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1,3-Dibenzyl-2-phenylperhydropyrimidine

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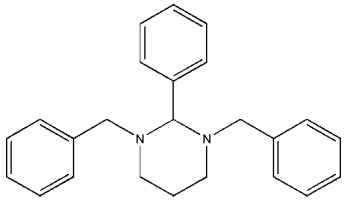
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.094; data-to-parameter ratio = 15.0.

In the title compound, $C_{24}H_{26}N_2$, the dihedral angles between the phenyl ring at the 2-position and the other two phenyl rings are 78.53 (10) and 79.37 (10)°. The heterocyclic ring adopts a chair conformation. Molecules are linked into chains of rings and a three-dimensional network by C—H$\cdots\pi$ hydrogen bonds.

Related literature

For bond-length data, see: Allen *et al.* (1987). For a related structure, see: Xia *et al.* (2007).



Experimental

Crystal data

$C_{24}H_{26}N_2$
M_r = 342.47
Monoclinic, $P2_1/n$
a = 6.0912 (11) Å
b = 16.900 (2) Å
c = 19.621 (3) Å
β = 98.304 (2)°
V = 1998.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.35 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.990
9972 measured reflections
3522 independent reflections
1341 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.094
S = 0.75
3522 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids of the C19–C24 and C12–C17 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C14—H14$\cdots$*Cg*1^{i}	0.93	2.85	3.55 (3)	132
C8—H8$\cdots$*Cg*1^{ii}	0.93	3.07	3.79 (3)	136
C21—H21$\cdots$*Cg*2^{iii}	0.93	3.00	3.63 (4)	126

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2159).

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supplementary materials

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1,3-Dibenzyl-2-phenylperhydropyrimidine

H.-T. Xia, Y.-F. Liu, D.-Q. Wang and W. Gao

Comment

As part of our investigation of crystal structures of diamine derivatives, we report here the crystal structure of a new diamine derivative.

The molecular structure of the title compound is illustrated in Fig. 1. The bond lengths and angles are normal (Allen *et al.*, 1987). A very closely related compound is 1,3-dibenzyl-2-phenylimidazolidine (Xia *et al.*, 2007); it and the title compound have similar crystal structures. In the title compound, the dihedral angles between the central phenyl ring (C5—C10) and the other two phenyl rings are 78.53 (10)° (C12—C1) and 79.37 (10)° (C19—C24) (Fig. 1). Molecules are linked into chains of rings and a three-dimensional network by C—H···π hydrogen bonds (Fig. 2 and Fig. 3).

Experimental

To a solution of benzaldehyde (20 mmol) in methanol (20 ml) propane-1,3-diamine (10 mmol) in methanol (10 ml) was added. The mixed solution was stirred for 10 min and then acetic acid catalyst was added. The reaction mixture was stirred continuously for 10 h at 338 K and then filtered. The solution was allowed to stand, slowly producing crystals of the title compound.

Refinement

All H atoms were located in difference Fourier maps. They were then treated as riding, with C—H distances of 0.93 Å (aryl), 0.97 Å (methylene) and 0.98 Å (methine); U_{iso}(H) = 1.2U_{eq}(C).

Figures

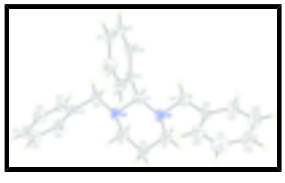

Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

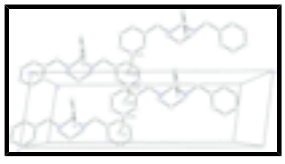

Fig. 2. A portion of the crystal structure of the title compound, showing the formation of a hydrogen-bonded (dashed lines) sheet built from three C—H···π interactions. For clarity, H atoms not involved in hydrogen bonding have been omitted. [Symmetry code: (B) −1/2 + *x*, 3/2 − *y*, 1/2 + *z*, (D) −1 + *x*, *y*, *z*, (E) −3/2 + *x*, 3/2 − *y*, 1/2 + *z*].

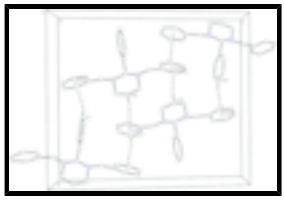

Fig. 3. The crystal structure of the title compound. Neighbouring sheets are connected by a pair of C—H···π hydrogen bonds (dashed lines). For clarity, H atoms not involved in the hydrogen bonding have been omitted. [Symmetry code: (A) (3/2 − *x*, −1/2 + *y*, 1/2 − *z*, (B) −1/2 + *x*, 3/2 − *y*, 1/2 + *z*, (C) 1 − *x*, 1 − *y*, 1 − *z*].

