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N-(2-Bromobenzyl)-2,6-diisopropylaniline

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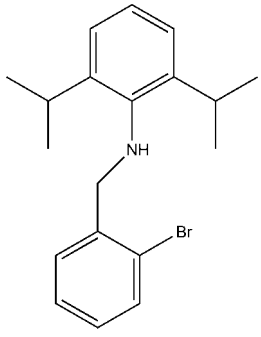
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.134; data-to-parameter ratio = 18.2.

The asymmetric unit of the title compound, $C_{19}H_{24}BrN$, contains two independent molecules that are linked into chains through intermolecular Br···H (3.06 Å) and H···phenyl contacts (3.15 Å). Furthermore, even stronger H···phenyl contacts (2.71–3.14 Å) between the chains and four neighbouring molecules result in a three-dimensional supramolecular architecture.

Related literature

For related literature see Balazs *et al.* (2003, 2004, 2006); Opris *et al.* (2004); Fernández *et al.* (2007); Soran *et al.* (2007); Kulcsar *et al.* (2007); Rotar *et al.* (2007).



Experimental

Crystal data

$C_{19}H_{24}BrN$
M_r = 346.30
Monoclinic, $P2_1/c$
a = 17.207 (17) Å
b = 14.742 (15) Å
c = 13.870 (14) Å
β = 94.650 (18)°
V = 3507 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.34 mm^{-1}
T = 297 (2) K
0.60 × 0.33 × 0.31 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker 2001)
T_{min} = 0.304, T_{max} = 0.483
27700 measured reflections
7183 independent reflections
4220 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.134
S = 1.03
7183 reflections
395 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry and X—H···π-ring interactions (Å, °).

$Cg1$ is a centroid of tthee benzene ring C1–C6, $Cg2$ is the centroid of the benzene ring C20–C25, $Cg3$ is the centroid of the benzene ring C27–C32.

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18C···Br2	0.96	3.06	3.928 (5)	151
C4—H4···$Cg3$	0.93	3.15	3.96 (1)	147
C25—H25···$Cg1^{i}$	0.93	2.71	3.55 (1)	151
C23—H23···$Cg2^{ii}$	0.93	2.97	3.79 (1)	147
C31—H31···$Cg2^{iii}$	0.93	3.14	3.89 (1)	140
C10—H10···$Cg3^{iv}$	0.93	3.04	3.79 (1)	139

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL* (Bruker, 2001); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2038).

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supplementary materials

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N-(2-Bromobenzyl)-2,6-diisopropylaniline

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Comment

Our interest in hypervalent organometalic compounds with aryl groups containing pendant arms with N atoms able to stabilize unusual species through intramolecular coordination to a metal atom (Balazs *et al.*, 2003, 2004, 2006; Opris *et al.*, 2004; Fernández *et al.*, 2007; Soran *et al.*, 2007; Kulcsar *et al.*, 2007; Rotar *et al.*, 2007) prompted us to design new organic molecules with steric hinderence. In this paper, we present the structure of the title compound, (I).

The asymmetric unit of (I) contains two independent molecules A and B (A containing Br1 and B conatining Br2, respectively) which are chemically identical, but differ slightly in their conformations (Fig. 1). The most importand difference is the value of the dihedral angle between the planes passing through the phenyl rings of the molecules [78 (1)° for A and 89 (1)° for B].

The two molecules are linked into a chain by a weak intermoleculare interaction (Br2···H18C 3.06 Å) and a *H*···phenyl contact (H4···*Cg*3 = 3.15 Å). These chains interact further through other four *H*···phenyl interactions (H···π range 2.71–3.14 Å, see Extra Table) (Fig.2), resulting in a three-dimensional supramolecular arhitecture.

Experimental

(2-Bromobezyl)-(2,6-diisopropylbenzyl)-amine was prepared from the reaction of brombenzyl-bromide and 2,6-diisopropil-aniline in 1:1 molar ratio, in CH_3CN in the presence of K_2CO_3. The mixture was refluxed for 48 h. The solvent was removed *in vacuo* and the solid residue was extracted with ethanol. Crystals suitable for single-crystal X-ray diffraction were obtained from ethanol.

Refinement

All hydrogen atoms were placed in calculated positions using a riding model, with C—H = 0.93–0.97 Å and with U_{iso}= 1.5U_{eq} (C) for methyl H and U_{iso}= 1.2U_{eq} (C) for aryl H. The methyl groups were allowed to rotate but not to tip. The hydrogen atoms bonded to N1 and N2 were found in a difference map and were allowed to refine with isotropic displacement parameters.

Figures

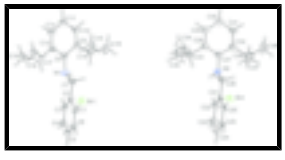


Fig. 1. A view of the title compound showing two molecules in the asymmetric unit with the atomic-numbering scheme; displacement ellipsoids are drawn at the 30% probability level.

