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1-Dehydroabietyl-4,5-diphenyl-1*H*-imidazole

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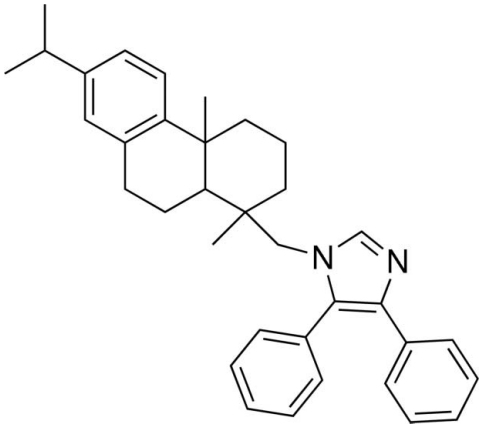
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.102; data-to-parameter ratio = 11.4.

The title compound [systematic name: 1-(7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-ylmethyl)-4,5-diphenyl-1*H*-imidazole], $C_{35}H_{40}N_2$, was obtained *via* the one-pot three-component condensation of benzil, formaldehyde and dehydroabietylamine, which is a fungal toxin. The two substituent phenyl groups and the imidazole ring form a conjugated system. The dihedral angles between the imidazole ring and the phenyl rings are 70.18 (9) and 12.77 (12)°. In the crystal structure, there are one intramolecular and two intermolecular hydrogen-bonding C—H···π contacts. Furthermore, a weak C—H···N intramolecular hydrogen bond is observed.

Related literature

For related structures of some imidazole derivatives, see: Thiruvalluvar *et al.* (2007); Seethalakshmi *et al.* (2006). For related literature, see: Bellina *et al.* (2007); Gassner *et al.* (2007); Harris *et al.* (1992); Zalkov & Girotra (1964).



Experimental

Crystal data

$C_{35}H_{40}N_2$
M_r = 488.69
Orthorhombic, $P2_12_12_1$
a = 9.9157 (9) Å
b = 12.3466 (11) Å
c = 23.058 (2) Å
V = 2822.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 273 (2) K
0.23 × 0.21 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.983, T_{max} = 0.996
17704 measured reflections
3860 independent reflections
2295 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.102
S = 0.79
3860 reflections
338 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

*Cg*1 is the centroid of the imidazole ring and *Cg*2 is the centroid of the C27–C32 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···N1	0.93	2.51	2.852 (3)	102
C17—H17*A*···*Cg*1	0.96	2.85	3.460 (2)	122
C12—H12···*Cg*2^{i}	0.93	2.65	3.570 (2)	170
C15—H15···*Cg*2^{ii}	0.93	2.81	3.685 (2)	157

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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: SI2025).

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supplementary materials

Acta Cryst. (2007). E**63**, o3623-o3624 [**doi:10.1107/S1600536807035878**]

1-Dehydroabietyl-4,5-diphenyl-1*H*-imidazole

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Comment

Dehydroabietic acid is a kind of natural product. A series of carboxylic acid group derivatives show biological activity (Zalkov *et al.*, 1964). Dehydroabietylamine could be obtained from Dehydroabietic acid and is a fungal toxin (Gassner *et al.*, 2007). Imidazoles are common scaffolds in highly significant biomolecules. Imidazole derivatives have been found to possess many pharmacological properties and are implicated in biochemical processes (Bellina *et al.*, 2007). For example, a mevalonate derivative containing a 4,5-diphenyl-1*H*-imidazole group has been shown to reduce cholesterol levels in rats (Harris *et al.*, 1992).

The title compound is a trisubstituted imidazole, and similar to 2-(2-chlorophenyl)-4,5-diphenyl-1*H*-imidazole (Thiruvalluvar *et al.*, 2007), except that the chlorophenyl ring is replaced by the Dehydroabietyl group (Fig. 1). The bond lengths and angles in the title compound are within normal ranges and are comparable to those in other derivatives (Seethalakshmi *et al.*, 2006). The dihedral angle between the imidazole ring and the 2-phenyl or 3-phenyl is 70.18 (9) ° or 12.77 (12) °.

