Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,4-Bis(4-*tert*-butylbenzyl)piperazine

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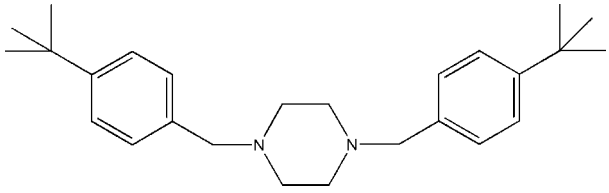
Received 14 October 2011; accepted 24 October 2011

Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.099; data-to-parameter ratio = 20.7.

The complete molecule of the title compound, $C_{26}H_{38}N_2$, is generated by a crystallographic inversion centre. The piperazine ring adopts a chair conformation with pseudo-equatorial substituents. In the crystal, molecules interact only by van der Waals forces.

Related literature

For related structures, see: Ma *et al.* (2007); Liu *et al.* (2011).



Experimental

Crystal data

$C_{26}H_{38}N_2$ M_r = 378.58
Triclinic, $P\overline{1}$
a = 6.162 (4) Å
b = 9.616 (5) Å
c = 10.656 (7) Å
α = 114.279 (19)°
β = 92.42 (5)°
γ = 96.50 (4)°
V = 569.1 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.06 mm^{-1}
T = 113 K
0.24 × 0.20 × 0.08 mm

Data collection

Rigaku Saturn724 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.985, T_{max} = 0.995
6003 measured reflections
2686 independent reflections
1481 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.099
S = 1.01
2686 reflections
130 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *CrystalStructure* (Rigaku/MSC, 2005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6451).

References

Liu, X.-F. & Liu, X.-H. (2011). *Acta Cryst.* E**67**, o202.
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supplementary materials

Acta Cryst. (2011). E**67**, o3094 [**doi:10.1107/S1600536811044114**]

1,4-Bis(4-*tert*-butylbenzyl)piperazine

L.-J. Luo and J.-Q. Weng

Experimental

Piperazine (50 mmol), dissolved in 20 ml 96% of ethanol, was added dropwise to a stirred solution of *tert*-butyl benzyl (50 mmol) at reflux. The mixture was stirred for 8 h at reflux, TLC monitored. The mixture was stirred overnight at room temperature, evaporated in vacuum and the residue was purified by recrystallization from ethanol to give the title compound, (I). Colourless prisms of (I) were grown from ethanol.

Refinement

All the H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

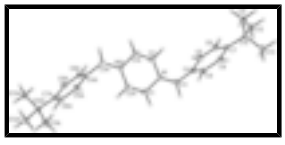


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

Fig. 2. The crystal packing for (I).

1,4-Bis(4-*tert*-butylbenzyl)piperazine

Crystal data

$C_{26}H_{38}N_2$	Z = 1
M_r = 378.58	F(000) = 208
Triclinic, $P\overline{1}$	D_x = 1.105 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 6.162 (4) Å	Cell parameters from 1980 reflections
b = 9.616 (5) Å	θ = 2.1–27.9°
c = 10.656 (7) Å	μ = 0.06 mm^{-1}
α = 114.279 (19)°	T = 113 K
β = 92.42 (5)°	Prism, colorless
γ = 96.50 (4)°	0.24 × 0.20 × 0.08 mm
V = 569.1 (6) Å^3	

Data collection

Rigaku Saturn724 CCD diffractometer	2686 independent reflections
Radiation source: rotating anode	1481 reflections with $I > 2\sigma(I)$
multilayer	$R_{int} = 0.041$
Detector resolution: 14.22 pixels mm^{-1}	$\theta_{max} = 27.9°$, $\theta_{min} = 2.1°$
ω and φ scans	$h = -8 \rightarrow 7$
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)	$k = -12 \rightarrow 12$
$T_{min} = 0.985$, $T_{max} = 0.995$	$l = -13 \rightarrow 14$
6003 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.041$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.099$	H-atom parameters constrained
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.034P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2686 reflections	$(\Delta/\sigma)_{max} < 0.001$
130 parameters	$\Delta\rho_{max} = 0.16$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.18$ e Å^{-3}

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	1.04698 (14)	0.10740 (11)	0.64238 (9)	0.0276 (3)
C1	1.19772 (18)	0.10329 (14)	0.53912 (12)	0.0304 (3)
H1A	1.3503	0.1354	0.5835	0.036*
H1B	1.1644	0.1765	0.4999	0.036*
C2	0.82344 (17)	0.05712 (14)	0.57527 (11)	0.0296 (3)

