



IUCrData

ISSN 2414-3146

Received 12 June 2016

Accepted 21 June 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

Keywords: crystal structure; 4-bromophenyl; dipyrromethane; C—H... π interactions; N—H... π interactions; C—Br... π interactions.

CCDC reference: 1486804

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

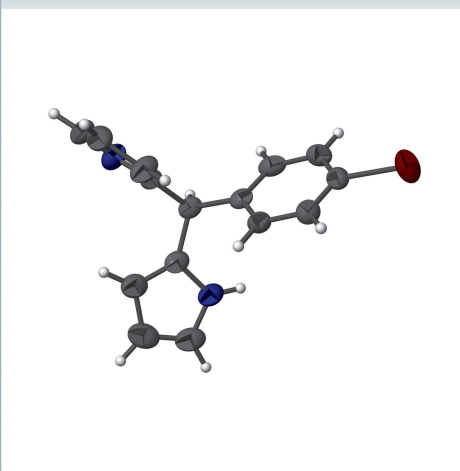
2,2'-[(4-Bromophenyl)methylene]bis(1*H*-pyrrole)

A. K. Bauri,^a Sabine Foro^b and Nhu Do Quynh Nguyen^{c*}

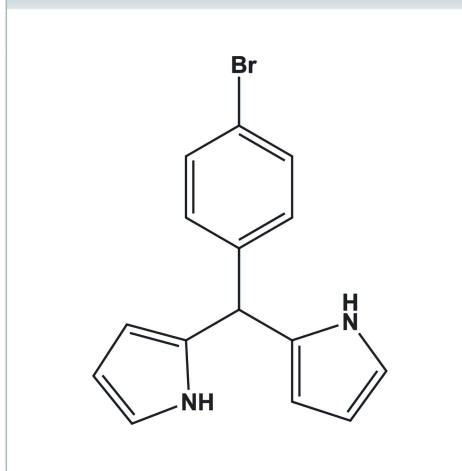
^aBio-Organic Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400 085, India, ^bInstitute of Materials Science, Darmstadt University of Technology, Alarich-Weiss-Strasse 2, D-64287 Darmstadt, Germany, and ^cInternational SOS Clinics, 167A Nam Ky Khoi Nghia Street, District-3, HoChiMinh City, Vietnam. *Correspondence e-mail: nguyendonhuquynh@yahoo.com

The title compound, C₁₅H₁₃BrN₂, is a substituted methane derivative. Three H atoms of the methane molecule have been substituted by means of two pyrrole rings and one 4-bromophenyl moiety. The two pyrrole rings are inclined to one another by 85.0 (3)°, and to the benzene ring by 71.4 (2)° and 69.5 (2)°. In the crystal, molecules are linked *via* N—H... π and C—H... π interactions, forming layers parallel to (101). The layers are linked by C—Br... π interactions, forming a three-dimensional structure.

3D view



Chemical scheme



Structure description

Dipyrromethanes, substituted dipyrromethanes and *meso*-substituted dipyrromethanes are the building blocks for the synthesis of porphyrins (Mukherjee *et al.*, 2015), fluorescent laser dyes (Loudet & Burgess, 2007) and fluorophores. They are also an important tool in a variety of imaging applications (Taki, 2013) and chemo-sensors (Nikola *et al.*, 2008). In general, they are synthesized by acid-catalysed condensation reaction of pyrrole or a substituted pyrrole and an aldehyde (Littler *et al.*, 1999). The crude product is purified to obtain the corresponding dipyrromethane which is used as precursor (Lee & Hupp, 2010) for syntheses of target host molecules such as molecular nanotweezers (Zhao *et al.* 2013), porphyrins and fluorescent dyes (Tram *et al.*, 2009). These host molecules are utilized as optoelectronic materials (Lee & Hupp, 2010; Rio *et al.*, 2009) in optical photovoltaic (OPV) cells, as organic light-emitting diodes (OLED), and for the purpose of material separation in supramolecular chemistry.