In the crystal structure of the title compound the following interactions are observed: one intramolecular hydrogen bonding C—H···π contact, C17—H17A···*Cg*1 (*Cg*1 is the centroid of the imidazole ring N1/C1/N2/C2/C3), and two intermolecular hydrogen bonds, C12—H12···*Cg*2 (*Cg*2 is the centroid of the abietyl ring C27—C32)^{i}), and C15—H15···*Cg*3 (*Cg*3 is the centroid of the same ring C27—C32)^{ii}). Details of the hydrogen bonds between molecules are shown in Fig. 2 and Table 1. symmetry codes: (i) −1/2 + *x*, 1/2 − *y*, −*z*; (ii) 1/2 + *x*, 1/2 − *y*, −*z*. And also a weak C9—H9···N1 intramolecular hydrogen bond is observed.

Experimental

A mixture of benzil (2.38 mmol), 0.2 mL formaldehyde (37% aqueous, 2.38 mmol), dehydroabietylamine (3.57 mmol) and ammonium acetate (11.9 mmol) in glacial acetic acid (15 mL) was heated at 385 K for 12 h. Then the dark solution was poured into a copious amount of water and neutralized with KOH until pH = 9. The resulting mixture was extracted with diethyl ether. The solvent of the organic layer was gradually removed by evaporation under vacuum until a solid product was obtained. The solid was then recrystallized from methanol and colorless crystals suitable for X-ray diffraction were obtained (Yield 55%, m.p. 415–416 K).

Refinement

H atoms attached to C atoms were all positioned geometrically and treated as riding on their parent atoms, with C—H = 0.93 − 0.98 Å. The U_{iso}(H) values were set at 1.5 U_{eq}(C) for the methyl H atoms and at 1.2 U_{eq}(C) for the other C-bound H atoms. Due to light atoms of the title compound and the X-ray source used, significant scattering effects were not observed and therefore Friedel pairs were merged.

Figures

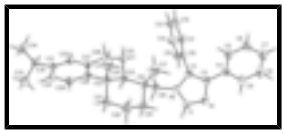

Fig. 1. The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

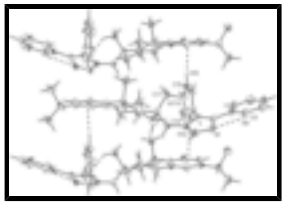

Fig. 2. C—H···N and C—H···π interactions in the crystal structure of the title compound. [Symmetry codes for the interactions: (i) −1/2 + *x*, 1/2 − *y*, −*z*; (ii) 1/2 + *x*, 1/2 − *y*, −*z*].

1-(7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10*a*-octahydrophenanthren- 1-ylmethyl)-4,5-diphenyl-1*H*-imidazole

Crystal data

$C_{35}H_{40}N_2$	F_{000} = 1056
M_r = 488.69	D_x = 1.150 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 3440 reflections
a = 9.9157 (9) Å	θ = 2.4–21.0º
b = 12.3466 (11) Å	μ = 0.07 mm^{-1}
c = 23.058 (2) Å	*T* = 273 (2) K
V = 2822.8 (4) Å^3	Block, colourless
Z = 4	0.23 × 0.21 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3860 independent reflections
Radiation source: fine-focus sealed tube	2295 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 273(2) K	θ_{max} = 28.3º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −13→11
T_{min} = 0.983, T_{max} = 0.996	*k* = −16→10
17704 measured reflections	*l* = −30→30

