N-(2-Aminobenzyl)-N,N-bis(quinolin-2-ylmethyl)amine

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The molecular conformation of (I), as it exists in the crystal, is influenced by several close intramolecular contacts. As shown in Fig. 1, the anilino H4B atom participates in a bifurcated contact with nearby tertiary amino (N1) and quinoline (N3) acceptor groups (Table 1). This hydrogen-bond motif results in the anilino and quinoline fragments adopting a roughly planar alignment with an interplanar angle of 16.66 (8)°. Selected geometric parameters are given in Table 2.

Inspection of the crystal structure reveals translationally related molecules linked by N–H⋅⋅⋅N hydrogen bonds to

![Figure 1](image1.png)

**Figure 1**
The molecular structure and labeling scheme of (I) (50% probability displacement ellipsoids), showing the intramolecular bifurcated interaction (dotted lines).

![Figure 2](image2.png)

**Figure 2**
A view of the packing of (I), showing the catemeric hydrogen-bond network and π-stacking of the quinoline fragments. H atoms have been omitted for clarity. [Symmetry codes: (i) −x, −y + 1, −z; (ii) −x + 1, −y + 2, −z; (iii) x, y − 1, z.]

The title new diquinaldine derivative, C27H24N4, forms molecular assemblies organized by intermolecular quinoline π–π stacking [3.356 (3) and 3.440 (3) Å] and both inter- and intramolecular N–H⋅⋅⋅N hydrogen bonds [3.039 (3)–3.104 (3) Å and 129 (2)–172 (2)°]. The combination of such interactions provides readily definable contacts that propagate along each crystallographic axis.

**Comment**

Different types of arene–arene non-covalent interactions lead to fascinating molecular architectures and supramolecular structure in solids. We have recently shown by NMR spectroscopy (Mitra, Seaton, Assarpour & Williamson et al., 1998; Mitra, Seaton, Capitani & Assarpour, 1998) that such interactions can also be a prevalent theme in solutions. In our continuing study of π–π interactions and their effect on 1H NMR spectra, we wanted to study the consequence of interactions between aromatic and heteroaromatic groups. To this end, we synthesized a molecule that contains both arene and quinoline components. 2-Aminobenzylamine is an interesting molecule that consists of two amino groups that have different reactivity profiles. Selective N-alkylation of the benzylic amine with two equivalents of 2-(bromomethyl)quinoline gave the title compound, (I).

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**Figure 1**
The molecular structure and labeling scheme of (I) (50% probability displacement ellipsoids), showing the intramolecular bifurcated interaction (dotted lines).
form a catemeric motif along the b axis (Fig. 2). These molecular assemblies, described by C(9) graph-set notation (Bernstein et al., 1995), result from the association of neighboring anilino (H4A) and quinoline (N2) groups. Another noteworthy feature of this structure is the contribution of \( \pi-\pi \) interactions to the crystal packing. As shown in Fig. 2, each of the quinoline groups forms centroymmetric dimeric motifs [for example quinoline(N3)–quinoline(N3')] = 3.356 (3) Å and quinoline(N2)–quinoline(N2') = 3.440 (3) Å; symmetry codes as in Fig. 2] that link the hydrogen-bonded molecular chains along the a and c axes. Since molecules of (I) contain two nearly orthogonally positioned quinoline fragments [the interplanar angle is 81.75 (4)°], the combination of such \( \pi-\pi \) interactions and hydrogen bonds provides readily definable contacts that contribute to the overall three-dimensional organization.

**Experimental**

2-(Bromomethyl)quinoline (0.222 g, 1.0 mmol) was reacted with 2-aminobenzylamine (0.061 g, 0.5 mmol) in CH\(_2\)CN (5 ml) in the presence of anhydrous K₂CO₃ (0.152 g, 1.1 mmol) under N\(_2\) at room temperature for 16 h. The reaction mixture was concentrated under reduced pressure and directly chromatographed by flash column chromatography (SiO\(_2\) gel) using a solvent gradient from 5 to 10% MeOH/CH\(_2\)Cl\(_2\). Fractions containing the pure product were collected, concentrated under reduced pressure and recrystallized from CHCl\(_3\)/n-heptane to give (I) (0.110 g, 55% yield) as a colorless powder (m.p. 473–477 K). UV–Vis [MeOH, \( \lambda_{\text{max}} \) nm, \( \epsilon \)]: 232 (5600), 303 (6570), 316 (6940). IR (KBr, cm\(^{-1}\)) : 3351, 3186, 1602, 1565, 743. 1H NMR (0.005 M in CDC\(_3\)); \( \delta \) 3.82 (t, 2H, benzyl-CH\(_2\)), 5.20 (br s, 2H, NH\(_2\)), 6.64 (t, \( J = 7.5 \) Hz, H-5), 7.66 (d, \( J = 6.9 \) Hz, 1H, H-3), 7.07 (t, \( J = 7.5 \) Hz, 1H, H-4), 7.11 (d, \( J = 7.5 \) Hz, 1H, H-6), 7.50 (m, 2H, H-5H-6), 7.51 (d, \( J = 8.1 \) Hz, 2H, H-3H-5), 7.69 (d, \( J = 8.3 \) Hz, 6.9 and 1.4 Hz, 1H, H-7), 7.75 (d, \( J = 8.1 \) Hz, 2H, H-5), 8.04 (d, \( J = 8.1 \) Hz, 2H, H-4), 8.06 (d, \( J = 8.3 \) Hz, 2H, H-8). 13C NMR (CDC\(_3\)); \( \delta \) 15.92 (C2), 147.6 (C8a), 147.0 (C2'), 136.3 (C4), 131.5 (C6'), 129.4 (C7), 128.6 (C4'), 127.5 (C5), 127.3 (C4a), 126.2 (C6), 122.2 (C1'), 121.3 (C3), 117.1 (C5'), 115.4 (C3'), 60.9 (CH\(_2\)), 58.4 (CH\(_2\)).