1,3-Dibenzyl-2-phenylperhydropyrimidine

Crystal data

$C_{24}H_{26}N_2$	F_{000} = 736
M_r = 342.47	D_x = 1.138 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 6.0912 (11) Å	Cell parameters from 926 reflections
b = 16.900 (2) Å	θ = 2.4–18.6º
c = 19.621 (3) Å	μ = 0.07 mm^{-1}
β = 98.304 (2)º	T = 298 (2) K
V = 1998.7 (5) Å^3	Block, colorless
Z = 4	0.35 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3522 independent reflections
Radiation source: fine-focus sealed tube	1341 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −7→6
T_{min} = 0.977, T_{max} = 0.990	k = −20→17
9972 measured reflections	l = −23→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.094	$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.75	$(\Delta/\sigma)_{max} < 0.001$
3522 reflections	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
235 parameters	$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
N1	0.7318 (3)	0.85935 (10)	0.06611 (9)	0.0516 (5)
N2	0.7249 (3)	0.88698 (10)	0.18657 (9)	0.0521 (6)
C1	0.8029 (4)	0.94061 (13)	0.05542 (11)	0.0692 (8)
H1A	0.6737	0.9739	0.0427	0.083*
H1B	0.8911	0.9418	0.0181	0.083*
C2	0.9374 (5)	0.97215 (13)	0.11995 (12)	0.0740 (9)
H2A	1.0714	0.9410	0.1314	0.089*
H2B	0.9799	1.0265	0.1129	0.089*
C3	0.8003 (4)	0.96792 (13)	0.17753 (12)	0.0671 (8)
H3A	0.8878	0.9860	0.2199	0.080*
H3B	0.6728	1.0026	0.1674	0.080*
C4	0.5999 (4)	0.85434 (12)	0.12315 (11)	0.0517 (7)
H4	0.4616	0.8841	0.1112	0.062*
C5	0.5463 (5)	0.76804 (13)	0.13427 (11)	0.0473 (6)
C6	0.7146 (4)	0.71554 (14)	0.15560 (11)	0.0591 (7)
H6	0.8593	0.7341	0.1661	0.071*
C7	0.6732 (5)	0.63590 (15)	0.16175 (12)	0.0708 (8)
H7	0.7893	0.6012	0.1759	0.085*
C8	0.4605 (6)	0.60803 (16)	0.14691 (13)	0.0718 (9)
H8	0.4320	0.5543	0.1506	0.086*
C9	0.2902 (5)	0.65937 (17)	0.12665 (12)	0.0683 (8)
H9	0.1459	0.6404	0.1164	0.082*
C10	0.3317 (5)	0.73931 (15)	0.12132 (10)	0.0583 (7)
H10	0.2144	0.7741	0.1089	0.070*
C11	0.6008 (4)	0.83060 (13)	0.00211 (11)	0.0606 (8)
H11A	0.4752	0.8657	−0.0100	0.073*
H11B	0.5428	0.7786	0.0106	0.073*
C12	0.7262 (5)	0.82518 (13)	−0.05768 (12)	0.0519 (7)
C13	0.9340 (5)	0.79109 (14)	−0.05116 (13)	0.0653 (8)
H13	1.0002	0.7736	−0.0081	0.078*
C14	1.0453 (5)	0.78237 (14)	−0.10665 (17)	0.0744 (9)