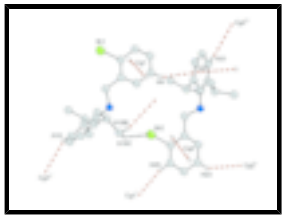


Fig. 2. Intermolecular interactions in the crystal structure of the title compound. Symmetry codes: (i) *x*, 1/2 − *y*, −1/2 + *z*, (ii) 1 − *x*, 1 − *y*, −*z*, (iii) 1 − *x*, 1/2 + *y*, 1/2 − *z*, (iv) −*x*, −1/2 + *y*, 1/2 − *z*

N-(2-Bromobenzyl)-2,6-diisopropylaniline

Crystal data

$C_{19}H_{24}BrN$	F_{000} = 1440
M_r = 346.30	D_x = 1.312 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4084 reflections
a = 17.207 (17) Å	θ = 2.3–20.6º
b = 14.742 (15) Å	μ = 2.34 mm^{-1}
c = 13.870 (14) Å	*T* = 297 (2) K
β = 94.650 (18)º	Block, yellow
V = 3507 (6) Å^3	0.60 × 0.33 × 0.31 mm
Z = 8	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	7183 independent reflections
Radiation source: fine-focus sealed tube	4220 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.058
T = 297(2) K	θ_{max} = 26.4º
ω and φ scans	θ_{min} = 1.2º
Absorption correction: multi-scan (SADABS; Bruker 2001)	*h* = −21→21
T_{min} = 0.304, T_{max} = 0.483	*k* = −18→17
27700 measured reflections	*l* = −17→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.134	$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
7183 reflections	$\Delta\rho_{max}$ = 0.36 e Å^{-3}

395 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. Spectroscopic analysis: ^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.59 (dd, 1H, H_3, $^3J_{HH}$ = 8.97), 7.429 (dd, 1H, H5, $^3J_{HH}$ = 6.7 Hz), 7.32 (d, 1H, H_5, $^3J_{HH}$ = 7.5 Hz), 7.29 (d, 2H, H_6), 7.12(m, 1H, H_{11}), 4.12 (s, 2H, CH_2), 3.45 (s, 1H, NH), 3.06 (sept, 1H, CH(CH_3)$_2$, ^{3}J = 6.85 Hz), 1.22 (d, 12 H, CH(CH_3)$_2$, ^{3}J = 6.87 Hz); ^{13}C NMR ($CDCl_3$, 75.47 MHz): 24,25 s [(CH$_3$)$_2$CH–]; 27,68 s [-CH(CH_3)$_2$]; 55,72 s [CH$_2$], 123,57 s [C_2]; 124,11 s [C_{10+12}]; 127,58 s [C_{11}]; 128,79 s [C_5]; 129,97 s [C_6]; 132,75 s [C_3]; 139,22 s [C_4]; 142,89 s [C_1]; 137,58 s [C_{9+13}];

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.08740 (3)	0.45571 (3)	0.59450 (3)	0.08102 (18)
Br2	0.27279 (3)	0.23566 (3)	0.17106 (3)	0.08471 (19)
C1	0.1518 (2)	0.4781 (2)	0.4920 (2)	0.0536 (9)
C2	0.14641 (17)	0.4235 (2)	0.4103 (2)	0.0451 (8)
C3	0.19723 (19)	0.4424 (2)	0.3403 (3)	0.0511 (8)
H3	0.1948	0.4073	0.2844	0.061*
C4	0.2511 (2)	0.5113 (2)	0.3510 (3)	0.0645 (10)
H4	0.2851	0.5219	0.3034	0.077*
C5	0.2545 (2)	0.5645 (3)	0.4324 (3)	0.0758 (12)
H5	0.2903	0.6118	0.4394	0.091*
C6	0.2059 (2)	0.5483 (2)	0.5032 (3)	0.0719 (11)
H6	0.2087	0.5840	0.5586	0.086*
C7	0.0881 (2)	0.3477 (2)	0.4003 (3)	0.0559 (9)
H7A	0.0918	0.3120	0.4592	0.067*
H7B	0.0360	0.3731	0.3921	0.067*
C8	0.05121 (19)	0.2092 (2)	0.3135 (2)	0.0476 (8)
C9	−0.0186 (2)	0.2083 (2)	0.2549 (3)	0.0534 (9)
C10	−0.0616 (2)	0.1296 (2)	0.2484 (3)	0.0618 (9)
H10	−0.1075	0.1278	0.2082	0.074*
C11	−0.0382 (2)	0.0542 (2)	0.2998 (3)	0.0638 (10)
H11	−0.0681	0.0016	0.2946	0.077*
C12	0.0298 (2)	0.0560 (2)	0.3593 (3)	0.0614 (9)