H2A	0.7838	0.1295	0.5366	0.036*
H2B	0.7205	0.0582	0.6444	0.036*
C3	1.0687 (2)	0.26252 (14)	0.75487 (12)	0.0349 (3)
H3A	1.0114	0.3328	0.7192	0.042*
H3B	1.2260	0.3006	0.7869	0.042*
C4	0.94701 (19)	0.26622 (13)	0.87580 (11)	0.0283 (3)
C5	0.7673 (2)	0.34155 (14)	0.91236 (12)	0.0354 (3)
H5	0.7138	0.3899	0.8579	0.042*
C6	0.66197 (19)	0.34862 (14)	1.02736 (12)	0.0325 (3)
H6	0.5377	0.4012	1.0492	0.039*
C7	0.73370 (17)	0.28090 (12)	1.11086 (11)	0.0244 (3)
C8	0.91275 (17)	0.20106 (13)	1.07092 (12)	0.0301 (3)
H8	0.9643	0.1500	1.1235	0.036*
C9	1.01657 (18)	0.19463 (14)	0.95659 (12)	0.0316 (3)
H9	1.1385	0.1398	0.9328	0.038*
C10	0.62717 (18)	0.28918 (14)	1.24015 (12)	0.0292 (3)
C11	0.5127 (2)	0.12960 (15)	1.21512 (15)	0.0519 (4)
H11A	0.4028	0.0923	1.1350	0.078*
H11B	0.4404	0.1356	1.2970	0.078*
H11C	0.6212	0.0584	1.1973	0.078*
C12	0.45875 (19)	0.40197 (14)	1.28026 (12)	0.0360 (3)
H12A	0.5309	0.5053	1.2976	0.054*
H12B	0.3964	0.4045	1.3641	0.054*
H12C	0.3413	0.3683	1.2047	0.054*
C13	0.8046 (2)	0.34597 (17)	1.36335 (12)	0.0448 (4)
H13A	0.9099	0.2723	1.3441	0.067*
H13B	0.7356	0.3547	1.4469	0.067*
H13C	0.8814	0.4470	1.3774	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0278 (5)	0.0292 (6)	0.0238 (5)	0.0025 (4)	0.0087 (4)	0.0089 (5)
C1	0.0275 (6)	0.0365 (8)	0.0272 (6)	0.0022 (5)	0.0094 (5)	0.0132 (6)
C2	0.0304 (7)	0.0347 (7)	0.0274 (6)	0.0078 (5)	0.0107 (5)	0.0151 (6)
C3	0.0433 (7)	0.0305 (7)	0.0271 (7)	−0.0004 (6)	0.0118 (6)	0.0090 (6)
C4	0.0344 (7)	0.0234 (6)	0.0229 (6)	−0.0004 (5)	0.0076 (5)	0.0061 (5)
C5	0.0478 (8)	0.0366 (8)	0.0275 (7)	0.0138 (6)	0.0079 (6)	0.0167 (6)
C6	0.0359 (7)	0.0354 (7)	0.0291 (7)	0.0147 (6)	0.0092 (5)	0.0134 (6)
C7	0.0269 (6)	0.0216 (6)	0.0204 (6)	0.0006 (5)	0.0029 (5)	0.0051 (5)
C8	0.0328 (7)	0.0318 (7)	0.0276 (6)	0.0060 (5)	0.0027 (5)	0.0139 (6)
C9	0.0297 (7)	0.0330 (7)	0.0312 (7)	0.0079 (5)	0.0099 (6)	0.0111 (6)
C10	0.0345 (7)	0.0302 (7)	0.0242 (6)	0.0061 (5)	0.0088 (5)	0.0118 (5)
C11	0.0698 (10)	0.0356 (8)	0.0532 (9)	0.0059 (7)	0.0367 (8)	0.0192 (7)
C12	0.0390 (7)	0.0395 (8)	0.0278 (7)	0.0099 (6)	0.0111 (6)	0.0105 (6)
C13	0.0510 (8)	0.0611 (10)	0.0255 (7)	0.0164 (7)	0.0073 (6)	0.0190 (7)

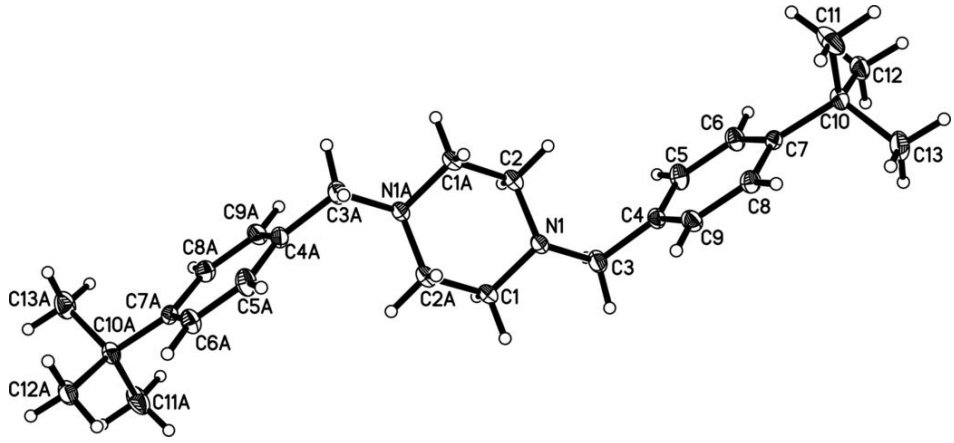
Geometric parameters (Å, °)