H14	1.1846	0.7588	−0.1011	0.089*
C15	0.9499 (6)	0.80870 (16)	−0.17072 (16)	0.0817 (10)
H15	1.0253	0.8038	−0.2085	0.098*
C16	0.7445 (6)	0.84185 (16)	−0.17795 (14)	0.0802 (10)
H16	0.6784	0.8590	−0.2211	0.096*
C17	0.6333 (5)	0.85023 (13)	−0.12196 (13)	0.0648 (8)
H17	0.4931	0.8732	−0.1278	0.078*
C18	0.5896 (4)	0.88619 (13)	0.24232 (11)	0.0629 (8)
H18A	0.5094	0.8365	0.2408	0.075*
H18B	0.4810	0.9284	0.2345	0.075*
C19	0.7200 (5)	0.89608 (13)	0.31294 (12)	0.0546 (7)
C20	0.9327 (5)	0.86625 (13)	0.32864 (14)	0.0680 (8)
H20	1.0010	0.8428	0.2943	0.082*
C21	1.0450 (5)	0.87117 (16)	0.39527 (18)	0.0851 (10)
H21	1.1887	0.8516	0.4054	0.102*
C22	0.9438 (7)	0.9048 (2)	0.44608 (17)	0.0984 (13)
H22	1.0182	0.9071	0.4909	0.118*
C23	0.7348 (7)	0.93502 (17)	0.43139 (16)	0.0968 (11)
H23	0.6671	0.9583	0.4660	0.116*
C24	0.6234 (5)	0.93087 (14)	0.36457 (14)	0.0732 (9)
H24	0.4814	0.9519	0.3546	0.088*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0641 (16)	0.0516 (12)	0.0404 (12)	−0.0082 (11)	0.0117 (11)	−0.0015 (9)
N2	0.0646 (16)	0.0502 (13)	0.0428 (12)	−0.0040 (11)	0.0117 (12)	−0.0028 (9)
C1	0.093 (2)	0.0613 (17)	0.0557 (17)	−0.0117 (16)	0.0182 (16)	0.0004 (13)
C2	0.104 (3)	0.0551 (17)	0.0645 (18)	−0.0254 (16)	0.0181 (18)	−0.0069 (13)
C3	0.090 (2)	0.0521 (17)	0.0596 (18)	−0.0055 (15)	0.0115 (17)	−0.0064 (13)
C4	0.056 (2)	0.0507 (15)	0.0484 (16)	0.0031 (13)	0.0064 (14)	0.0011 (12)
C5	0.0499 (19)	0.0489 (16)	0.0443 (15)	−0.0022 (15)	0.0106 (13)	−0.0009 (11)
C6	0.056 (2)	0.0550 (18)	0.0674 (18)	−0.0019 (16)	0.0131 (15)	0.0020 (13)
C7	0.073 (3)	0.0581 (19)	0.083 (2)	0.0035 (17)	0.0167 (17)	0.0032 (15)
C8	0.099 (3)	0.0528 (18)	0.0680 (19)	−0.010 (2)	0.0271 (18)	−0.0052 (14)
C9	0.069 (2)	0.075 (2)	0.0628 (19)	−0.0212 (18)	0.0157 (16)	−0.0071 (15)
C10	0.058 (2)	0.0631 (19)	0.0537 (16)	0.0000 (16)	0.0094 (14)	0.0011 (13)
C11	0.066 (2)	0.0688 (17)	0.0466 (16)	−0.0071 (14)	0.0057 (15)	−0.0015 (13)
C12	0.059 (2)	0.0531 (15)	0.0438 (17)	−0.0041 (14)	0.0073 (15)	−0.0037 (12)
C13	0.073 (3)	0.0735 (19)	0.0478 (18)	−0.0067 (17)	0.0042 (17)	−0.0040 (13)
C14	0.072 (2)	0.0720 (19)	0.080 (2)	−0.0004 (16)	0.014 (2)	−0.0170 (17)
C15	0.106 (3)	0.081 (2)	0.065 (2)	−0.024 (2)	0.035 (2)	−0.0200 (17)
C16	0.103 (3)	0.090 (2)	0.0460 (19)	−0.008 (2)	0.007 (2)	0.0081 (15)
C17	0.077 (2)	0.0652 (18)	0.0518 (18)	−0.0026 (15)	0.0084 (17)	0.0077 (14)
C18	0.072 (2)	0.0606 (16)	0.0574 (18)	0.0007 (14)	0.0125 (16)	−0.0042 (13)
C19	0.071 (2)	0.0518 (15)	0.0434 (17)	−0.0032 (15)	0.0146 (16)	−0.0002 (13)
C20	0.080 (3)	0.0595 (17)	0.065 (2)	0.0001 (17)	0.0114 (17)	0.0063 (14)
C21	0.090 (3)	0.076 (2)	0.083 (2)	−0.0110 (18)	−0.009 (2)	0.0248 (18)

