SM-4 computer and using the X-Y recorder as a plotter.

Discussion. Table 1 presents the atomic coordinates and isotropic temperature factors.* Table 2 lists bond lengths and angles. Fig. 1 shows a plot of the molecule. All the bulky side substituents are situated in equatorial positions. Most are nearly perpendicular to the mean plane of the cyclohexane ring (Table 3).

The aromatic rings are essentially planar but some atoms still deviate significantly from planarity, the maximal deviations being 0·011 (5) C(42), 0·009 (3) C(44), 0·09 (4) C(51), 0·09 C(54), 0·08 (4) C(41), 0·07 (5) Å C(43). Bond lengths and angles in the molecule under investigation are in good agreement with standard values for organic compounds.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52697 (18 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of *N'*,*N'*-Dibenzylbenzohydrazide

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Abstract. $C_{21}H_{20}N_2O$, $M_r = 316{\cdot}4$, monoclinic, $P2_1/c$, $a = 9{\cdot}985$ (2), $b = 17{\cdot}070$ (3), $c = 10{\cdot}119$ (2) Å, $\beta = 95{\cdot}99$ (1)°, $V = 1715{\cdot}3$ Å^3, $Z = 4$, $D_x = 1{\cdot}225$ g cm^{-3}, Mo $K\alpha$ ($\lambda = 0{\cdot}71069$ Å), $\mu = 0{\cdot}82$ cm^{-1}, $F(000) = 672$, $T = 295$ K. Final $R = 0{\cdot}043$, $wR = 0{\cdot}042$ for 1139 reflections with $I > 3\sigma(I)$. There is one hydrogen bond in the structure with N—H···O = 2·05 (4) and N···O = 2·923 (5) Å.

Experimental. Colorless needles from dilute ethanol, CAD-4 diffractometer, graphite monochromator, 0·5 × 0·3 × 0·25 mm crystal, cell parameters from 25 reflections automatically centered in the range $8{\cdot}3 < \theta < 15{\cdot}6°$, θ–2θ scan at variable θ speed of 1·03 to 8·24° min^{-1}; 5 standard reflections measured every 2 h, each scan recorded in 96 steps over the θ range of $1{\cdot}5 \times (1{\cdot}2 + 0{\cdot}35\tan\theta)°$, $\theta_{max} = 25°$, 3129 unique reflections measured, 2462 with $F_o > 0{\cdot}0$, 1647 reflections with $I > \sigma(I)$, $R_{int} = 0{\cdot}008$ for 134 reflections; index range for h, k, $l = -10$ to 11; 0 to 20, 0 to 12. All crystallographic calculations performed with the *TEXSAN* program system (Molecular Structure Corporation, 1985) on DEC MicroVAX II computer; structure solved by *MITHRIL* (Gilmore, 1983) incorporated in *TEXSAN*. Full-matrix least-squares refinement; atomic scattering factors from *International Tables for X-ray Crystallography* (1974), anisotropic temperature factors for C, N and O, individual isotropic terms for H; $\sum w(F_o - F_c)^2$ minimized, $w = 1/\sigma^2(F_o)$, reflections with $I < \sigma(I)$ excluded from refinement; maximum Δ/σ of 0·66 in the final least-squares cycle; $\Delta/\rho_{min,max} = -0{\cdot}31$, 0·28 e Å^{-3}. Final R, wR and S are 0·078, 0·053 and 1·19 for 1647 reflections with $I > \sigma(I)$. Atomic

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Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
O	−0·5698 (3)	0·2251 (2)	0·4595 (3)	4·2 (2)
N1	−0·5486 (4)	0·2272 (2)	0·2385 (4)	3·1 (2)
N2	−0·4335 (4)	0·1794 (2)	0·2513 (3)	3·0 (2)
C1	−0·6016 (5)	0·2525 (3)	0·3476 (4)	3·0 (2)
C2	−0·7014 (4)	0·3169 (3)	0·3253 (4)	3·0 (2)
C3	−0·8084 (5)	0·3205 (3)	0·4016 (5)	4·1 (3)
C4	−0·8992 (6)	0·3812 (4)	0·3869 (7)	5·1 (3)
C5	−0·8828 (6)	0·4403 (4)	0·2974 (6)	5·0 (3)
C6	−0·7773 (6)	0·4384 (3)	0·2224 (6)	4·7 (3)
C7	−0·6872 (6)	0·3765 (3)	0·2343 (5)	3·7 (3)
C8	−0·3141 (6)	0·2264 (3)	0·2272 (6)	4·0 (3)
C9	−0·1852 (5)	0·1874 (3)	0·2771 (5)	3·4 (2)
C10	−0·0784 (6)	0·1834 (3)	0·2016 (6)	4·6 (3)
C11	0·0425 (6)	0·1508 (3)	0·2494 (7)	5·0 (3)
C12	0·0581 (7)	0·1216 (3)	0·3758 (7)	5·4 (4)
C13	−0·0473 (7)	0·1241 (4)	0·4539 (7)	5·6 (3)
C14	−0·1673 (6)	0·1571 (3)	0·4032 (6)	4·3 (3)
C15	−0·4529 (5)	0·1141 (3)	0·1569 (5)	3·2 (2)
C16	−0·5574 (5)	0·0561 (2)	0·1929 (4)	2·8 (2)
C17	−0·6389 (5)	0·0188 (3)	0·0944 (5)	3·9 (3)
C18	−0·7298 (6)	−0·0379 (3)	0·1236 (6)	4·8 (3)
C19	−0·7403 (6)	−0·0576 (3)	0·2521 (6)	4·5 (3)
C20	−0·6636 (6)	−0·0198 (4)	0·3513 (6)	4·8 (3)
C21	−0·5718 (6)	0·0373 (3)	0·3227 (5)	4·3 (3)