The title compound, Fig. 1, can be considered as a substituted methane derivative. Three H atoms of the methane molecule have been substituted by means of two pyrrole rings and one 4-bromophenyl moiety. The two pyrrole rings, N1/C8–C11 and N2/C12–

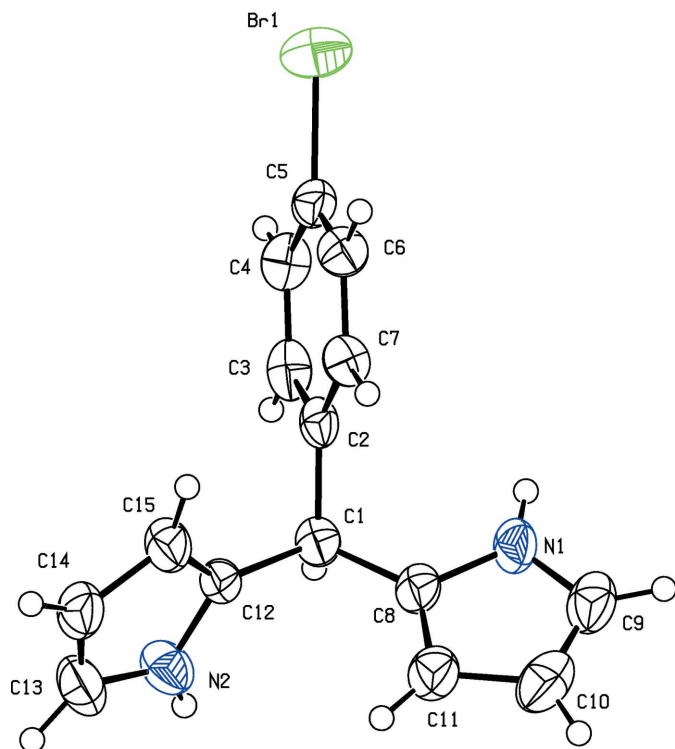


Figure 1
A view of the molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

C15, are inclined to one another by $85.0(3)^\circ$, and to the benzene ring, C2–C7, by $71.4(2)$ and $69.5(2)^\circ$, respectively.

In the crystal, molecules are linked *via* N–H $\cdots\pi$ and C–H $\cdots\pi$ interactions, forming layers parallel to (101), Table 1 and Fig. 2. The layers are linked by C–Br $\cdots\pi$ interactions, forming a three-dimensional structure, Table 1 and Fig. 3.

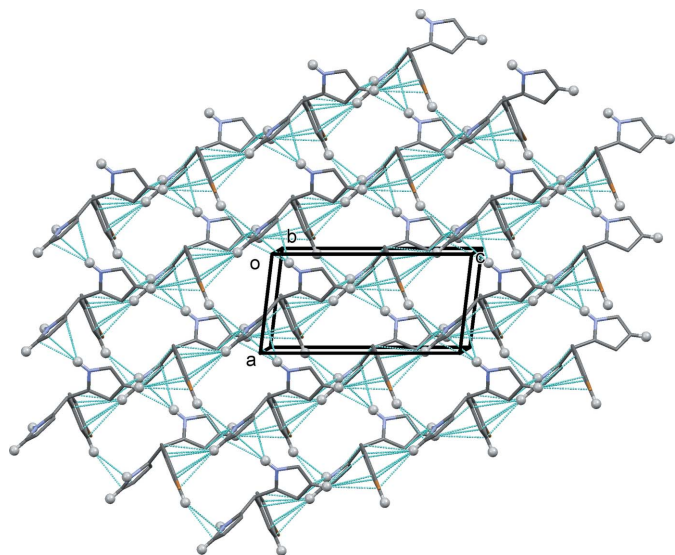


Figure 2
The crystal packing of the title compound, viewed along the *b* axis, with the intermolecular interactions shown as dashed lines (see Table 1).