H12	0.0452	0.0047	0.3950	0.074*
C13	0.07529 (19)	0.1330 (2)	0.3665 (2)	0.0521 (8)
C14	−0.0486 (2)	0.2900 (3)	0.1966 (3)	0.0710 (11)
H14	−0.0119	0.3400	0.2111	0.085*
C15	−0.0516 (3)	0.2724 (3)	0.0888 (4)	0.1121 (18)
H15A	−0.0860	0.2225	0.0726	0.168*
H15B	−0.0002	0.2580	0.0710	0.168*
H15C	−0.0704	0.3256	0.0544	0.168*
C16	−0.1270 (3)	0.3199 (4)	0.2250 (5)	0.137 (2)
H16A	−0.1656	0.2759	0.2032	0.206*
H16B	−0.1400	0.3775	0.1959	0.206*
H16C	−0.1254	0.3253	0.2941	0.206*
C17	0.1525 (2)	0.1301 (3)	0.4277 (3)	0.0667 (10)
H17	0.1717	0.1925	0.4354	0.080*
C18	0.2125 (2)	0.0761 (3)	0.3792 (3)	0.0883 (13)
H18A	0.1977	0.0133	0.3772	0.132*
H18B	0.2623	0.0825	0.4150	0.132*
H18C	0.2157	0.0981	0.3145	0.132*
C19	0.1435 (3)	0.0919 (4)	0.5285 (3)	0.119 (2)
H19A	0.1085	0.1296	0.5612	0.178*
H19B	0.1934	0.0906	0.5647	0.178*
H19C	0.1228	0.0314	0.5229	0.178*
C20	0.33447 (19)	0.2507 (2)	0.0648 (2)	0.0488 (8)
C21	0.38118 (18)	0.3273 (2)	0.0587 (2)	0.0437 (7)
C22	0.4236 (2)	0.3337 (2)	−0.0213 (2)	0.0583 (9)
H22	0.4555	0.3839	−0.0280	0.070*
C23	0.4198 (3)	0.2671 (3)	−0.0916 (3)	0.0779 (12)
H23	0.4490	0.2726	−0.1449	0.093*
C24	0.3734 (2)	0.1936 (3)	−0.0826 (3)	0.0732 (11)
H24	0.3709	0.1488	−0.1300	0.088*
C25	0.3306 (2)	0.1846 (2)	−0.0050 (3)	0.0619 (10)
H25	0.2990	0.1341	0.0007	0.074*
C26	0.3839 (2)	0.3989 (2)	0.1358 (2)	0.0534 (8)
H26A	0.3317	0.4221	0.1414	0.064*
H26B	0.4020	0.3720	0.1973	0.064*
C27	0.43522 (19)	0.5466 (2)	0.1832 (2)	0.0481 (8)
C28	0.38287 (19)	0.6181 (2)	0.1681 (2)	0.0522 (8)
C29	0.3880 (2)	0.6892 (2)	0.2329 (3)	0.0674 (10)
H29	0.3539	0.7379	0.2237	0.081*
C30	0.4422 (3)	0.6892 (3)	0.3101 (3)	0.0753 (12)
H30	0.4450	0.7383	0.3524	0.090*
C31	0.4920 (2)	0.6186 (3)	0.3261 (3)	0.0705 (11)
H31	0.5280	0.6194	0.3799	0.085*
C32	0.4900 (2)	0.5453 (2)	0.2633 (3)	0.0565 (9)
C33	0.3235 (2)	0.6204 (3)	0.0810 (3)	0.0704 (11)
H33	0.3168	0.5578	0.0581	0.084*
C34	0.2454 (3)	0.6534 (6)	0.1035 (4)	0.161 (3)
H34A	0.2496	0.7146	0.1269	0.241*
H34B	0.2256	0.6154	0.1521	0.241*