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.102$

$S = 0.79$

3860 reflections

338 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.10$ e Å^{-3}

$\Delta\rho_{min} = -0.14$ e Å^{-3}

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 $F^2 > 2$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}
N2	0.66925 (19)	1.09095 (14)	1.00629 (8)	0.0538 (5)
N1	0.6547 (2)	1.27059 (15)	1.00804 (8)	0.0601 (5)
C4	0.7757 (2)	1.31473 (19)	1.09868 (9)	0.0533 (5)
C9	0.7729 (3)	1.42402 (19)	1.08533 (11)	0.0652 (7)
H9	0.7405	1.4460	1.0494	0.078*
C8	0.8173 (3)	1.5010 (2)	1.12431 (13)	0.0784 (8)
H8	0.8148	1.5739	1.1143	0.094*
C7	0.8648 (3)	1.4709 (3)	1.17748 (14)	0.0813 (8)
H7	0.8956	1.5226	1.2037	0.098*
C6	0.8662 (3)	1.3623 (3)	1.19170 (12)	0.0812 (8)
H6	0.8970	1.3409	1.2280	0.097*
C5	0.8228 (3)	1.2857 (2)	1.15309 (10)	0.0678 (7)
H5	0.8249	1.2130	1.1635	0.081*
C3	0.7271 (2)	1.23573 (17)	1.05611 (10)	0.0516 (5)
C2	0.7372 (2)	1.12421 (17)	1.05551 (9)	0.0486 (5)
C1	0.6228 (2)	1.18223 (19)	0.98034 (10)	0.0613 (6)
H1	0.5731	1.1818	0.9461	0.074*
C10	0.7937 (2)	1.04442 (17)	1.09639 (9)	0.0476 (5)
C11	0.9320 (2)	1.0304 (2)	1.10340 (10)	0.0594 (6)
H11	0.9918	1.0733	1.0825	0.071*
C12	0.9804 (3)	0.9533 (2)	1.14101 (11)	0.0719 (7)
H12	1.0730	0.9445	1.1454	0.086*

C13	0.8935 (3)	0.8892 (2)	1.17225 (12)	0.0775 (8)
H13	0.9267	0.8364	1.1972	0.093*
C14	0.7569 (3)	0.9039 (2)	1.16618 (11)	0.0731 (8)
H14	0.6976	0.8617	1.1878	0.088*
C15	0.7072 (2)	0.9802 (2)	1.12860 (10)	0.0610 (6)
H15	0.6144	0.9888	1.1247	0.073*
C16	0.6709 (2)	0.98173 (17)	0.98190 (10)	0.0550 (6)
H16A	0.5825	0.9662	0.9659	0.066*
H16B	0.6870	0.9306	1.0131	0.066*
C17	0.9114 (2)	1.0160 (2)	0.95018 (11)	0.0689 (7)
H17A	0.8950	1.0890	0.9626	0.103*
H17B	0.9704	1.0167	0.9171	0.103*
H17C	0.9528	0.9760	0.9811	0.103*
C18	0.7783 (2)	0.96272 (17)	0.93371 (9)	0.0514 (5)
C19	0.7213 (3)	1.01225 (19)	0.87775 (10)	0.0699 (7)
H19A	0.6262	0.9943	0.8753	0.084*
H19B	0.7282	1.0905	0.8804	0.084*
C20	0.7898 (4)	0.97588 (19)	0.82200 (11)	0.0853 (9)
H20A	0.8821	1.0018	0.8214	0.102*
H20B	0.7431	1.0067	0.7889	0.102*
C21	0.7886 (3)	0.85255 (18)	0.81759 (10)	0.0697 (7)
H21A	0.8330	0.8309	0.7820	0.084*
H21B	0.6959	0.8275	0.8158	0.084*
C22	0.8594 (2)	0.79845 (17)	0.86912 (9)	0.0515 (5)
C23	0.7889 (2)	0.83724 (16)	0.92572 (8)	0.0480 (5)
H23	0.6955	0.8119	0.9224	0.058*
C24	1.0115 (3)	0.8217 (2)	0.86585 (12)	0.0798 (8)
H24A	1.0261	0.8986	0.8653	0.120*
H24B	1.0478	0.7902	0.8311	0.120*
H24C	1.0555	0.7909	0.8991	0.120*
C25	0.8479 (3)	0.77547 (17)	0.97744 (9)	0.0570 (6)
H25A	0.9454	0.7811	0.9772	0.068*
H25B	0.8149	0.8065	1.0134	0.068*
C26	0.8063 (3)	0.65741 (17)	0.97348 (9)	0.0598 (6)
H26A	0.8588	0.6158	1.0011	0.072*
H26B	0.7121	0.6511	0.9843	0.072*
C27	0.8253 (2)	0.60948 (17)	0.91382 (9)	0.0494 (5)
C28	0.8468 (2)	0.67438 (16)	0.86538 (8)	0.0468 (5)
C29	0.8636 (2)	0.62312 (17)	0.81187 (9)	0.0542 (6)
H29	0.8804	0.6649	0.7791	0.065*
C30	0.8558 (2)	0.51188 (17)	0.80653 (9)	0.0533 (6)
H30	0.8673	0.4803	0.7702	0.064*
C31	0.8312 (2)	0.44639 (16)	0.85419 (9)	0.0485 (5)
C32	0.8179 (2)	0.49714 (17)	0.90716 (9)	0.0511 (5)
H32	0.8034	0.4547	0.9399	0.061*
C33	0.7107 (3)	0.2938 (2)	0.80477 (13)	0.0856 (9)
H33A	0.7334	0.3220	0.7672	0.128*
H33B	0.6259	0.3235	0.8171	0.128*
H33C	0.7039	0.2163	0.8027	0.128*

