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Ethyl 1-benzyl-3-phenyl-1*H*-pyrazole-5-carboxylate

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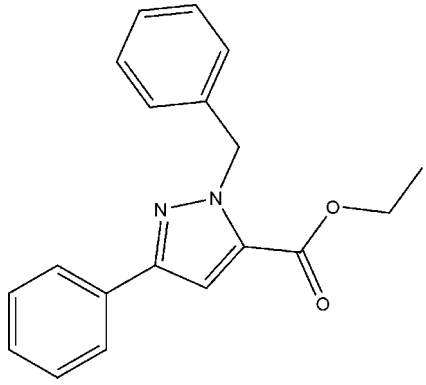
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.120; data-to-parameter ratio = 18.0.

In the title compound, $C_{19}H_{18}N_2O_2$, the dihedral angles made by the central pyrazole ring with the benzyl and phenyl rings are 87.00 (9) and 15.23 (9)°, respectively. There is a short intermolecular interaction between a C—H bond and the benzyl ring.

Related literature

For related literature, see: Altomare *et al.* (1999); Cottineau *et al.* (2006); Farrugia (1999); Qiao *et al.* (2007); Singh *et al.* (2006); Wei *et al.* (2006); Xia *et al.* (2007).



Experimental

Crystal data

$C_{19}H_{18}N_2O_2$
M_r = 306.35
Orthorhombic, *Pbca*
a = 10.7352 (2) Å
b = 14.9914 (2) Å
c = 20.4561 (3) Å
V = 3292.12 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.28 × 0.22 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.95, T_{max} = 0.98
14925 measured reflections
3753 independent reflections
1983 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.120
S = 0.98
3753 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
X—H···π ring interactions.

Values were calculated using *PLATON* (Spek, 2003). *Cg* is the centroid of the benzyl ring C14–C19.

X—H···*Cg*	X—H	H···*Cg*	X···*Cg*	X—H···*Cg*
C3—H3···*Cg*3^{i}	0.93	2.91	3.785 (2)	157

Symmetry code: (i) 1 − x, 1 − y, − z.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2070).

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supplementary materials

Acta Cryst. (2007). E**63**, o3298 [**doi:10.1107/S1600536807030139**]

Ethyl 1-benzyl-3-phenyl-1*H*-pyrazole-5-carboxylate

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Comment

The pyrazole unit is one of the core structures in a number of natural products. Pyrazole derivatives have a broad spectrum of biological activities being used as antidiabetic (Cottineau *et al.*, 2006), antitumour (Wei *et al.*, 2006), antithrombotic (Qiao *et al.*, 2007), gastric secretion stimulatory, antidepressant and against rheumatoid arthritis agents. Many of them are also currently being used as herbicides, fungicides, pesticides, insecticides and dyestuffs, in sunscreen materials and as analytical reagents (Singh *et al.*, 2006). We report here the crystal structure of the title compound $C_{19}H_{18}N_2O_2$ (I) (Fig. 1). The most relevant features in the structure are the dihedral angles made by the central pyrazole ring and the lateral benzyl and phenyl rings, which amount 87.00 (9)° and 15.23 (9)°, respectively. There is a short C3—H3···Cg^{i} intermolecular interaction in the structure, where (i): 1 − *x*,1 − *y*,-*z* and *Cg*: the centroid of the benzyl ring.

Experimental

The compound was synthesized according to the literature procedure (Xia *et al*., 2007). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a solution of the solid in ethyl acetate/petroleum ether (1:2 *v*/*v*) at room temperature over a period of 4 d.

Refinement

All H atoms were placed in geometrically calculated positions and refined using a riding model with C—H = 0.97%A (for CH_2 groups) and 0.96%A (for CH_3 groups), their isotropic displacement parameters were set to 1.2 times (1.5times for CH_3 groups) the equivalent displacement parameter of their parent atoms.

Figures

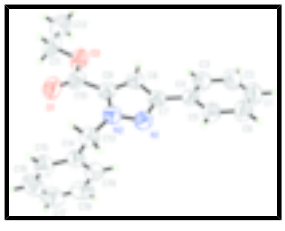


Fig. 1. The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level.