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

Cg1, Cg2 and Cg3 are the centroids of the N1/C8–C11, N2/C12–C15 and C2–C7 rings, respectively.

<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>
N2–H2N \cdots Cg1 ⁱ	0.86	2.43	3.262 (4)	163
C6–H6 \cdots Cg1 ⁱⁱ	0.93	2.89	3.656 (5)	141
C9–H9 \cdots Cg3 ⁱⁱⁱ	0.93	2.71	3.590 (5)	159
C14–H14 \cdots Cg3 ^{iv}	0.93	2.79	3.564 (5)	142
C5–Br1 \cdots Cg2 ^v	1.91 (1)	3.70 (1)	5.595 (4)	171 (1)

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

A search of the Cambridge Structural Database (CSD, Version 5.37, last update February 2016; Groom *et al.*, 2016), found 19 hits for 5-phenyldipyrromethanes. 5-Phenyldipyrromethane itself (CSD refcode LAYIA; Littler *et al.*, 1999) has a very similar structural skeleton to the title molecule: the two pyrrole rings are inclined to one another by $87.1(1)^\circ$, and to the benzene ring by $71.6(1)$ and $67.8(1)^\circ$.

Synthesis and crystallization

A suspension of 4-bromobenzaldehyde (3.24 g, 57.7 mmol) in pyrrole (100 ml, 1.44 mol) was placed in a 250 ml two-necked round-bottom flask equipped with an internal thermometer and a water condenser in the reflux position. The solution was heated to 323 K, and then the heat source was removed and TFA (444 μL , 5.77 mmol) was added immediately. A sharp increase in the temperature of the solution was observed and the solution rapidly became clear and dark. After 5 min the reaction was quenched and the product was purified following

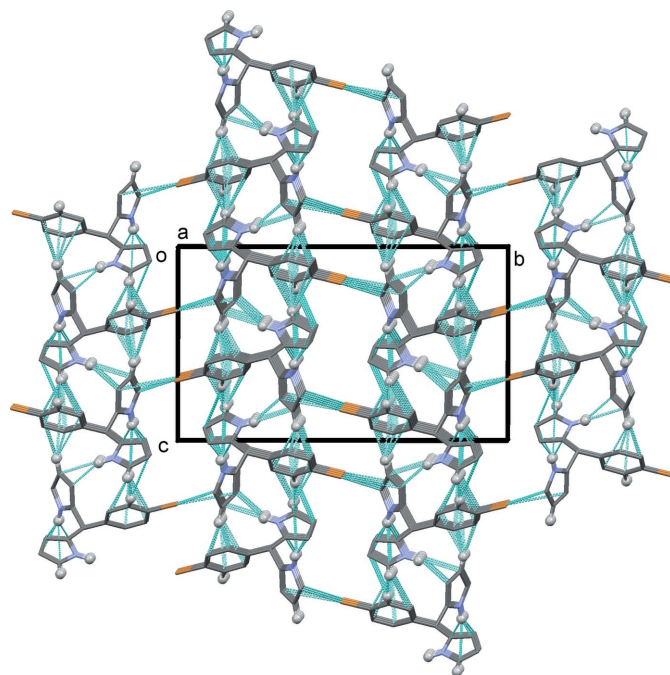


Figure 3
The crystal packing of the title compound, viewed along the *a* axis, with the intermolecular interactions shown as dashed lines (see Table 1).

