 (17)	0.0415 (17)	0.0049 (13)	0.0136 (14)	0.0070 (13)
C20	0.0315 (15)	0.0360 (15)	0.0465 (18)	0.0015 (12)	0.0140 (13)	0.0089 (13)
C2	0.0389 (17)	0.0494 (18)	0.0401 (17)	-0.0023 (14)	0.0133 (14)	0.0030 (14)
C8	0.052 (2)	0.054 (2)	0.0379 (17)	0.0078 (16)	0.0188 (15)	0.0020 (15)
C21	0.0286 (15)	0.0322 (15)	0.059 (2)	-0.0012 (12)	0.0069 (14)	0.0050 (14)
C13	0.0433 (18)	0.0419 (17)	0.0410 (18)	-0.0080 (14)	0.0098 (14)	-0.0061 (13)
C6	0.0469 (18)	0.0389 (16)	0.0379 (17)	-0.0039 (14)	0.0059 (14)	-0.0037 (13)
C7	0.062 (2)	0.0439 (18)	0.0373 (18)	0.0047 (16)	0.0093 (16)	-0.0058 (14)
C16	0.0389 (17)	0.0378 (17)	0.061 (2)	0.0031 (14)	0.0050 (15)	0.0133 (15)
C26	0.0388 (17)	0.0457 (18)	0.056 (2)	0.0000 (14)	0.0074 (15)	0.0072 (16)
C18	0.051 (2)	0.0384 (18)	0.065 (2)	-0.0136 (15)	0.0232 (18)	0.0003 (15)
C1	0.0504 (19)	0.060 (2)	0.0377 (18)	0.0041 (16)	0.0181 (15)	-0.0013 (15)
C19	0.0313 (16)	0.0508 (19)	0.066 (2)	-0.0044 (14)	0.0145 (16)	0.0070 (17)
C22	0.049 (2)	0.0476 (19)	0.056 (2)	-0.0016 (16)	0.0134 (17)	0.0038 (16)
C17	0.060 (2)	0.0309 (16)	0.070 (2)	-0.0027 (15)	0.0140 (19)	0.0133 (16)
C14	0.057 (2)	0.054 (2)	0.0386 (18)	-0.0039 (16)	0.0151 (16)	-0.0098 (15)
C23	0.065 (2)	0.045 (2)	0.090 (3)	-0.0036 (18)	0.043 (2)	-0.009 (2)
C25	0.045 (2)	0.052 (2)	0.095 (3)	0.0124 (17)	0.002 (2)	0.024 (2)
C24	0.048 (2)	0.052 (2)	0.121 (4)	0.0122 (18)	0.035 (3)	0.006 (2)

Geometric parameters (Å, °)

Br1—C4	1.896 (3)	C21—C22	1.388 (5)
N1—C20	1.401 (4)	C13—C14	1.353 (5)
N1—C21	1.404 (4)	C13—H13	0.9300
N1—H55	0.78 (4)	C6—C7	1.352 (5)
C3—C4	1.396 (4)	C6—H6	0.9300
C3—C2	1.430 (4)	C7—H7	0.9300
C3—C12	1.432 (4)	C16—C17	1.383 (5)
C12—C11	1.405 (4)	C16—H16	0.9300

C12—C13	1.429 (4)	C26—C25	1.385 (5)
C11—C10	1.405 (4)	C26—H26	0.9300
C11—C15	1.497 (4)	C18—C17	1.366 (5)
C5—C4	1.400 (4)	C18—C19	1.375 (5)
C5—C6	1.428 (4)	C18—H18	0.9300
C5—C10	1.437 (4)	C1—C14	1.392 (5)
C10—C9	1.427 (4)	C1—H1	0.9300
C15—C20	1.386 (4)	C19—H19	0.9300
C15—C16	1.390 (4)	C22—C23	1.371 (5)
C9—C8	1.351 (5)	C22—H22	0.9300
C9—H9	0.9300	C17—H17	0.9300
C20—C19	1.395 (4)	C14—H14	0.9300
C2—C1	1.353 (4)	C23—C24	1.352 (6)
C2—H2	0.9300	C23—H23	0.9300
C8—C7	1.400 (5)	C25—C24	1.381 (6)
C8—H8	0.9300	C25—H25	0.9300
C21—C26	1.376 (5)	C24—H24	0.9300
C20—N1—C21	124.8 (3)	C12—C13—H13	119.6
C20—N1—H55	122 (3)	C7—C6—C5	121.0 (3)
C21—N1—H55	113 (3)	C7—C6—H6	119.5
C4—C3—C2	123.6 (3)	C5—C6—H6	119.5
C4—C3—C12	118.0 (2)	C6—C7—C8	120.8 (3)
C2—C3—C12	118.4 (3)	C6—C7—H7	119.6
C11—C12—C13	121.2 (3)	C8—C7—H7	119.6
C11—C12—C3	120.6 (3)	C17—C16—C15	121.5 (3)
C13—C12—C3	118.2 (3)	C17—C16—H16	119.2
C10—C11—C12	120.1 (2)	C15—C16—H16	119.2
C10—C11—C15	120.1 (2)	C21—C26—C25	119.7 (4)
C12—C11—C15	119.8 (2)	C21—C26—H26	120.2
C4—C5—C6	123.7 (3)	C25—C26—H26	120.2
C4—C5—C10	118.1 (2)	C17—C18—C19	120.2 (3)
C6—C5—C10	118.2 (3)	C17—C18—H18	119.9
C11—C10—C9	121.9 (3)	C19—C18—H18	119.9
C11—C10—C5	120.2 (2)	C2—C1—C14	121.1 (3)
C9—C10—C5	118.0 (3)	C2—C1—H1	119.5
C3—C4—C5	123.0 (3)	C14—C1—H1	119.5
C3—C4—Br1	118.7 (2)	C18—C19—C20	120.8 (3)
C5—C4—Br1	118.3 (2)	C18—C19—H19	119.6
C20—C15—C16	118.6 (3)	C20—C19—H19	119.6
C20—C15—C11	120.8 (3)	C23—C22—C21	120.1 (3)
C16—C15—C11	120.6 (3)	C23—C22—H22	119.9
C8—C9—C10	121.3 (3)	C21—C22—H22	119.9
C8—C9—H9	119.4	C18—C17—C16	119.4 (3)
C10—C9—H9	119.4	C18—C17—H17	120.3
C15—C20—C19	119.4 (3)	C16—C17—H17	120.3
C15—C20—N1	118.9 (3)	C13—C14—C1	120.9 (3)
C19—C20—N1	121.7 (3)	C13—C14—H14	119.5