Ethyl 1-benzyl-3-phenyl-1*H*-pyrazole-5-carboxylate

Crystal data

$C_{19}H_{18}N_2O_2$	F_{000} = 1296
M_r = 306.35	D_x = 1.236 Mg m^{-3}

Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 2989 reflections
a = 10.7352 (2) Å	θ = 2.5–20.6º
b = 14.9914 (2) Å	μ = 0.08 mm^{-1}
c = 20.4561 (3) Å	*T* = 293 (2) K
V = 3292.12 (9) $Å^3$	Prism, colourless
Z = 8	0.28 × 0.22 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	3753 independent reflections
Radiation source: fine-focus sealed tube	1983 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
T = 293(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (APEX2; Bruker, 2005)	*h* = −12→13
T_{min} = 0.95, T_{max} = 0.98	*k* = −14→19
14925 measured reflections	*l* = −23→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H-atom parameters constrained
$wR(F^2)$ = 0.120	$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 0.4671P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.98	$(\Delta/\sigma)_{max} < 0.001$
3753 reflections	$\Delta\rho_{max}$ = 0.17 e $Å^{-3}$
209 parameters	$\Delta\rho_{min}$ = −0.16 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}
C1	0.4305 (3)	0.23696 (14)	0.25853 (11)	0.0897 (7)
H1	0.4039	0.2536	0.2170	0.108*
C2	0.3550 (2)	0.18657 (14)	0.29793 (11)	0.0831 (6)
H2	0.2768	0.1692	0.2830	0.100*
C3	0.39371 (19)	0.16145 (12)	0.35920 (10)	0.0692 (5)
H3	0.3415	0.1272	0.3854	0.083*
C4	0.50986 (17)	0.18666 (10)	0.38243 (9)	0.0579 (4)
C5	0.5860 (2)	0.23772 (12)	0.34255 (10)	0.0745 (5)
H5	0.6642	0.2552	0.3572	0.089*
C6	0.5459 (2)	0.26281 (14)	0.28082 (11)	0.0893 (7)
H6	0.5972	0.2973	0.2543	0.107*
C7	0.55031 (16)	0.16023 (10)	0.44805 (8)	0.0546 (4)
C8	0.47946 (16)	0.12737 (11)	0.49970 (8)	0.0578 (4)
H8	0.3941	0.1167	0.4998	0.069*
C9	0.56075 (16)	0.11390 (10)	0.55025 (8)	0.0556 (4)
C10	0.5378 (2)	0.08303 (11)	0.61744 (9)	0.0628 (5)
C11	0.3818 (2)	0.02637 (14)	0.68818 (9)	0.0815 (6)
H11A	0.3969	0.0722	0.7207	0.098*
H11B	0.4288	−0.0264	0.7002	0.098*
C12	0.2485 (2)	0.00559 (17)	0.68466 (12)	0.1118 (8)
H12A	0.2037	0.0571	0.6696	0.168*
H12B	0.2189	−0.0110	0.7272	0.168*
H12C	0.2355	−0.0429	0.6548	0.168*
C13	0.79636 (15)	0.13233 (11)	0.56062 (9)	0.0628 (5)
H13A	0.7897	0.1571	0.6043	0.075*
H13B	0.8565	0.1678	0.5366	0.075*
C14	0.84326 (14)	0.03803 (11)	0.56537 (8)	0.0544 (4)
C15	0.89934 (18)	0.00852 (14)	0.62189 (10)	0.0741 (5)