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₅ H ₁₃ BrN ₂
<i>M_r</i>	301.18
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	299
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.8132 (8), 19.763 (2), 11.656 (1)
β (°)	96.85 (1)
<i>V</i> (Å ³)	1329.6 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	3.08
Crystal size (mm)	0.34 × 0.26 × 0.12
Data collection	
Diffractometer	Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction	Multi-scan (<i>CrysAlis RED</i> ; Oxford Diffraction, 2009)
<i>T</i> _{min} , <i>T</i> _{max}	0.421, 0.709
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	4326, 2289, 1685
<i>R</i> _{int}	0.039
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.602
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.063, 0.176, 1.20
No. of reflections	2289
No. of parameters	163
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.59, -1.22

Computer programs: *CrysAlis CCD* (Oxford Diffraction, 2009), *CrysAlis RED* (Oxford Diffraction, 2009), *SHELXS97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008), *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

the general procedure [distilled at 360 K (0.01 mm/Hg); recrystallized from ethyl acetate:hexane (1:4)] giving the desired product as colourless crystals (yield 3.48 g, 41%; m.p. 403 K). ¹H NMR (200 MHz, CDCl₃): δ_{H} 5.43 (s, 1H, H-1), 5.92 (s, 2H, β H, H-11 & H-15), 6.16 (*dd*, *J* = 2.7 & 5.6 Hz, 2H, β H, H-10 & H-14), 6.67 (*dd*, *J* = 2.6 & 4.2 Hz, 2H, α H, H-9 & H-13), 7.15 (*d*, *J* = 8.2 Hz, 2H, H-6 & H-4/Ar-H), 7.48 (*d*, *J* = 8.2 Hz, 2H, H-3 & H-7/Ar-H), 7.81 (*brs*, 2H, >NH).

Refinement

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

Acknowledgements

The authors thank Professor Dr Hartmut, FG Struktur-forschung, Material-und Geowissenschaften, Technische Universit at Darmstadt, for his kind cooperation to record the XRD of the crystal, and for providing diffractometer time.

References

- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Lee, C. Y. & Hupp, J. T. (2010). *Langmuir*, **26**, 3760–3765.
- Littler, B. J., Miller, M. A., Hung, C.-H., Wagner, R. W., O'Shea, D. F., Boyle, P. D. & Lindsey, J. S. (1999). *J. Org. Chem.* **64**, 1391–1396.
- Loudet, A. & Burgess, K. (2007). *Chem. Rev.* **107**, 4891–4932.
- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
- Mukherjee, S., Bauri, A. K., Banerjee, S. & Bhattacharya, S. (2015). *ScienceJet*, **100**, 1–9.
- Nikola, B., Marija, R. & Kata, M. (2008). US Patent No. WO2008114067A1.
- Oxford Diffraction (2009). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.
- Rio, Y., Sánchez-García, D., Seitz, W., Torres, T., Sessler, J. L. & Guldi, D. M. (2009). *Chem. Eur. J.* **15**, 3956–3959.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Taki, M. (2013). *Cadmium: From Toxicity to Essentiality*, Vol. 11, *Metal ions in Life Sciences*, edited by A. Sigel, H. Sigel & R. K. O. Sigel, pp. 99–115. Berlin: Springer.
- Tram, K., Yan, H., Jenkins, H. A., Vassiliev, S. & Bruce, D. (2009). *Dyes Pigments*, **82**, 392–395.
- Zhao, H., Liao, J., Yang, D., Xie, Y., Xu, Y., Wang, H. & Wang, B. (2013). *Aust. J. Chem.* **66**, 972–982.

full crystallographic data

IUCrData (2016). **1**, x161005 [doi:10.1107/S2414314616010051]

2,2'-[(4-Bromophenyl)methylene]bis(1*H*-pyrrole)

A. K. Bauri, Sabine Foro and Nhu Do Quynh Nguyen

2,2'-[(4-Bromophenyl)methylene]bis(1*H*-pyrrole)*Crystal data*

$C_{15}H_{13}BrN_2$

$M_r = 301.18$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 5.8132$ (8) Å

$b = 19.763$ (2) Å

$c = 11.656$ (1) Å

$\beta = 96.85$ (1)°

$V = 1329.6$ (3) Å³

$Z = 4$

$F(000) = 608$

$D_x = 1.505$ Mg m⁻³

Melting point: 403 K

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

Cell parameters from 1789 reflections

$\theta = 2.7$ – 27.8 °

$\mu = 3.08$ mm⁻¹

$T = 299$ K

Prism, colourless

$0.34 \times 0.26 \times 0.12$ mm

Data collection

Oxford Diffraction Xcalibur

diffractometer with a Sapphire CCD detector

Radiation source: fine-focus sealed tube

Graphite monochromator

Rotation method data acquisition using ω scans.