C22	0.131 (4)	0.101 (3)	0.060 (2)	−0.036 (3)	0.003 (3)	0.0060 (19)
C23	0.128 (4)	0.102 (3)	0.065 (3)	−0.021 (2)	0.033 (2)	−0.0185 (19)
C24	0.089 (3)	0.0736 (19)	0.0603 (19)	−0.0089 (16)	0.0198 (18)	−0.0079 (15)

Geometric parameters (Å, °)

N1—C1	1.464 (2)	C11—H11A	0.9700
N1—C11	1.470 (2)	C11—H11B	0.9700
N1—C4	1.472 (3)	C12—C17	1.373 (3)
N2—C18	1.462 (3)	C12—C13	1.380 (3)
N2—C3	1.462 (2)	C13—C14	1.371 (3)
N2—C4	1.469 (2)	C13—H13	0.9300
C1—C2	1.503 (3)	C14—C15	1.380 (3)
C1—H1A	0.9700	C14—H14	0.9300
C1—H1B	0.9700	C15—C16	1.359 (4)
C2—C3	1.501 (3)	C15—H15	0.9300
C2—H2A	0.9700	C16—C17	1.379 (4)
C2—H2B	0.9700	C16—H16	0.9300
C3—H3A	0.9700	C17—H17	0.9300
C3—H3B	0.9700	C18—C19	1.504 (3)
C4—C5	1.517 (3)	C18—H18A	0.9700
C4—H4	0.9800	C18—H18B	0.9700
C5—C6	1.375 (3)	C19—C24	1.375 (3)
C5—C10	1.383 (3)	C19—C20	1.383 (3)
C6—C7	1.378 (3)	C20—C21	1.388 (3)
C6—H6	0.9300	C20—H20	0.9300
C7—C8	1.370 (3)	C21—C22	1.369 (4)
C7—H7	0.9300	C21—H21	0.9300
C8—C9	1.366 (3)	C22—C23	1.364 (4)
C8—H8	0.9300	C22—H22	0.9300
C9—C10	1.381 (3)	C23—C24	1.388 (3)
C9—H9	0.9300	C23—H23	0.9300
C10—H10	0.9300	C24—H24	0.9300
C11—C12	1.492 (3)		
C1—N1—C11	108.85 (17)	N1—C11—C12	114.5 (2)
C1—N1—C4	111.60 (18)	N1—C11—H11A	108.6
C11—N1—C4	110.00 (19)	C12—C11—H11A	108.6
C18—N2—C3	108.68 (18)	N1—C11—H11B	108.6
C18—N2—C4	110.6 (2)	C12—C11—H11B	108.6
C3—N2—C4	112.45 (17)	H11A—C11—H11B	107.6
N1—C1—C2	110.40 (18)	C17—C12—C13	117.7 (3)
N1—C1—H1A	109.6	C17—C12—C11	120.9 (3)
C2—C1—H1A	109.6	C13—C12—C11	121.3 (2)
N1—C1—H1B	109.6	C14—C13—C12	121.6 (3)
C2—C1—H1B	109.6	C14—C13—H13	119.2
H1A—C1—H1B	108.1	C12—C13—H13	119.2
C3—C2—C1	108.8 (2)	C13—C14—C15	119.8 (3)
C3—C2—H2A	109.9	C13—C14—H14	120.1
C1—C2—H2A	109.9	C15—C14—H14	120.1