C34	0.9531 (3)	0.2747 (2)	0.83175 (16)	0.0957 (10)
H34A	1.0184	0.2912	0.8612	0.144*
H34B	0.9829	0.3036	0.7953	0.144*
H34C	0.9431	0.1976	0.8286	0.144*
C35	0.8192 (2)	0.32465 (17)	0.84779 (9)	0.0556 (6)
H35	0.7929	0.2953	0.8856	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0570 (11)	0.0462 (10)	0.0582 (11)	0.0065 (9)	−0.0050 (10)	−0.0043 (9)
N1	0.0703 (13)	0.0498 (11)	0.0602 (11)	0.0123 (10)	−0.0059 (10)	−0.0049 (10)
C4	0.0510 (12)	0.0535 (13)	0.0554 (12)	0.0021 (11)	0.0085 (11)	−0.0069 (11)
C9	0.0742 (16)	0.0538 (15)	0.0677 (15)	−0.0009 (13)	0.0077 (13)	−0.0080 (13)
C8	0.0857 (19)	0.0578 (16)	0.092 (2)	−0.0044 (15)	0.0162 (17)	−0.0191 (16)
C7	0.0745 (18)	0.084 (2)	0.086 (2)	−0.0121 (16)	0.0081 (17)	−0.0375 (18)
C6	0.0842 (19)	0.094 (2)	0.0657 (16)	0.0024 (17)	−0.0048 (15)	−0.0212 (16)
C5	0.0788 (18)	0.0612 (15)	0.0635 (15)	0.0029 (14)	−0.0022 (14)	−0.0095 (13)
C3	0.0532 (13)	0.0479 (12)	0.0537 (12)	0.0057 (10)	0.0044 (11)	−0.0028 (11)
C2	0.0460 (12)	0.0510 (13)	0.0489 (12)	0.0029 (10)	0.0024 (10)	−0.0046 (11)
C1	0.0671 (15)	0.0564 (14)	0.0604 (13)	0.0142 (13)	−0.0101 (12)	−0.0020 (13)
C10	0.0483 (13)	0.0470 (12)	0.0474 (11)	0.0000 (10)	0.0000 (10)	−0.0019 (10)
C11	0.0493 (13)	0.0632 (15)	0.0659 (14)	−0.0043 (11)	0.0001 (12)	0.0078 (13)
C12	0.0534 (14)	0.0782 (18)	0.0842 (17)	0.0007 (13)	−0.0122 (14)	0.0134 (16)
C13	0.078 (2)	0.0751 (19)	0.0796 (18)	−0.0042 (15)	−0.0217 (15)	0.0276 (15)
C14	0.0679 (19)	0.0822 (19)	0.0692 (16)	−0.0204 (14)	−0.0070 (13)	0.0220 (15)
C15	0.0503 (13)	0.0744 (17)	0.0584 (13)	−0.0038 (12)	−0.0010 (11)	0.0101 (13)
C16	0.0572 (13)	0.0442 (12)	0.0635 (13)	−0.0030 (11)	−0.0054 (12)	−0.0067 (11)
C17	0.0722 (16)	0.0558 (14)	0.0786 (16)	−0.0147 (13)	0.0122 (14)	−0.0168 (13)
C18	0.0615 (13)	0.0413 (11)	0.0515 (12)	−0.0040 (11)	−0.0003 (11)	−0.0033 (10)
C19	0.105 (2)	0.0441 (13)	0.0606 (14)	0.0086 (14)	0.0028 (14)	0.0024 (12)
C20	0.149 (3)	0.0466 (14)	0.0604 (14)	0.0039 (18)	0.0080 (18)	0.0056 (12)
C21	0.114 (2)	0.0464 (13)	0.0487 (12)	0.0029 (14)	0.0055 (15)	0.0012 (11)
C22	0.0658 (14)	0.0383 (11)	0.0503 (11)	−0.0059 (10)	0.0024 (11)	−0.0028 (10)
C23	0.0536 (12)	0.0425 (11)	0.0478 (11)	−0.0028 (10)	−0.0038 (10)	−0.0016 (9)
C24	0.0783 (17)	0.0618 (15)	0.0995 (19)	−0.0162 (14)	0.0253 (16)	−0.0194 (16)
C25	0.0696 (15)	0.0504 (13)	0.0511 (12)	0.0047 (12)	−0.0087 (12)	−0.0066 (11)
C26	0.0845 (17)	0.0498 (13)	0.0452 (11)	0.0063 (13)	−0.0036 (12)	0.0025 (11)
C27	0.0572 (14)	0.0446 (12)	0.0464 (11)	0.0039 (11)	−0.0035 (10)	−0.0008 (9)
C28	0.0533 (12)	0.0407 (11)	0.0464 (11)	−0.0019 (10)	−0.0020 (10)	−0.0028 (10)
C29	0.0677 (15)	0.0453 (12)	0.0496 (12)	−0.0027 (12)	0.0035 (12)	0.0012 (10)
C30	0.0654 (14)	0.0463 (12)	0.0483 (11)	−0.0017 (12)	0.0041 (11)	−0.0060 (10)
C31	0.0510 (12)	0.0412 (11)	0.0533 (12)	−0.0006 (10)	−0.0027 (11)	−0.0027 (10)
C32	0.0613 (14)	0.0428 (12)	0.0492 (12)	0.0009 (11)	−0.0021 (11)	0.0062 (10)
C33	0.091 (2)	0.0505 (15)	0.116 (2)	−0.0060 (15)	−0.0305 (18)	−0.0086 (16)
C34	0.080 (2)	0.0528 (15)	0.155 (3)	0.0104 (14)	−0.005 (2)	−0.0058 (18)
C35	0.0670 (15)	0.0422 (12)	0.0575 (12)	−0.0035 (12)	−0.0012 (12)	0.0020 (11)