Absorption correction: multi-scan

(CrysAlis RED; Oxford Diffraction, 2009)

$T_{\min} = 0.421$, $T_{\max} = 0.709$

4326 measured reflections

2289 independent reflections

1685 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 25.4$ °, $\theta_{\min} = 2.7$ °

$h = -7 \rightarrow 5$

$k = -23 \rightarrow 17$

$l = -12 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.063$

$wR(F^2) = 0.176$

$S = 1.20$

2289 reflections

163 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

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$

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

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

$\Delta\rho_{\max} = 0.59$ e Å⁻³

$\Delta\rho_{\min} = -1.22$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.86594 (9)	0.49826 (2)	0.17591 (5)	0.0642 (3)
N1	0.7634 (6)	0.19396 (18)	-0.0868 (3)	0.0443 (9)
H1N	0.7680	0.2357	-0.1070	0.053*
N2	0.1873 (6)	0.14504 (19)	0.1458 (3)	0.0481 (9)
H2N	0.0954	0.1383	0.0834	0.058*
C1	0.4652 (6)	0.2148 (2)	0.0487 (3)	0.0355 (9)
H1	0.3273	0.2214	-0.0074	0.043*
C2	0.5648 (6)	0.28383 (19)	0.0784 (3)	0.0338 (9)
C3	0.4351 (7)	0.3416 (2)	0.0523 (4)	0.0417 (10)
H3	0.2867	0.3373	0.0133	0.050*
C4	0.5182 (7)	0.4049 (2)	0.0820 (4)	0.0432 (10)
H4	0.4270	0.4430	0.0642	0.052*
C5	0.7386 (7)	0.41107 (19)	0.1385 (3)	0.0395 (10)
C6	0.8724 (6)	0.3555 (2)	0.1673 (4)	0.0402 (10)
H6	1.0198	0.3603	0.2073	0.048*
C7	0.7871 (6)	0.29211 (19)	0.1364 (3)	0.0364 (9)
H7	0.8794	0.2543	0.1545	0.044*
C8	0.6299 (7)	0.1687 (2)	-0.0082 (3)	0.0387 (9)
C9	0.8879 (8)	0.1435 (3)	-0.1283 (4)	0.0541 (12)
H9	0.9927	0.1481	-0.1822	0.065*
C10	0.8336 (8)	0.0863 (3)	-0.0785 (4)	0.0620 (13)
H10	0.8927	0.0436	-0.0914	0.074*
C11	0.6677 (7)	0.1020 (2)	-0.0013 (4)	0.0500 (11)
H11	0.5990	0.0716	0.0451	0.060*
C12	0.3867 (6)	0.18121 (19)	0.1531 (3)	0.0351 (9)
C13	0.1542 (8)	0.1208 (2)	0.2525 (4)	0.0555 (12)
H13	0.0296	0.0948	0.2698	0.067*
C14	0.3335 (8)	0.1414 (2)	0.3281 (4)	0.0491 (11)
H14	0.3554	0.1322	0.4069	0.059*
C15	0.4810 (7)	0.1791 (2)	0.2662 (4)	0.0478 (11)
H15	0.6194	0.1992	0.2968	0.057*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0775 (5)	0.0397 (4)	0.0728 (5)	-0.0020 (2)	-0.0020 (3)	-0.0044 (2)
N1	0.048 (2)	0.059 (2)	0.028 (2)	-0.0062 (17)	0.0100 (16)	-0.0044 (16)
N2	0.039 (2)	0.059 (2)	0.045 (2)	-0.0109 (17)	0.0019 (17)	0.0040 (17)
C1	0.031 (2)	0.049 (2)	0.026 (2)	-0.0040 (17)	-0.0014 (16)	-0.0007 (17)
C2	0.033 (2)	0.047 (2)	0.022 (2)	-0.0015 (17)	0.0055 (16)	0.0024 (15)