H15	0.9054	0.0466	0.6577	0.089*
C16	0.9465 (2)	−0.07644 (17)	0.62605 (13)	0.0942 (7)
H16	0.9847	−0.0954	0.6644	0.113*
C17	0.9375 (2)	−0.13319 (15)	0.57405 (15)	0.0940 (7)
H17	0.9694	−0.1907	0.5770	0.113*
C18	0.88155 (19)	−0.10520 (14)	0.51756 (12)	0.0826 (6)
H18	0.8748	−0.1439	0.4822	0.099*
C19	0.83502 (16)	−0.01959 (12)	0.51301 (9)	0.0642 (5)
H19	0.7979	−0.0006	0.4744	0.077*
N1	0.67075 (13)	0.16654 (8)	0.46589 (7)	0.0592 (4)
N2	0.67539 (12)	0.13894 (8)	0.52832 (7)	0.0559 (4)
O1	0.61277 (14)	0.08151 (10)	0.66085 (6)	0.0862 (4)
O2	0.41949 (12)	0.05760 (9)	0.62380 (6)	0.0762 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.126 (2)	0.0814 (15)	0.0617 (14)	0.0286 (15)	−0.0070 (14)	−0.0002 (12)
C2	0.1004 (16)	0.0739 (13)	0.0749 (15)	0.0142 (12)	−0.0148 (13)	−0.0095 (12)
C3	0.0794 (13)	0.0613 (11)	0.0668 (13)	0.0047 (9)	−0.0005 (10)	−0.0043 (9)
C4	0.0701 (12)	0.0466 (9)	0.0570 (11)	0.0106 (9)	0.0082 (9)	−0.0004 (8)
C5	0.0825 (14)	0.0720 (12)	0.0691 (14)	0.0079 (10)	0.0102 (11)	0.0132 (10)
C6	0.1150 (19)	0.0806 (14)	0.0722 (15)	0.0160 (14)	0.0191 (14)	0.0187 (12)
C7	0.0592 (10)	0.0445 (9)	0.0600 (11)	0.0031 (7)	0.0060 (9)	−0.0019 (8)
C8	0.0552 (10)	0.0552 (10)	0.0630 (11)	−0.0004 (8)	0.0054 (9)	−0.0004 (8)
C9	0.0624 (11)	0.0462 (9)	0.0583 (11)	−0.0015 (8)	0.0062 (9)	−0.0035 (8)
C10	0.0771 (14)	0.0547 (10)	0.0566 (12)	0.0002 (9)	0.0061 (10)	−0.0069 (9)
C11	0.1074 (17)	0.0797 (13)	0.0574 (12)	−0.0056 (12)	0.0229 (11)	0.0042 (10)
C12	0.1035 (18)	0.138 (2)	0.0938 (18)	−0.0042 (16)	0.0361 (14)	0.0293 (15)
C13	0.0612 (11)	0.0553 (10)	0.0719 (13)	−0.0078 (8)	−0.0047 (9)	−0.0068 (9)
C14	0.0493 (9)	0.0546 (10)	0.0593 (11)	−0.0057 (8)	−0.0004 (8)	−0.0017 (8)
C15	0.0749 (13)	0.0791 (13)	0.0683 (13)	−0.0028 (11)	−0.0092 (10)	0.0024 (10)
C16	0.0843 (16)	0.0905 (17)	0.108 (2)	0.0080 (13)	−0.0148 (14)	0.0280 (15)
C17	0.0756 (15)	0.0621 (13)	0.144 (2)	0.0085 (11)	0.0097 (15)	0.0158 (16)
C18	0.0742 (14)	0.0639 (13)	0.1098 (18)	−0.0034 (10)	0.0115 (13)	−0.0203 (12)
C19	0.0626 (11)	0.0598 (12)	0.0703 (13)	−0.0057 (9)	−0.0001 (9)	−0.0082 (9)
N1	0.0664 (10)	0.0493 (8)	0.0619 (10)	0.0002 (7)	0.0075 (7)	0.0044 (7)
N2	0.0578 (9)	0.0475 (8)	0.0623 (9)	−0.0007 (6)	0.0007 (7)	−0.0017 (7)
O1	0.0895 (10)	0.1121 (11)	0.0569 (9)	−0.0023 (8)	−0.0046 (8)	−0.0046 (8)
O2	0.0781 (9)	0.0909 (9)	0.0597 (9)	−0.0135 (7)	0.0103 (7)	0.0107 (7)