H34C	0.2104	0.6515	0.0459	0.241*
C35	0.3519 (3)	0.6745 (4)	−0.0009 (3)	0.1128 (18)
H35A	0.3122	0.6761	−0.0536	0.169*
H35B	0.3980	0.6467	−0.0222	0.169*
H35C	0.3638	0.7352	0.0206	0.169*
C36	0.5474 (2)	0.4683 (3)	0.2809 (3)	0.0757 (12)
H36	0.5248	0.4147	0.2475	0.091*
C37	0.6232 (3)	0.4892 (4)	0.2376 (4)	0.1159 (18)
H37A	0.6135	0.4976	0.1691	0.174*
H37B	0.6589	0.4397	0.2500	0.174*
H37C	0.6454	0.5436	0.2662	0.174*
C38	0.5624 (3)	0.4441 (3)	0.3879 (4)	0.128 (2)
H38A	0.5928	0.3895	0.3943	0.191*
H38B	0.5135	0.4349	0.4152	0.191*
H38C	0.5903	0.4927	0.4213	0.191*
N1	0.10011 (18)	0.2884 (2)	0.3183 (2)	0.0568 (8)
N2	0.43507 (18)	0.47372 (19)	0.1151 (2)	0.0542 (7)
H2	0.428 (3)	0.482 (3)	0.0571 (15)	0.109 (18)*
H1	0.092 (2)	0.322 (2)	0.267 (2)	0.092 (15)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0975 (4)	0.0830 (3)	0.0650 (3)	0.0026 (2)	0.0213 (2)	−0.0153 (2)
Br2	0.1145 (4)	0.0704 (3)	0.0735 (3)	−0.0334 (2)	0.0336 (3)	−0.0005 (2)
C1	0.057 (2)	0.0439 (19)	0.060 (2)	0.0026 (16)	0.0021 (17)	−0.0036 (16)
C2	0.0443 (19)	0.0374 (17)	0.053 (2)	0.0013 (14)	−0.0015 (15)	0.0014 (15)
C3	0.052 (2)	0.0438 (19)	0.056 (2)	−0.0004 (16)	0.0000 (16)	0.0046 (16)
C4	0.056 (2)	0.053 (2)	0.084 (3)	−0.0081 (18)	0.002 (2)	0.016 (2)
C5	0.071 (3)	0.056 (2)	0.098 (3)	−0.020 (2)	−0.005 (3)	0.000 (2)
C6	0.078 (3)	0.056 (2)	0.079 (3)	−0.007 (2)	−0.010 (2)	−0.015 (2)
C7	0.056 (2)	0.048 (2)	0.065 (2)	−0.0078 (16)	0.0126 (18)	−0.0139 (17)
C8	0.049 (2)	0.0422 (18)	0.053 (2)	−0.0100 (15)	0.0095 (17)	−0.0102 (15)
C9	0.054 (2)	0.0411 (19)	0.065 (2)	−0.0045 (16)	0.0055 (18)	−0.0031 (16)
C10	0.055 (2)	0.056 (2)	0.074 (2)	−0.0089 (18)	−0.0058 (19)	−0.0026 (19)
C11	0.064 (3)	0.046 (2)	0.081 (3)	−0.0148 (17)	−0.005 (2)	−0.0007 (19)
C12	0.063 (2)	0.048 (2)	0.071 (2)	−0.0078 (18)	−0.006 (2)	0.0029 (18)
C13	0.048 (2)	0.052 (2)	0.056 (2)	−0.0046 (16)	0.0005 (16)	−0.0087 (17)
C14	0.072 (3)	0.051 (2)	0.089 (3)	−0.0002 (19)	−0.001 (2)	0.009 (2)
C15	0.150 (5)	0.093 (4)	0.093 (4)	0.017 (3)	0.009 (3)	0.031 (3)
C16	0.142 (5)	0.100 (4)	0.176 (6)	0.063 (4)	0.047 (4)	0.039 (4)
C17	0.057 (2)	0.064 (2)	0.076 (3)	−0.0052 (19)	−0.009 (2)	−0.007 (2)
C18	0.055 (3)	0.115 (4)	0.095 (3)	0.002 (2)	0.008 (2)	−0.010 (3)
C19	0.079 (3)	0.209 (6)	0.066 (3)	0.015 (4)	−0.008 (2)	−0.001 (4)
C20	0.053 (2)	0.049 (2)	0.0435 (19)	−0.0018 (15)	−0.0020 (15)	0.0021 (15)
C21	0.0465 (19)	0.0418 (18)	0.0415 (18)	−0.0037 (14)	−0.0040 (15)	0.0008 (14)
C22	0.060 (2)	0.058 (2)	0.058 (2)	−0.0121 (17)	0.0119 (18)	−0.0073 (18)
C23	0.087 (3)	0.092 (3)	0.057 (2)	−0.015 (2)	0.021 (2)	−0.023 (2)