C1—C2—C3	120.6 (3)	C1—C14—H14	119.5
C1—C2—H2	119.7	C24—C23—C22	121.3 (4)
C3—C2—H2	119.7	C24—C23—H23	119.3
C9—C8—C7	120.7 (3)	C22—C23—H23	119.3
C9—C8—H8	119.6	C24—C25—C26	120.7 (4)
C7—C8—H8	119.6	C24—C25—H25	119.7
C26—C21—C22	119.1 (3)	C26—C25—H25	119.7
C26—C21—N1	119.3 (3)	C23—C24—C25	119.1 (4)
C22—C21—N1	121.5 (3)	C23—C24—H24	120.4
C14—C13—C12	120.8 (3)	C25—C24—H24	120.4
C14—C13—H13	119.6		
C4—C3—C12—C11	-0.2 (4)	C11—C15—C20—N1	-2.8 (5)
C2—C3—C12—C11	178.7 (3)	C21—N1—C20—C15	148.5 (3)
C4—C3—C12—C13	-179.9 (3)	C21—N1—C20—C19	-32.9 (5)
C2—C3—C12—C13	-1.0 (4)	C4—C3—C2—C1	178.5 (3)
C13—C12—C11—C10	178.9 (3)	C12—C3—C2—C1	-0.3 (4)
C3—C12—C11—C10	-0.8 (4)	C10—C9—C8—C7	-0.3 (5)
C13—C12—C11—C15	-1.1 (4)	C20—N1—C21—C26	144.7 (4)
C3—C12—C11—C15	179.2 (2)	C20—N1—C21—C22	-38.2 (5)
C12—C11—C10—C9	-179.0 (3)	C11—C12—C13—C14	-178.4 (3)
C15—C11—C10—C9	1.0 (4)	C3—C12—C13—C14	1.3 (5)
C12—C11—C10—C5	1.9 (4)	C4—C5—C6—C7	-179.1 (3)
C15—C11—C10—C5	-178.1 (2)	C10—C5—C6—C7	0.8 (4)
C4—C5—C10—C11	-2.0 (4)	C5—C6—C7—C8	-0.2 (5)
C6—C5—C10—C11	178.1 (3)	C9—C8—C7—C6	0.0 (5)
C4—C5—C10—C9	178.8 (2)	C20—C15—C16—C17	1.9 (5)
C6—C5—C10—C9	-1.0 (4)	C11—C15—C16—C17	-178.4 (3)
C2—C3—C4—C5	-178.8 (3)	C22—C21—C26—C25	-0.4 (5)
C12—C3—C4—C5	0.0 (4)	N1—C21—C26—C25	176.8 (3)
C2—C3—C4—Br1	1.3 (4)	C3—C2—C1—C14	1.6 (5)
C12—C3—C4—Br1	-179.9 (2)	C17—C18—C19—C20	1.0 (5)
C6—C5—C4—C3	-179.1 (3)	C15—C20—C19—C18	0.4 (5)
C10—C5—C4—C3	1.1 (4)	N1—C20—C19—C18	-178.3 (3)
C6—C5—C4—Br1	0.8 (4)	C26—C21—C22—C23	-0.5 (5)
C10—C5—C4—Br1	-179.03 (19)	N1—C21—C22—C23	-177.5 (3)
C10—C11—C15—C20	-86.9 (3)	C19—C18—C17—C16	-0.9 (6)
C12—C11—C15—C20	93.1 (3)	C15—C16—C17—C18	-0.5 (6)
C10—C11—C15—C16	93.3 (4)	C12—C13—C14—C1	-0.1 (5)
C12—C11—C15—C16	-86.7 (4)	C2—C1—C14—C13	-1.3 (5)
C11—C10—C9—C8	-178.3 (3)	C21—C22—C23—C24	1.1 (6)
C5—C10—C9—C8	0.8 (4)	C21—C26—C25—C24	0.6 (6)
C16—C15—C20—C19	-1.8 (5)	C22—C23—C24—C25	-0.9 (6)
C11—C15—C20—C19	178.5 (3)	C26—C25—C24—C23	0.0 (6)
C16—C15—C20—N1	176.9 (3)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C17—H17 \cdots Cg3 ⁱ	0.93	2.77	3.598 (4)	148
C18—H18 \cdots Cg5 ⁱ	0.93	2.85	3.661 (4)	146

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