C3—C2—H2B	109.9	C16—C15—C14	119.2 (3)
C1—C2—H2B	109.9	C16—C15—H15	120.4
H2A—C2—H2B	108.3	C14—C15—H15	120.4
N2—C3—C2	110.77 (19)	C15—C16—C17	120.7 (3)
N2—C3—H3A	109.5	C15—C16—H16	119.7
C2—C3—H3A	109.5	C17—C16—H16	119.7
N2—C3—H3B	109.5	C12—C17—C16	121.0 (3)
C2—C3—H3B	109.5	C12—C17—H17	119.5
H3A—C3—H3B	108.1	C16—C17—H17	119.5
N2—C4—N1	110.4 (2)	N2—C18—C19	114.1 (2)
N2—C4—C5	109.58 (17)	N2—C18—H18A	108.7
N1—C4—C5	108.50 (18)	C19—C18—H18A	108.7
N2—C4—H4	109.4	N2—C18—H18B	108.7
N1—C4—H4	109.4	C19—C18—H18B	108.7
C5—C4—H4	109.4	H18A—C18—H18B	107.6
C6—C5—C10	118.2 (2)	C24—C19—C20	118.6 (3)
C6—C5—C4	119.8 (2)	C24—C19—C18	120.1 (3)
C10—C5—C4	121.9 (2)	C20—C19—C18	121.2 (2)
C5—C6—C7	121.3 (2)	C19—C20—C21	120.4 (3)
C5—C6—H6	119.4	C19—C20—H20	119.8
C7—C6—H6	119.4	C21—C20—H20	119.8
C8—C7—C6	119.8 (3)	C22—C21—C20	119.9 (3)
C8—C7—H7	120.1	C22—C21—H21	120.0
C6—C7—H7	120.1	C20—C21—H21	120.0
C9—C8—C7	119.9 (3)	C23—C22—C21	120.4 (3)
C9—C8—H8	120.1	C23—C22—H22	119.8
C7—C8—H8	120.1	C21—C22—H22	119.8
C8—C9—C10	120.3 (3)	C22—C23—C24	119.7 (3)
C8—C9—H9	119.9	C22—C23—H23	120.2
C10—C9—H9	119.9	C24—C23—H23	120.2
C9—C10—C5	120.5 (2)	C19—C24—C23	121.0 (3)
C9—C10—H10	119.7	C19—C24—H24	119.5
C5—C10—H10	119.7	C23—C24—H24	119.5
C11—N1—C1—C2	179.9 (2)	C4—C5—C10—C9	174.78 (19)
C4—N1—C1—C2	58.3 (3)	C1—N1—C11—C12	63.4 (3)
N1—C1—C2—C3	−57.8 (3)	C4—N1—C11—C12	−173.99 (19)
C18—N2—C3—C2	−179.1 (2)	N1—C11—C12—C17	−137.0 (2)
C4—N2—C3—C2	−56.4 (3)	N1—C11—C12—C13	46.5 (3)
C1—C2—C3—N2	56.7 (3)	C17—C12—C13—C14	0.1 (4)
C18—N2—C4—N1	176.79 (17)	C11—C12—C13—C14	176.7 (2)
C3—N2—C4—N1	55.1 (2)	C12—C13—C14—C15	0.6 (4)
C18—N2—C4—C5	−63.7 (2)	C13—C14—C15—C16	−1.1 (4)
C3—N2—C4—C5	174.6 (2)	C14—C15—C16—C17	0.9 (4)
C1—N1—C4—N2	−56.0 (2)	C13—C12—C17—C16	−0.3 (3)
C11—N1—C4—N2	−176.92 (16)	C11—C12—C17—C16	−176.9 (2)
C1—N1—C4—C5	−176.11 (18)	C15—C16—C17—C12	−0.2 (4)
C11—N1—C4—C5	63.0 (2)	C3—N2—C18—C19	−72.8 (2)
N2—C4—C5—C6	−56.2 (3)	C4—N2—C18—C19	163.38 (17)
N1—C4—C5—C6	64.5 (3)	N2—C18—C19—C24	150.9 (2)

N2—C4—C5—C10	126.1 (2)	N2—C18—C19—C20	−33.2 (3)
N1—C4—C5—C10	−113.3 (2)	C24—C19—C20—C21	0.3 (4)
C10—C5—C6—C7	2.2 (3)	C18—C19—C20—C21	−175.6 (2)
C4—C5—C6—C7	−175.6 (2)	C19—C20—C21—C22	0.8 (4)
C5—C6—C7—C8	−0.5 (4)	C20—C21—C22—C23	−1.3 (5)
C6—C7—C8—C9	−0.6 (4)	C21—C22—C23—C24	0.6 (5)
C7—C8—C9—C10	−0.3 (4)	C20—C19—C24—C23	−1.0 (4)
C8—C9—C10—C5	2.1 (4)	C18—C19—C24—C23	174.9 (2)
C6—C5—C10—C9	−3.0 (3)	C22—C23—C24—C19	0.6 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···Cg1^{i}	0.93	2.85	3.55 (3)	132
C8—H8···Cg1^{ii}	0.93	3.07	3.79 (3)	136
C21—H21···Cg2^{iii}	0.93	3.00	3.63 (4)	126

Symmetry codes: (i) *x*+1/2, −*y*+3/2, *z*−1/2; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iii) *x*+1/2, −*y*+3/2, *z*+1/2.