C24	0.086 (3)	0.072 (3)	0.061 (2)	−0.017 (2)	0.006 (2)	−0.026 (2)
C25	0.069 (3)	0.052 (2)	0.063 (2)	−0.0127 (18)	−0.007 (2)	−0.0057 (18)
C26	0.060 (2)	0.0476 (19)	0.053 (2)	−0.0115 (16)	0.0066 (17)	−0.0043 (16)
C27	0.051 (2)	0.0449 (19)	0.050 (2)	−0.0129 (16)	0.0118 (16)	−0.0045 (15)
C28	0.051 (2)	0.048 (2)	0.059 (2)	−0.0067 (16)	0.0111 (17)	0.0016 (17)
C29	0.070 (3)	0.051 (2)	0.084 (3)	0.0049 (19)	0.020 (2)	−0.003 (2)
C30	0.092 (3)	0.063 (3)	0.072 (3)	−0.011 (2)	0.018 (3)	−0.022 (2)
C31	0.082 (3)	0.069 (3)	0.059 (2)	−0.017 (2)	−0.002 (2)	−0.011 (2)
C32	0.053 (2)	0.054 (2)	0.063 (2)	−0.0114 (17)	0.0042 (18)	−0.0030 (18)
C33	0.063 (3)	0.069 (3)	0.079 (3)	−0.005 (2)	−0.001 (2)	0.016 (2)
C34	0.066 (3)	0.295 (9)	0.120 (5)	0.017 (5)	0.007 (3)	0.050 (5)
C35	0.102 (4)	0.149 (5)	0.086 (3)	−0.016 (3)	−0.003 (3)	0.039 (3)
C36	0.066 (3)	0.061 (2)	0.098 (3)	−0.007 (2)	−0.008 (2)	−0.001 (2)
C37	0.075 (3)	0.113 (4)	0.161 (5)	0.018 (3)	0.023 (3)	0.019 (4)
C38	0.132 (5)	0.108 (4)	0.139 (5)	0.007 (3)	−0.019 (4)	0.052 (4)
N1	0.070 (2)	0.0464 (17)	0.0551 (19)	−0.0163 (15)	0.0106 (16)	−0.0071 (15)
N2	0.067 (2)	0.0471 (17)	0.0500 (19)	−0.0166 (14)	0.0114 (15)	−0.0080 (14)

Geometric parameters (Å, °)

Br1—C1	1.901 (4)	C20—C25	1.371 (5)
Br2—C20	1.898 (4)	C20—C21	1.393 (4)
C1—C2	1.387 (5)	C21—C22	1.380 (4)
C1—C6	1.393 (5)	C21—C26	1.500 (4)
C2—C3	1.386 (4)	C22—C23	1.381 (5)
C2—C7	1.501 (4)	C22—H22	0.9300
C3—C4	1.376 (5)	C23—C24	1.358 (6)
C3—H3	0.9300	C23—H23	0.9300
C4—C5	1.372 (6)	C24—C25	1.359 (5)
C4—H4	0.9300	C24—H24	0.9300
C5—C6	1.362 (6)	C25—H25	0.9300
C5—H5	0.9300	C26—N2	1.454 (4)
C6—H6	0.9300	C26—H26A	0.9700
C7—N1	1.462 (4)	C26—H26B	0.9700
C7—H7A	0.9700	C27—C28	1.392 (5)
C7—H7B	0.9700	C27—C32	1.398 (5)
C8—C13	1.387 (5)	C27—N2	1.430 (4)
C8—C9	1.396 (5)	C28—C29	1.378 (5)
C8—N1	1.438 (4)	C28—C33	1.518 (5)
C9—C10	1.374 (5)	C29—C30	1.361 (6)
C9—C14	1.518 (5)	C29—H29	0.9300
C10—C11	1.364 (5)	C30—C31	1.355 (6)
C10—H10	0.9300	C30—H30	0.9300
C11—C12	1.375 (5)	C31—C32	1.386 (5)
C11—H11	0.9300	C31—H31	0.9300
C12—C13	1.378 (5)	C32—C36	1.512 (5)
C12—H12	0.9300	C33—C34	1.487 (6)
C13—C17	1.519 (5)	C33—C35	1.502 (6)
C14—C16	1.502 (6)	C33—H33	0.9800