### Table 1

Hydrogen-bond geometry (Å, °).

<table>
<thead>
<tr>
<th>D–H···A</th>
<th>D–H</th>
<th>H···A</th>
<th>D···A</th>
<th>D–H···A</th>
</tr>
</thead>
<tbody>
<tr>
<td>N4–H4A···N3</td>
<td>0.95</td>
<td>2.17</td>
<td>3.09</td>
<td>152 (2)</td>
</tr>
<tr>
<td>N4–H4B···N1</td>
<td>0.95</td>
<td>2.42</td>
<td>3.10</td>
<td>129 (2)</td>
</tr>
<tr>
<td>N4–H4A···N2(_\text{av})</td>
<td>0.96</td>
<td>2.15</td>
<td>3.10</td>
<td>172 (2)</td>
</tr>
</tbody>
</table>

Symmetry code: (iii) \( x, y - 1, z \).

### Table 2

Selected geometric parameters (Å, °).

<table>
<thead>
<tr>
<th>N1–C1</th>
<th>1.457 (3)</th>
<th>N1–C21</th>
<th>1.469 (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1–C11</td>
<td>1.458 (3)</td>
<td>N4–C23</td>
<td>1.370 (3)</td>
</tr>
<tr>
<td>C1–N1–C11</td>
<td>111.7 (2)</td>
<td>C11–N1–C21</td>
<td>111.5 (2)</td>
</tr>
<tr>
<td>C1–N1–C21</td>
<td>112.1 (2)</td>
<td>C11–N1–C21</td>
<td>111.5 (2)</td>
</tr>
</tbody>
</table>

Crystal data

\[ C_{20}H_{24}N_4 \]

\( M_r = 404.50 \)

Monoclinic, \( P2_1/n \)

\( a = 12.4071 (16) \) Å

\( b = 7.9834 (10) \) Å

\( c = 21.376 (3) \) Å

\( \beta = 98.041 (2)^\circ \)

\( V = 2096.5 (5) \) Å\(^3\)

Data collection

Bruker APEX-II CCD area-detector diffractometer

\( \varphi \) and \( \omega \) scans

Absorption correction: multi-scan

\( R_{\text{min}} = 0.058 \)

\( \theta_{\text{max}} = 27.5^\circ \)

Reﬁnement

Reﬁnement on \( F^2 \)

\[ R(F^2 > 2\sigma(F^2)) = 0.057 \]

\[ wR(F^2) = 0.134 \]

\( S = 1.02 \)

4699 reﬁnements

288 parameters

H atoms treated by a mixture of independent and constrained reﬁnement

The anilino H atoms (H4A and H4B) were located in a difference density map and their parameters were reﬁned freely. The remaining H atoms were treated as riding, with C–H distances of 0.95 (aromatic) and 0.99 Å (CH\(_2\)) [\( U_{eq}(H) = 1.2U_{eq}(C) \)].

Data collection: SMART (Bruker, 2001); cell reﬁnement: SMART; data reduction: SAINT (Bruker, 2002) and XPREP (Bruker, 2001); program(s) used to solve structure: SHELXL (Bruker, 2000); program(s) used to reﬁne structure: SHELXL; molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: X-SEED.

The authors thank Professor Arnold Rheingold of UC San Diego, CA, for use of his X-ray laboratory and ACS–PRF for funding the X-ray Crystallography Summer 2004 Workshop at UCSD. We also thank Dr Charles Campana of Bruker AXS and Dr Lev Zhakarov for all their help in acquiring the data, and Professor Richard Kirchner for helpful discussions.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SF3012). Services for accessing these data are described at the back of the journal.

**References**


Bruker (2000). SADABS (Version 2.05) and SHELXTL (Version 6.10).

Bruker AXS Inc., Madison, Wisconsin, USA.


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