Fig. 1

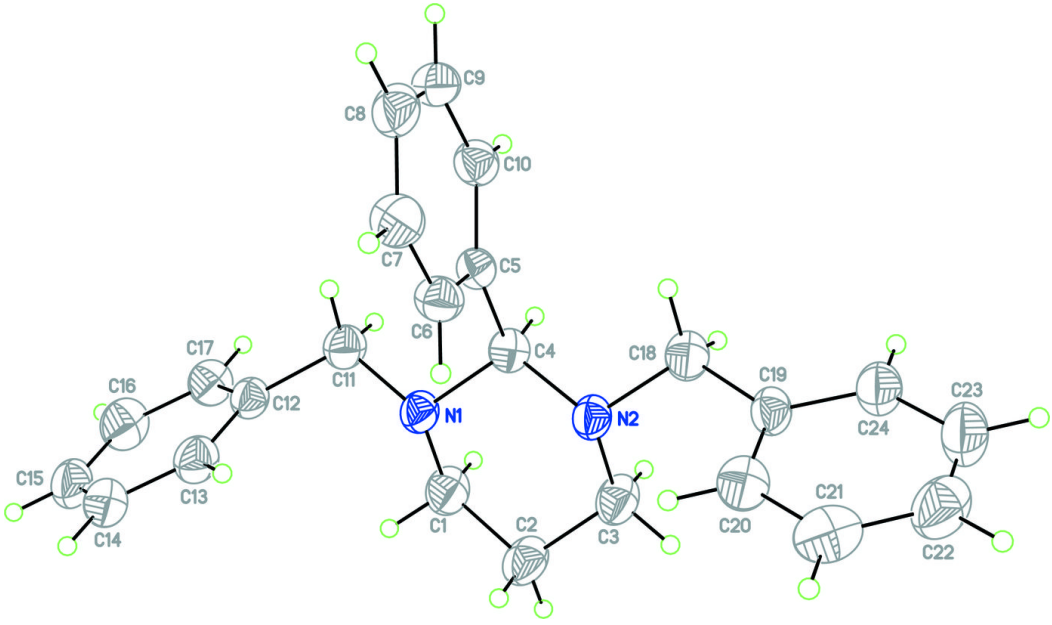
C9
C8
C10
C7
C5
C6
C4
C18
C19
C24
C23
C17
C16
C12
C11
N1
N2
C15
C13
C1
C2
C3
C20
C21
C22
C14

Fig. 2

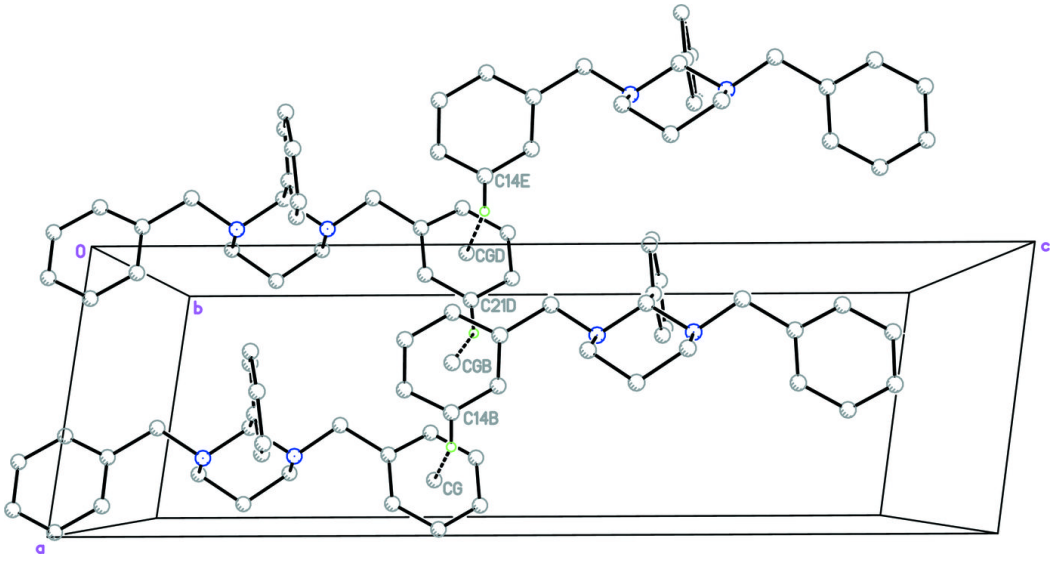

Fig. 3