C14—C15	1.514 (6)	C34—H34A	0.9600
C14—H14	0.9800	C34—H34B	0.9600
C15—H15A	0.9600	C34—H34C	0.9600
C15—H15B	0.9600	C35—H35A	0.9600
C15—H15C	0.9600	C35—H35B	0.9600
C16—H16A	0.9600	C35—H35C	0.9600
C16—H16B	0.9600	C36—C37	1.511 (6)
C16—H16C	0.9600	C36—C38	1.527 (6)
C17—C18	1.505 (5)	C36—H36	0.9800
C17—C19	1.526 (6)	C37—H37A	0.9600
C17—H17	0.9800	C37—H37B	0.9600
C18—H18A	0.9600	C37—H37C	0.9600
C18—H18B	0.9600	C38—H38A	0.9600
C18—H18C	0.9600	C38—H38B	0.9600
C19—H19A	0.9600	C38—H38C	0.9600
C19—H19B	0.9600	N1—H1	0.863 (18)
C19—H19C	0.9600	N2—H2	0.814 (19)
C2—C1—C6	121.5 (3)	C22—C21—C20	116.7 (3)
C2—C1—Br1	120.4 (3)	C22—C21—C26	122.5 (3)
C6—C1—Br1	118.1 (3)	C20—C21—C26	120.8 (3)
C3—C2—C1	116.9 (3)	C21—C22—C23	121.4 (3)
C3—C2—C7	122.7 (3)	C21—C22—H22	119.3
C1—C2—C7	120.5 (3)	C23—C22—H22	119.3
C4—C3—C2	122.0 (3)	C24—C23—C22	119.8 (4)
C4—C3—H3	119.0	C24—C23—H23	120.1
C2—C3—H3	119.0	C22—C23—H23	120.1
C5—C4—C3	119.7 (4)	C23—C24—C25	120.7 (4)
C5—C4—H4	120.2	C23—C24—H24	119.6
C3—C4—H4	120.2	C25—C24—H24	119.6
C6—C5—C4	120.3 (4)	C24—C25—C20	119.5 (3)
C6—C5—H5	119.8	C24—C25—H25	120.3
C4—C5—H5	119.8	C20—C25—H25	120.3
C5—C6—C1	119.7 (4)	N2—C26—C21	112.2 (3)
C5—C6—H6	120.2	N2—C26—H26A	109.2
C1—C6—H6	120.2	C21—C26—H26A	109.2
N1—C7—C2	112.4 (3)	N2—C26—H26B	109.2
N1—C7—H7A	109.1	C21—C26—H26B	109.2
C2—C7—H7A	109.1	H26A—C26—H26B	107.9
N1—C7—H7B	109.1	C28—C27—C32	121.0 (3)
C2—C7—H7B	109.1	C28—C27—N2	120.2 (3)
H7A—C7—H7B	107.9	C32—C27—N2	118.7 (3)
C13—C8—C9	120.5 (3)	C29—C28—C27	118.1 (3)
C13—C8—N1	119.0 (3)	C29—C28—C33	120.4 (3)
C9—C8—N1	120.5 (3)	C27—C28—C33	121.4 (3)
C10—C9—C8	118.7 (3)	C30—C29—C28	121.1 (4)
C10—C9—C14	118.5 (3)	C30—C29—H29	119.4
C8—C9—C14	122.8 (3)	C28—C29—H29	119.4
C11—C10—C9	121.3 (3)	C31—C30—C29	120.8 (4)
C11—C10—H10	119.4	C31—C30—H30	119.6

C9—C10—H10	119.4	C29—C30—H30	119.6
C10—C11—C12	119.9 (3)	C30—C31—C32	120.8 (4)
C10—C11—H11	120.0	C30—C31—H31	119.6
C12—C11—H11	120.0	C32—C31—H31	119.6
C11—C12—C13	120.6 (3)	C31—C32—C27	118.0 (3)
C11—C12—H12	119.7	C31—C32—C36	120.1 (3)
C13—C12—H12	119.7	C27—C32—C36	121.9 (3)
C12—C13—C8	119.0 (3)	C34—C33—C35	109.9 (4)
C12—C13—C17	118.9 (3)	C34—C33—C28	113.7 (4)
C8—C13—C17	122.0 (3)	C35—C33—C28	112.0 (3)
C16—C14—C15	110.5 (4)	C34—C33—H33	107.0
C16—C14—C9	111.5 (4)	C35—C33—H33	107.0
C15—C14—C9	111.9 (3)	C28—C33—H33	107.0
C16—C14—H14	107.6	C33—C34—H34A	109.5
C15—C14—H14	107.6	C33—C34—H34B	109.5
C9—C14—H14	107.6	H34A—C34—H34B	109.5
C14—C15—H15A	109.5	C33—C34—H34C	109.5
C14—C15—H15B	109.5	H34A—C34—H34C	109.5
H15A—C15—H15B	109.5	H34B—C34—H34C	109.5
C14—C15—H15C	109.5	C33—C35—H35A	109.5
H15A—C15—H15C	109.5	C33—C35—H35B	109.5
H15B—C15—H15C	109.5	H35A—C35—H35B	109.5
C14—C16—H16A	109.5	C33—C35—H35C	109.5
C14—C16—H16B	109.5	H35A—C35—H35C	109.5
H16A—C16—H16B	109.5	H35B—C35—H35C	109.5
C14—C16—H16C	109.5	C37—C36—C32	110.9 (4)
H16A—C16—H16C	109.5	C37—C36—C38	110.5 (4)
H16B—C16—H16C	109.5	C32—C36—C38	112.9 (4)
C18—C17—C13	111.4 (3)	C37—C36—H36	107.4
C18—C17—C19	109.8 (4)	C32—C36—H36	107.4
C13—C17—C19	111.9 (3)	C38—C36—H36	107.4
C18—C17—H17	107.8	C36—C37—H37A	109.5
C13—C17—H17	107.8	C36—C37—H37B	109.5
C19—C17—H17	107.8	H37A—C37—H37B	109.5
C17—C18—H18A	109.5	C36—C37—H37C	109.5
C17—C18—H18B	109.5	H37A—C37—H37C	109.5
H18A—C18—H18B	109.5	H37B—C37—H37C	109.5
C17—C18—H18C	109.5	C36—C38—H38A	109.5
H18A—C18—H18C	109.5	C36—C38—H38B	109.5
H18B—C18—H18C	109.5	H38A—C38—H38B	109.5
C17—C19—H19A	109.5	C36—C38—H38C	109.5
C17—C19—H19B	109.5	H38A—C38—H38C	109.5
H19A—C19—H19B	109.5	H38B—C38—H38C	109.5
C17—C19—H19C	109.5	C8—N1—C7	113.7 (3)
H19A—C19—H19C	109.5	C8—N1—H1	112 (3)
H19B—C19—H19C	109.5	C7—N1—H1	106 (3)
C25—C20—C21	121.9 (3)	C27—N2—C26	114.1 (3)
C25—C20—Br2	117.9 (3)	C27—N2—H2	122 (3)
C21—C20—Br2	120.2 (2)	C26—N2—H2	106 (3)