C3	0.031 (2)	0.065 (3)	0.029 (2)	0.0060 (19)	0.0012 (18)	0.0050 (19)
C4	0.041 (2)	0.048 (3)	0.040 (3)	0.0109 (19)	0.0034 (19)	0.0049 (19)
C5	0.049 (2)	0.038 (2)	0.033 (2)	-0.0005 (18)	0.0112 (19)	-0.0012 (17)
C6	0.038 (2)	0.045 (3)	0.037 (2)	-0.0014 (18)	-0.0002 (19)	0.0006 (17)
C7	0.0279 (19)	0.043 (2)	0.038 (2)	0.0034 (17)	0.0009 (17)	0.0046 (17)
C8	0.037 (2)	0.053 (3)	0.025 (2)	-0.0065 (19)	0.0006 (16)	-0.0072 (18)
C9	0.049 (3)	0.078 (4)	0.036 (3)	-0.002 (2)	0.005 (2)	-0.014 (2)
C10	0.065 (3)	0.070 (4)	0.051 (3)	0.006 (3)	0.004 (2)	-0.021 (2)
C11	0.049 (3)	0.058 (3)	0.043 (3)	-0.004 (2)	0.007 (2)	-0.009 (2)
C12	0.031 (2)	0.040 (2)	0.035 (2)	-0.0054 (16)	0.0081 (17)	-0.0051 (16)
C13	0.052 (3)	0.055 (3)	0.065 (3)	-0.003 (2)	0.026 (2)	0.012 (2)
C14	0.063 (3)	0.051 (3)	0.037 (3)	0.001 (2)	0.017 (2)	0.0028 (19)
C15	0.046 (2)	0.069 (3)	0.029 (2)	-0.017 (2)	0.0059 (19)	-0.006 (2)

Geometric parameters (Å, °)

Br1—C5	1.905 (4)	C5—C6	1.365 (5)
N1—C9	1.355 (6)	C6—C7	1.379 (5)
N1—C8	1.364 (5)	C6—H6	0.9300
N1—H1N	0.8600	C7—H7	0.9300
N2—C12	1.356 (5)	C8—C11	1.336 (6)
N2—C13	1.368 (6)	C9—C10	1.326 (7)
N2—H2N	0.8600	C9—H9	0.9300
C1—C12	1.505 (5)	C10—C11	1.430 (6)
C1—C2	1.506 (5)	C10—H10	0.9300
C1—C8	1.529 (6)	C11—H11	0.9300
C1—H1	0.9800	C12—C15	1.366 (5)
C2—C3	1.381 (5)	C13—C14	1.344 (6)
C2—C7	1.395 (5)	C13—H13	0.9300
C3—C4	1.372 (6)	C14—C15	1.400 (5)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.374 (6)	C15—H15	0.9300
C4—H4	0.9300		
C9—N1—C8	110.0 (4)	C6—C7—C2	121.1 (4)
C9—N1—H1N	125.0	C6—C7—H7	119.4
C8—N1—H1N	125.0	C2—C7—H7	119.4
C12—N2—C13	109.8 (4)	C11—C8—N1	107.4 (4)
C12—N2—H2N	125.1	C11—C8—C1	131.9 (4)
C13—N2—H2N	125.1	N1—C8—C1	120.6 (4)
C12—C1—C2	111.0 (3)	C10—C9—N1	107.8 (4)
C12—C1—C8	110.7 (3)	C10—C9—H9	126.1
C2—C1—C8	113.4 (3)	N1—C9—H9	126.1
C12—C1—H1	107.1	C9—C10—C11	107.7 (4)
C2—C1—H1	107.1	C9—C10—H10	126.2
C8—C1—H1	107.1	C11—C10—H10	126.2
C3—C2—C7	117.4 (4)	C8—C11—C10	107.2 (4)
C3—C2—C1	120.8 (3)	C8—C11—H11	126.4