Geometric parameters (Å, °)

N2—C1	1.356 (3)	C19—H19A	0.97
N2—C2	1.382 (3)	C19—H19B	0.97
N2—C16	1.461 (3)	C20—C21	1.526 (3)
N1—C1	1.303 (3)	C20—H20A	0.97
N1—C3	1.389 (3)	C20—H20B	0.97
C4—C5	1.386 (3)	C21—C22	1.533 (3)
C4—C9	1.384 (3)	C21—H21A	0.97
C4—C3	1.465 (3)	C21—H21B	0.97
C9—C8	1.380 (3)	C22—C24	1.537 (3)
C9—H9	0.93	C22—C28	1.539 (3)
C8—C7	1.365 (4)	C22—C23	1.556 (3)
C8—H8	0.93	C23—C25	1.532 (3)
C7—C6	1.380 (4)	C23—H23	0.98
C7—H7	0.93	C24—H24A	0.96
C6—C5	1.368 (3)	C24—H24B	0.96
C6—H6	0.93	C24—H24C	0.96
C5—H5	0.93	C25—C26	1.518 (3)
C3—C2	1.381 (3)	C25—H25A	0.97
C2—C10	1.474 (3)	C25—H25B	0.97
C1—H1	0.93	C26—C27	1.509 (3)
C10—C15	1.384 (3)	C26—H26A	0.97
C10—C11	1.392 (3)	C26—H26B	0.97
C11—C12	1.374 (3)	C27—C32	1.397 (3)
C11—H11	0.93	C27—C28	1.391 (3)
C12—C13	1.375 (3)	C28—C29	1.397 (3)
C12—H12	0.93	C29—C30	1.381 (3)
C13—C14	1.373 (4)	C29—H29	0.93
C13—H13	0.93	C30—C31	1.386 (3)
C14—C15	1.372 (3)	C30—H30	0.93
C14—H14	0.93	C31—C32	1.379 (3)
C15—H15	0.93	C31—C35	1.515 (3)
C16—C18	1.557 (3)	C32—H32	0.93
C16—H16A	0.97	C33—C35	1.512 (3)
C16—H16B	0.97	C33—H33A	0.96
C17—C18	1.523 (3)	C33—H33B	0.96
C17—H17A	0.96	C33—H33C	0.96
C17—H17B	0.96	C34—C35	1.510 (3)
C17—H17C	0.96	C34—H34A	0.96
C18—C19	1.536 (3)	C34—H34B	0.96
C18—C23	1.564 (3)	C34—H34C	0.96
C19—C20	1.521 (4)	C35—H35	0.98
C1—N2—C2	106.31 (18)	C19—C20—H20B	109.6
C1—N2—C16	126.93 (19)	C21—C20—H20B	109.6
C2—N2—C16	125.78 (18)	H20A—C20—H20B	108.1
C1—N1—C3	104.89 (19)	C20—C21—C22	112.3 (2)
C5—C4—C9	117.4 (2)	C20—C21—H21A	109.1