C6—C1—C2—C3	−0.2 (5)	Br2—C20—C21—C26	0.3 (4)
Br1—C1—C2—C3	−177.8 (2)	C20—C21—C22—C23	0.0 (5)
C6—C1—C2—C7	179.5 (3)	C26—C21—C22—C23	−179.7 (4)
Br1—C1—C2—C7	1.8 (4)	C21—C22—C23—C24	0.1 (6)
C1—C2—C3—C4	0.5 (5)	C22—C23—C24—C25	−0.1 (7)
C7—C2—C3—C4	−179.1 (3)	C23—C24—C25—C20	0.0 (6)
C2—C3—C4—C5	−1.0 (5)	C21—C20—C25—C24	0.0 (5)
C3—C4—C5—C6	1.1 (6)	Br2—C20—C25—C24	179.4 (3)
C4—C5—C6—C1	−0.8 (6)	C22—C21—C26—N2	0.5 (5)
C2—C1—C6—C5	0.3 (6)	C20—C21—C26—N2	−179.1 (3)
Br1—C1—C6—C5	178.0 (3)	C32—C27—C28—C29	1.9 (5)
C3—C2—C7—N1	9.6 (5)	N2—C27—C28—C29	−176.5 (3)
C1—C2—C7—N1	−170.1 (3)	C32—C27—C28—C33	179.6 (3)
C13—C8—C9—C10	−2.0 (5)	N2—C27—C28—C33	1.2 (5)
N1—C8—C9—C10	176.6 (3)	C27—C28—C29—C30	−0.7 (5)
C13—C8—C9—C14	179.0 (3)	C33—C28—C29—C30	−178.4 (3)
N1—C8—C9—C14	−2.4 (5)	C28—C29—C30—C31	−0.8 (6)
C8—C9—C10—C11	1.7 (5)	C29—C30—C31—C32	1.1 (6)
C14—C9—C10—C11	−179.3 (4)	C30—C31—C32—C27	0.1 (6)
C9—C10—C11—C12	−0.2 (6)	C30—C31—C32—C36	178.4 (4)
C10—C11—C12—C13	−1.0 (6)	C28—C27—C32—C31	−1.6 (5)
C11—C12—C13—C8	0.7 (5)	N2—C27—C32—C31	176.8 (3)
C11—C12—C13—C17	−176.0 (3)	C28—C27—C32—C36	−179.9 (3)
C9—C8—C13—C12	0.9 (5)	N2—C27—C32—C36	−1.5 (5)
N1—C8—C13—C12	−177.7 (3)	C29—C28—C33—C34	−43.1 (5)
C9—C8—C13—C17	177.4 (3)	C27—C28—C33—C34	139.3 (5)
N1—C8—C13—C17	−1.2 (5)	C29—C28—C33—C35	82.3 (5)
C10—C9—C14—C16	60.7 (5)	C27—C28—C33—C35	−95.4 (4)
C8—C9—C14—C16	−120.3 (5)	C31—C32—C36—C37	−85.3 (5)
C10—C9—C14—C15	−63.6 (5)	C27—C32—C36—C37	93.0 (5)
C8—C9—C14—C15	115.4 (4)	C31—C32—C36—C38	39.4 (5)
C12—C13—C17—C18	73.0 (5)	C27—C32—C36—C38	−142.4 (4)
C8—C13—C17—C18	−103.5 (4)	C13—C8—N1—C7	−85.2 (4)
C12—C13—C17—C19	−50.4 (5)	C9—C8—N1—C7	96.2 (4)
C8—C13—C17—C19	133.1 (4)	C2—C7—N1—C8	173.0 (3)
C25—C20—C21—C22	0.0 (5)	C28—C27—N2—C26	−90.3 (4)
Br2—C20—C21—C22	−179.4 (2)	C32—C27—N2—C26	91.2 (4)
C25—C20—C21—C26	179.6 (3)	C21—C26—N2—C27	175.8 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18C···Br2	0.96	3.06	3.928 (5)	151