C7—C2—C1	121.8 (3)	C10—C11—H11	126.4
C4—C3—C2	122.1 (4)	N2—C12—C15	106.6 (4)
C4—C3—H3	118.9	N2—C12—C1	121.4 (3)
C2—C3—H3	118.9	C15—C12—C1	132.0 (3)
C3—C4—C5	118.8 (4)	C14—C13—N2	107.9 (4)
C3—C4—H4	120.6	C14—C13—H13	126.0
C5—C4—H4	120.6	N2—C13—H13	126.0
C6—C5—C4	121.2 (4)	C13—C14—C15	107.4 (4)
C6—C5—Br1	118.5 (3)	C13—C14—H14	126.3
C4—C5—Br1	120.3 (3)	C15—C14—H14	126.3
C5—C6—C7	119.4 (4)	C12—C15—C14	108.3 (4)
C5—C6—H6	120.3	C12—C15—H15	125.9
C7—C6—H6	120.3	C14—C15—H15	125.9
C12—C1—C2—C3	-100.7 (4)	C12—C1—C8—N1	-164.7 (3)
C8—C1—C2—C3	133.9 (4)	C2—C1—C8—N1	-39.2 (5)
C12—C1—C2—C7	77.2 (4)	C8—N1—C9—C10	0.8 (5)
C8—C1—C2—C7	-48.1 (5)	N1—C9—C10—C11	-0.4 (6)
C7—C2—C3—C4	-0.4 (5)	N1—C8—C11—C10	0.6 (5)
C1—C2—C3—C4	177.7 (4)	C1—C8—C11—C10	176.9 (4)
C2—C3—C4—C5	0.7 (6)	C9—C10—C11—C8	-0.1 (5)
C3—C4—C5—C6	-1.4 (6)	C13—N2—C12—C15	0.5 (5)
C3—C4—C5—Br1	177.4 (3)	C13—N2—C12—C1	-179.1 (4)
C4—C5—C6—C7	1.7 (6)	C2—C1—C12—N2	139.7 (4)
Br1—C5—C6—C7	-177.2 (3)	C8—C1—C12—N2	-93.5 (4)
C5—C6—C7—C2	-1.3 (6)	C2—C1—C12—C15	-39.8 (6)
C3—C2—C7—C6	0.7 (5)	C8—C1—C12—C15	87.0 (5)
C1—C2—C7—C6	-177.3 (3)	C12—N2—C13—C14	-0.3 (5)
C9—N1—C8—C11	-0.8 (5)	N2—C13—C14—C15	-0.1 (5)
C9—N1—C8—C1	-177.7 (4)	N2—C12—C15—C14	-0.6 (5)
C12—C1—C8—C11	19.3 (6)	C1—C12—C15—C14	179.0 (4)
C2—C1—C8—C11	144.8 (4)	C13—C14—C15—C12	0.4 (5)

Hydrogen-bond geometry (\AA , $^\circ$)

$Cg1$, $Cg2$ and $Cg3$ are the centroids of the N1/C8—C11, N2/C12—C15 and C2—C7 rings, respectively.

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N2—H2N \cdots Cg1 ⁱ	0.86	2.43	3.262 (4)	163
C6—H6 \cdots Cg1 ⁱⁱ	0.93	2.89	3.656 (5)	141
C9—H9 \cdots Cg3 ⁱⁱⁱ	0.93	2.71	3.590 (5)	159
C14—H14 \cdots Cg3 ^{iv}	0.93	2.79	3.564 (5)	142
C5—Br1 \cdots Cg2 ^v	1.91 (1)	3.70 (1)	5.595 (4)	171 (1)

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