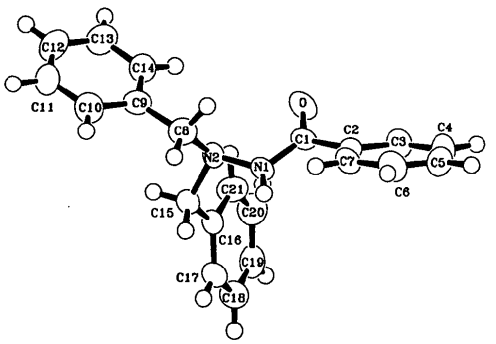

Fig. 1. An *ORTEP* diagram for the molecule of *N′,N′*-dibenzylbenzohydrazide. The C, O and N atoms are shown as 50% boundary ellipsoids; H atoms are drawn as spheres with B = 1·5 Å^2.

coordinates are listed in Table 1.* Bond lengths and angles are given in Table 2; an *ORTEP* (Johnson, 1965) drawing is shown in Fig. 1. There is only one hydrogen bond in the structure with N1···O (x, $\frac{1}{2}-y$, $-\frac{1}{2}+z$) = 2·923 (5) and H···O = 2·05 (4) Å.

Related literature. There is interest in the synthesis, chemistry and spectral and insecticidal studies on *N*-acyl-*N′,N′*-dibenzylhydrazines (Prasad, Sinha & Prasad, 1985; Palenik, 1965).

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52954 (25 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond distances* (Å), *angles* (°) *and selected torsion angles* (°) *with e.s.d.'s in parentheses*

O—C1	1·233 (4)	C9—C14	1·371 (6)
N1—C1	1·346 (4)	C9—C10	1·379 (6)
N1—N2	1·405 (4)	C10—C11	1·374 (7)
N2—C15	1·468 (5)	C11—C12	1·361 (7)
N2—C8	1·478 (5)	C12—C13	1·384 (7)
C1—C2	1·489 (5)	C13—C14	1·373 (7)
C2—C3	1·384 (5)	C15—C16	1·508 (6)
C2—C7	1·389 (6)	C16—C17	1·375 (6)
C3—C4	1·374 (6)	C16—C21	1·377 (6)
C4—C5	1·380 (7)	C17—C18	1·382 (6)
C5—C6	1·360 (7)	C18—C19	1·360 (6)
C6—C7	1·387 (6)	C19—C20	1·361 (7)
C8—C9	1·489 (6)	C20—C21	1·391 (7)

C1—N1—N2	119·8 (3)	C14—C9—C8	120·6 (5)
N1—N2—C15	109·4 (3)	C10—C9—C8	121·8 (4)
N1—N2—C8	109·4 (3)	C11—C10—C9	121·9 (5)
C15—N2—C8	111·0 (3)	C12—C11—C10	119·4 (5)
O—C1—N1	123·3 (4)	C11—C12—C13	120·2 (6)
O—C1—C2	121·6 (4)	C14—C13—C12	119·2 (6)
N1—C1—C2	115·1 (4)	C9—C14—C13	121·8 (5)
C3—C2—C7	118·4 (4)	N2—C15—C16	112·6 (4)
C3—C2—C1	119·6 (4)	C17—C16—C21	118·2 (4)
C7—C2—C1	121·9 (4)	C17—C16—C15	119·8 (4)
C4—C3—C2	120·5 (5)	C21—C16—C15	121·9 (4)
C3—C4—C5	120·5 (5)	C16—C17—C18	121·5 (5)
C6—C5—C4	119·7 (6)	C19—C18—C17	119·8 (5)
C5—C6—C7	120·3 (5)	C18—C19—C20	119·6 (5)
C6—C7—C2	120·5 (5)	C19—C20—C21	121·0 (5)
N2—C8—C9	112·8 (4)	C16—C21—C20	119·8 (5)
C14—C9—C10	117·5 (5)		

O—C1—N1—N2	−13·2 (6)	N2—C15—C16—C21	−36·7 (6)
O—C1—C2—C3	−33·9 (6)	N2—C8—C9—C14	−48·4 (6)
O—C1—C2—C7	142·4 (4)	N2—C8—C9—C10	133·9 (5)
N1—C1—C2—C7	−37·2 (6)	C1—N1—N2—C15	134·9 (4)
N1—N2—C15—C16	−69·6 (5)	C8—N2—C15—C16	169·5 (4)
N1—N2—C8—C9	162·8 (3)		
N2—C15—C16—C17	145·5 (4)		
N2—N1—C1—C2	166·4 (4)		

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