C5—C4—C3	123.0 (2)	C22—C21—H21A	109.1
C9—C4—C3	119.6 (2)	C20—C21—H21B	109.1
C8—C9—C4	121.3 (3)	C22—C21—H21B	109.1
C8—C9—H9	119.3	H21A—C21—H21B	107.9
C4—C9—H9	119.3	C21—C22—C24	109.3 (2)
C7—C8—C9	120.5 (3)	C21—C22—C28	110.67 (18)
C7—C8—H8	119.8	C24—C22—C28	105.22 (18)
C9—C8—H8	119.8	C21—C22—C23	108.06 (18)
C8—C7—C6	118.8 (3)	C24—C22—C23	115.12 (19)
C8—C7—H7	120.6	C28—C22—C23	108.48 (17)
C6—C7—H7	120.6	C25—C23—C22	109.17 (17)
C5—C6—C7	120.9 (3)	C25—C23—C18	115.28 (17)
C5—C6—H6	119.6	C22—C23—C18	115.72 (17)
C7—C6—H6	119.6	C25—C23—H23	105.2
C6—C5—C4	121.1 (3)	C22—C23—H23	105.2
C6—C5—H5	119.4	C18—C23—H23	105.2
C4—C5—H5	119.4	C22—C24—H24A	109.5
C2—C3—N1	109.8 (2)	C22—C24—H24B	109.5
C2—C3—C4	130.3 (2)	H24A—C24—H24B	109.5
N1—C3—C4	119.89 (19)	C22—C24—H24C	109.5
N2—C2—C3	105.60 (19)	H24A—C24—H24C	109.5
N2—C2—C10	120.77 (19)	H24B—C24—H24C	109.5
C3—C2—C10	133.5 (2)	C26—C25—C23	109.12 (18)
N1—C1—N2	113.4 (2)	C26—C25—H25A	109.9
N1—C1—H1	123.3	C23—C25—H25A	109.9
N2—C1—H1	123.3	C26—C25—H25B	109.9
C15—C10—C11	118.5 (2)	C23—C25—H25B	109.9
C15—C10—C2	119.39 (19)	H25A—C25—H25B	108.3
C11—C10—C2	122.1 (2)	C27—C26—C25	113.43 (19)
C12—C11—C10	120.3 (2)	C27—C26—H26A	108.9
C12—C11—H11	119.9	C25—C26—H26A	108.9
C10—C11—H11	119.9	C27—C26—H26B	108.9
C13—C12—C11	120.7 (2)	C25—C26—H26B	108.9
C13—C12—H12	119.7	H26A—C26—H26B	107.7
C11—C12—H12	119.7	C32—C27—C28	119.45 (19)
C12—C13—C14	119.3 (2)	C32—C27—C26	118.86 (19)
C12—C13—H13	120.4	C28—C27—C26	121.67 (18)
C14—C13—H13	120.4	C29—C28—C27	117.81 (18)
C13—C14—C15	120.7 (3)	C29—C28—C22	119.39 (18)
C13—C14—H14	119.7	C27—C28—C22	122.73 (18)
C15—C14—H14	119.7	C30—C29—C28	121.5 (2)
C14—C15—C10	120.6 (2)	C30—C29—H29	119.2
C14—C15—H15	119.7	C28—C29—H29	119.2
C10—C15—H15	119.7	C29—C30—C31	121.28 (19)
N2—C16—C18	114.93 (18)	C29—C30—H30	119.4
N2—C16—H16A	108.5	C31—C30—H30	119.4
C18—C16—H16A	108.5	C32—C31—C30	117.01 (18)
N2—C16—H16B	108.5	C32—C31—C35	121.98 (19)
C18—C16—H16B	108.5	C30—C31—C35	121.02 (19)