N1—C2	1.4575 (17)	C7—C8	1.3968 (16)
N1—C1	1.4609 (17)	C7—C10	1.5275 (18)
N1—C3	1.4665 (16)	C8—C9	1.3821 (17)
C1—C2^{i}	1.5089 (17)	C8—H8	0.9500
C1—H1A	0.9900	C9—H9	0.9500
C1—H1B	0.9900	C10—C11	1.5251 (19)
C2—C1^{i}	1.5090 (17)	C10—C12	1.5321 (17)
C2—H2A	0.9900	C10—C13	1.540 (2)
C2—H2B	0.9900	C11—H11A	0.9800
C3—C4	1.5079 (18)	C11—H11B	0.9800
C3—H3A	0.9900	C11—H11C	0.9800
C3—H3B	0.9900	C12—H12A	0.9800
C4—C5	1.3742 (17)	C12—H12B	0.9800
C4—C9	1.3863 (17)	C12—H12C	0.9800
C5—C6	1.3916 (18)	C13—H13A	0.9800
C5—H5	0.9500	C13—H13B	0.9800
C6—C7	1.3855 (17)	C13—H13C	0.9800
C6—H6	0.9500		
C2—N1—C1	109.05 (10)	C8—C7—C10	119.97 (11)
C2—N1—C3	111.16 (11)	C9—C8—C7	121.48 (12)
C1—N1—C3	110.69 (10)	C9—C8—H8	119.3
N1—C1—C2^{i}	110.36 (10)	C7—C8—H8	119.3
N1—C1—H1A	109.6	C8—C9—C4	121.58 (11)
C2^{i}—C1—H1A	109.6	C8—C9—H9	119.2
N1—C1—H1B	109.6	C4—C9—H9	119.2
C2^{i}—C1—H1B	109.6	C11—C10—C7	109.50 (10)
H1A—C1—H1B	108.1	C11—C10—C12	108.72 (11)
N1—C2—C1^{i}	110.74 (11)	C7—C10—C12	112.36 (11)
N1—C2—H2A	109.5	C11—C10—C13	109.56 (12)
C1^{i}—C2—H2A	109.5	C7—C10—C13	109.51 (10)
N1—C2—H2B	109.5	C12—C10—C13	107.14 (11)
C1^{i}—C2—H2B	109.5	C10—C11—H11A	109.5
H2A—C2—H2B	108.1	C10—C11—H11B	109.5
N1—C3—C4	112.51 (11)	H11A—C11—H11B	109.5
N1—C3—H3A	109.1	C10—C11—H11C	109.5
C4—C3—H3A	109.1	H11A—C11—H11C	109.5
N1—C3—H3B	109.1	H11B—C11—H11C	109.5
C4—C3—H3B	109.1	C10—C12—H12A	109.5
H3A—C3—H3B	107.8	C10—C12—H12B	109.5
C5—C4—C9	117.25 (11)	H12A—C12—H12B	109.5
C5—C4—C3	122.29 (12)	C10—C12—H12C	109.5
C9—C4—C3	120.46 (11)	H12A—C12—H12C	109.5
C4—C5—C6	121.51 (12)	H12B—C12—H12C	109.5
C4—C5—H5	119.2	C10—C13—H13A	109.5

C6—C5—H5	119.2	C10—C13—H13B	109.5
C7—C6—C5	121.68 (11)	H13A—C13—H13B	109.5
C7—C6—H6	119.2	C10—C13—H13C	109.5
C5—C6—H6	119.2	H13A—C13—H13C	109.5
C6—C7—C8	116.46 (11)	H13B—C13—H13C	109.5
C6—C7—C10	123.57 (11)		
C2—N1—C1—C2^{i}	−58.15 (14)	C5—C6—C7—C10	178.35 (10)
C3—N1—C1—C2^{i}	179.26 (9)	C6—C7—C8—C9	2.03 (16)
C1—N1—C2—C1^{i}	58.37 (14)	C10—C7—C8—C9	−178.31 (10)
C3—N1—C2—C1^{i}	−179.32 (10)	C7—C8—C9—C4	−0.42 (18)
C2—N1—C3—C4	68.92 (14)	C5—C4—C9—C8	−1.27 (17)
C1—N1—C3—C4	−169.72 (9)	C3—C4—C9—C8	177.64 (10)
N1—C3—C4—C5	−113.26 (14)	C6—C7—C10—C11	111.43 (14)
N1—C3—C4—C9	67.89 (15)	C8—C7—C10—C11	−68.21 (14)
C9—C4—C5—C6	1.30 (17)	C6—C7—C10—C12	−9.49 (16)
C3—C4—C5—C6	−177.58 (11)	C8—C7—C10—C12	170.87 (10)
C4—C5—C6—C7	0.36 (19)	C6—C7—C10—C13	−128.42 (13)
C5—C6—C7—C8	−2.00 (17)	C8—C7—C10—C13	51.94 (14)

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

Fig. 1


C11
C12
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C7
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C2
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C4
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C9
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C3
C13A
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C5A
C2A
C1
C10A
C6A
C12A
C11A

Fig. 2