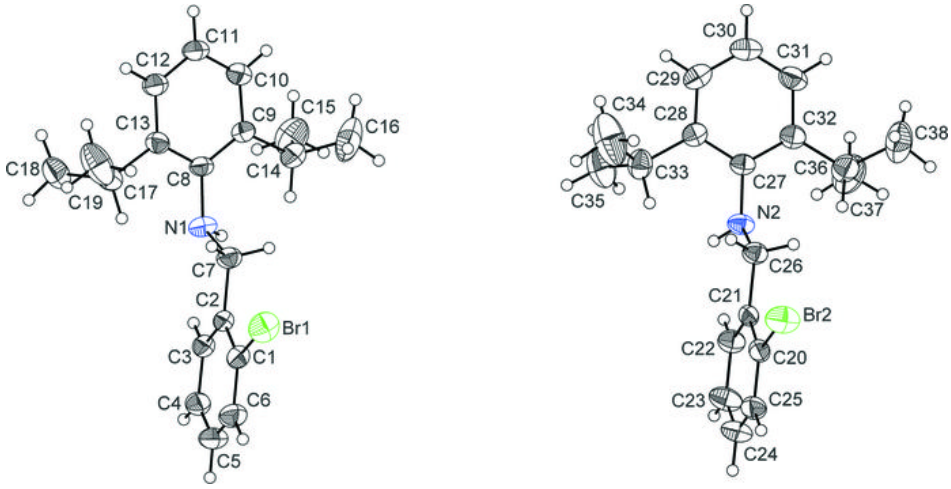
X—H···π-ring interactions. Cg1 is a centroid of the benzene ring C1–C6, Cg2 is a centroid of the benzene ring C20–C25, Cg3 is a centroid of the benzene ring C27–C32

Y—*X*···*Cg*	*X*—H	H···*Cg*	*X*···*Cg*	*X*—H···*Cg*
C4—H4···*Cg*3	0.93	3.15	3.96 (1)	147

C25—H25···$Cg1^{i}$	0.93	2.71	3.55 (1)	151
C23—H23···$Cg2^{ii}$	0.93	2.97	3.79 (1)	147
C31—H31···$Cg2^{iii}$	0.93	3.14	3.89 (1)	140
C10—H10···$Cg3^{iv}$	0.93	3.04	3.79 (1)	139

Symmetry code: (i) x, 1/2 − y, −1/2 + z, (ii) 1 − x, 1 − y, −z, (iii) 1 − x, 1/2 + y, 1/2 − z, (iv) −x, −1/2 + y, 1/2 − z

Fig. 1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C12
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C13
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C16
C18
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C14
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C19
N1
C7
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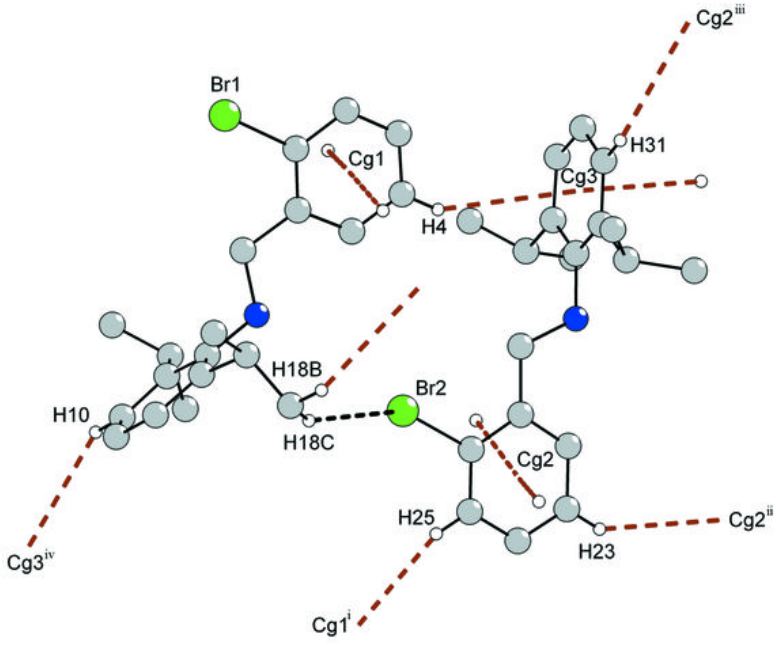
C3
C1
C4
C6
C5
C30
C31
C29
C34
C28
C32
C38
C33
C27
C36
C35
N2
C37
C26
C21
Br2
C22
C20
C23
C25
C24

Fig. 2


Cg2iii
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Cg1
H31
Cg3
H4
H18B
Br2
H10
H18C
Cg2
H25
Cg2ii
H23
Cg3iv
Cg1i