H16A—C16—H16B	107.5	C31—C32—C27	122.9 (2)
C18—C17—H17A	109.5	C31—C32—H32	118.6
C18—C17—H17B	109.5	C27—C32—H32	118.6
H17A—C17—H17B	109.5	C35—C33—H33A	109.5
C18—C17—H17C	109.5	C35—C33—H33B	109.5
H17A—C17—H17C	109.5	H33A—C33—H33B	109.5
H17B—C17—H17C	109.5	C35—C33—H33C	109.5
C17—C18—C19	110.9 (2)	H33A—C33—H33C	109.5
C17—C18—C16	110.48 (18)	H33B—C33—H33C	109.5
C19—C18—C16	106.73 (18)	C35—C34—H34A	109.5
C17—C18—C23	113.54 (19)	C35—C34—H34B	109.5
C19—C18—C23	108.67 (17)	H34A—C34—H34B	109.5
C16—C18—C23	106.23 (17)	C35—C34—H34C	109.5
C20—C19—C18	115.3 (2)	H34A—C34—H34C	109.5
C20—C19—H19A	108.4	H34B—C34—H34C	109.5
C18—C19—H19A	108.4	C34—C35—C31	111.10 (19)
C20—C19—H19B	108.4	C34—C35—C33	111.2 (2)
C18—C19—H19B	108.4	C31—C35—C33	111.71 (19)
H19A—C19—H19B	107.5	C34—C35—H35	107.5
C19—C20—C21	110.3 (2)	C31—C35—H35	107.5
C19—C20—H20A	109.6	C33—C35—H35	107.5
C21—C20—H20A	109.6		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···N1	0.93	2.51	2.852 (3)	102
C17—H17A···Cg1	0.96	2.85	3.460 (2)	122
C12—H12···Cg2^{i}	0.93	2.65	3.570 (2)	170
C15—H15···Cg3^{ii}	0.93	2.81	3.685 (2)	157

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

Fig. 1

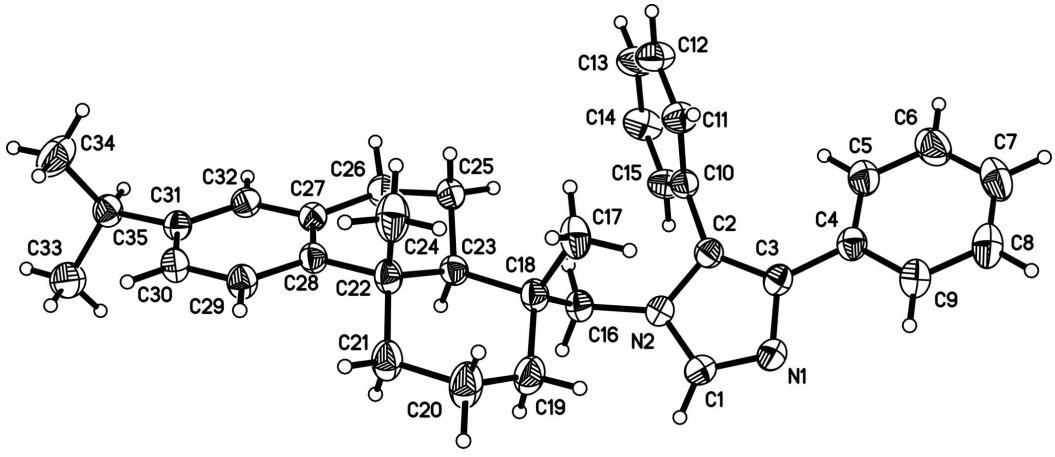
C12
C13
C14
C11
C6
C34
C5
C7
C15
C10
C32
C26
C25
C31
C27
C17
C2
C4
C35
C24
C23
C3
C8
C33
C18
C30
C28
C22
C29
C9
C16
N2
C21
N1
C20
C19
C1

Fig. 2