Geometric parameters (Å, °)

C1—C2	1.370 (3)	C11—H11A	0.9700
C1—C6	1.375 (3)	C11—H11B	0.9700
C1—H1	0.9300	C12—H12A	0.9600
C2—C3	1.373 (3)	C12—H12B	0.9600
C2—H2	0.9300	C12—H12C	0.9600
C3—C4	1.387 (2)	C13—N2	1.460 (2)
C3—H3	0.9300	C13—C14	1.504 (2)
C4—C5	1.385 (2)	C13—H13A	0.9700
C4—C7	1.465 (2)	C13—H13B	0.9700
C5—C6	1.386 (3)	C14—C15	1.376 (2)
C5—H5	0.9300	C14—C19	1.379 (2)
C6—H6	0.9300	C15—C16	1.373 (3)
C7—N1	1.347 (2)	C15—H15	0.9300
C7—C8	1.392 (2)	C16—C17	1.366 (3)
C8—C9	1.368 (2)	C16—H16	0.9300
C8—H8	0.9300	C17—C18	1.368 (3)
C9—N2	1.363 (2)	C17—H17	0.9300
C9—C10	1.471 (2)	C18—C19	1.380 (3)
C10—O1	1.198 (2)	C18—H18	0.9300

C10—O2	1.333 (2)	C19—H19	0.9300
C11—O2	1.455 (2)	N1—N2	1.3433 (19)
C11—C12	1.467 (3)		
C2—C1—C6	119.5 (2)	C11—C12—H12A	109.5
C2—C1—H1	120.2	C11—C12—H12B	109.5
C6—C1—H1	120.2	H12A—C12—H12B	109.5
C1—C2—C3	120.6 (2)	C11—C12—H12C	109.5
C1—C2—H2	119.7	H12A—C12—H12C	109.5
C3—C2—H2	119.7	H12B—C12—H12C	109.5
C2—C3—C4	120.67 (19)	N2—C13—C14	113.00 (13)
C2—C3—H3	119.7	N2—C13—H13A	109.0
C4—C3—H3	119.7	C14—C13—H13A	109.0
C3—C4—C5	118.63 (18)	N2—C13—H13B	109.0
C3—C4—C7	120.43 (16)	C14—C13—H13B	109.0
C5—C4—C7	120.94 (17)	H13A—C13—H13B	107.8
C4—C5—C6	120.2 (2)	C15—C14—C19	118.63 (17)
C4—C5—H5	119.9	C15—C14—C13	120.18 (16)
C6—C5—H5	119.9	C19—C14—C13	121.15 (16)
C1—C6—C5	120.3 (2)	C14—C15—C16	120.8 (2)
C1—C6—H6	119.8	C14—C15—H15	119.6
C5—C6—H6	119.8	C16—C15—H15	119.6
N1—C7—C8	110.11 (15)	C17—C16—C15	120.2 (2)
N1—C7—C4	120.91 (15)	C17—C16—H16	119.9
C8—C7—C4	128.98 (16)	C15—C16—H16	119.9
C9—C8—C7	106.11 (16)	C18—C17—C16	119.8 (2)
C9—C8—H8	126.9	C18—C17—H17	120.1
C7—C8—H8	126.9	C16—C17—H17	120.1
N2—C9—C8	106.65 (15)	C17—C18—C19	120.1 (2)
N2—C9—C10	123.05 (16)	C17—C18—H18	120.0
C8—C9—C10	130.24 (17)	C19—C18—H18	120.0
O1—C10—O2	124.21 (18)	C14—C19—C18	120.45 (19)
O1—C10—C9	125.87 (18)	C14—C19—H19	119.8
O2—C10—C9	109.91 (17)	C18—C19—H19	119.8
O2—C11—C12	107.16 (18)	C7—N1—N2	105.76 (13)
O2—C11—H11A	110.3	N1—N2—C9	111.37 (13)
C12—C11—H11A	110.3	N1—N2—C13	118.95 (13)
O2—C11—H11B	110.3	C9—N2—C13	129.45 (15)
C12—C11—H11B	110.3	C10—O2—C11	116.43 (16)
H11A—C11—H11B	108.5		
C6—C1—C2—C3	−0.3 (3)	C19—C14—C15—C16	0.2 (3)
C1—C2—C3—C4	0.1 (3)	C13—C14—C15—C16	−177.69 (17)
C2—C3—C4—C5	0.0 (3)	C14—C15—C16—C17	−0.4 (3)
C2—C3—C4—C7	179.54 (16)	C15—C16—C17—C18	0.1 (3)
C3—C4—C5—C6	0.1 (3)	C16—C17—C18—C19	0.5 (3)
C7—C4—C5—C6	−179.44 (17)	C15—C14—C19—C18	0.4 (3)
C2—C1—C6—C5	0.4 (3)	C13—C14—C19—C18	178.24 (16)
C4—C5—C6—C1	−0.3 (3)	C17—C18—C19—C14	−0.7 (3)
C3—C4—C7—N1	165.11 (15)	C8—C7—N1—N2	−0.70 (17)

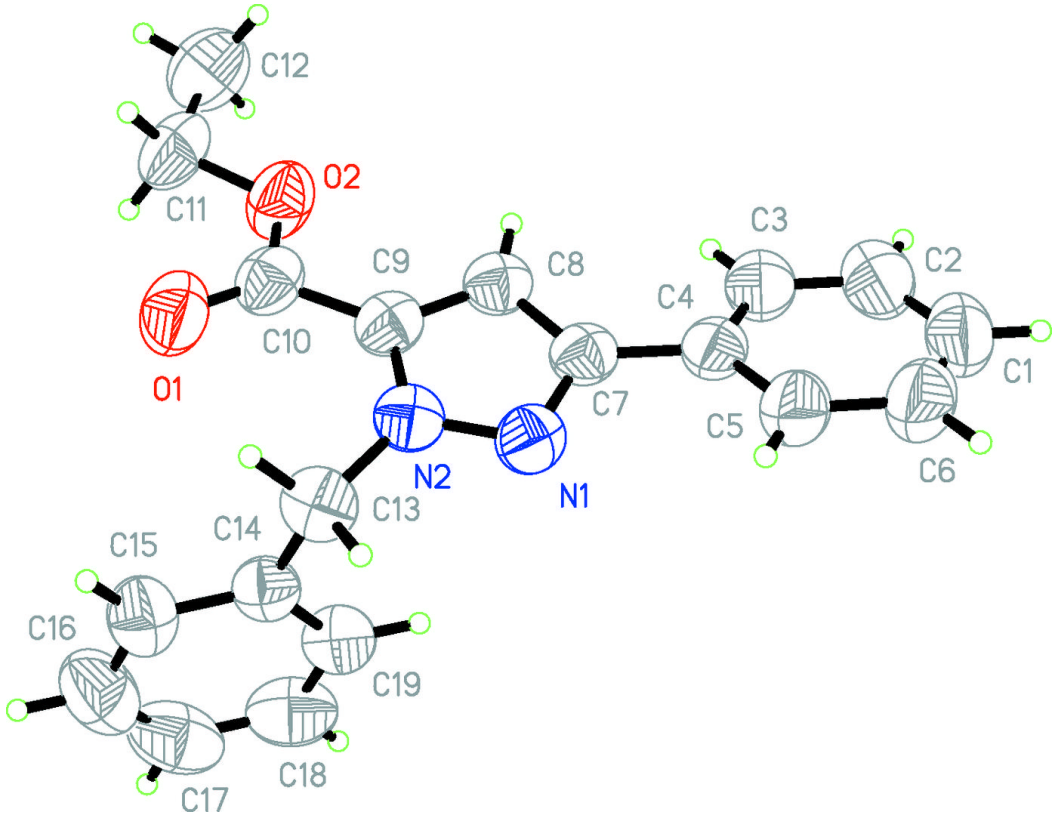
C5—C4—C7—N1	−15.4 (2)	C4—C7—N1—N2	178.93 (13)
C3—C4—C7—C8	−15.3 (2)	C7—N1—N2—C9	0.95 (17)
C5—C4—C7—C8	164.16 (17)	C7—N1—N2—C13	175.92 (13)
N1—C7—C8—C9	0.20 (18)	C8—C9—N2—N1	−0.84 (17)
C4—C7—C8—C9	−179.39 (15)	C10—C9—N2—N1	−178.36 (14)
C7—C8—C9—N2	0.37 (17)	C8—C9—N2—C13	−175.13 (14)
C7—C8—C9—C10	177.64 (16)	C10—C9—N2—C13	7.4 (2)
N2—C9—C10—O1	4.9 (3)	C14—C13—N2—N1	−102.49 (17)
C8—C9—C10—O1	−171.99 (18)	C14—C13—N2—C9	71.4 (2)
N2—C9—C10—O2	−175.95 (14)	O1—C10—O2—C11	0.0 (3)
C8—C9—C10—O2	7.2 (2)	C9—C10—O2—C11	−179.15 (14)
N2—C13—C14—C15	−138.32 (16)	C12—C11—O2—C10	177.76 (17)
N2—C13—C14—C19	43.9 (2)		

X—H···π ring interactions

X—H···*Cg*	*X*—H	H···*Cg*	*X*···*Cg*	*X*—H···*Cg*
C3—H3···*Cg*3^{i}	0.93	2.91	3.785 (2)	157

Symmetry code: (i) 1 − *x*, 1 − *y*, −*z*. Values were calculated by *PLATON* (Spek, 2003). *Cg* is the centroid of the benzyl ring C14–C19.

Fig. 1


C12
O2
C11
C9
C8
C3
C2
C4
C10
O1
C7
C1
C5
C6
N2
N1
C13
C14
C15
C16
C19
C18
C17