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(*S*)-*N*-(1-Benzyl-2-hydroxyethyl)benzamide

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.089
Data-to-parameter ratio = 7.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Colorless crystals of the title compound, $C_{16}H_{17}NO_2$, have been obtained by the reaction of benzoyl chloride and (*S*)-2-amino-3-phenylpropan-1-ol. The crystal packing is stabilized by O—H···O and N—H···O intermolecular hydrogen-bonding interactions.

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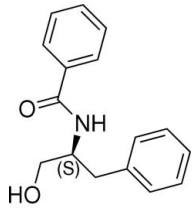
Comment

In the course of our studies directed to the development of new chiral ligands for asymmetric synthesis (Zeng, Liu, Cui *et al.*, 2002; Zeng, Liu, Mi *et al.*, 2002), we have synthesized a new and useful chiral ligand, namely (*S*)-*N*-(1-benzyl-2-hydroxyethyl)benzamide, (I), from the reaction of benzoyl chloride with (*S*)-2-amino-3-phenyl-propan-1-ol. An X-ray crystal structure determination of (I) was carried out in order to elucidate the structure and the results are presented here.0



(I)

Bond lengths and angles in (I) are in agreement with the values reported in the literature (Allen, 1987). The crystal packing is stabilized by strong O—H···O and N—H···O intermolecular hydrogen-bonding interactions (Table 2 and Fig. 2).

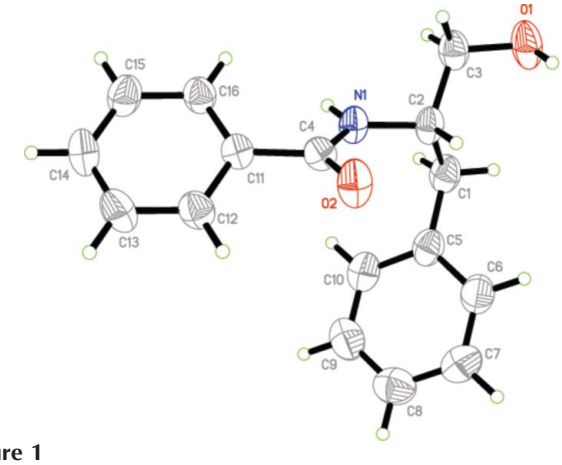


Figure 1
ORTEP3 (Farrugia, 1997) plot of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

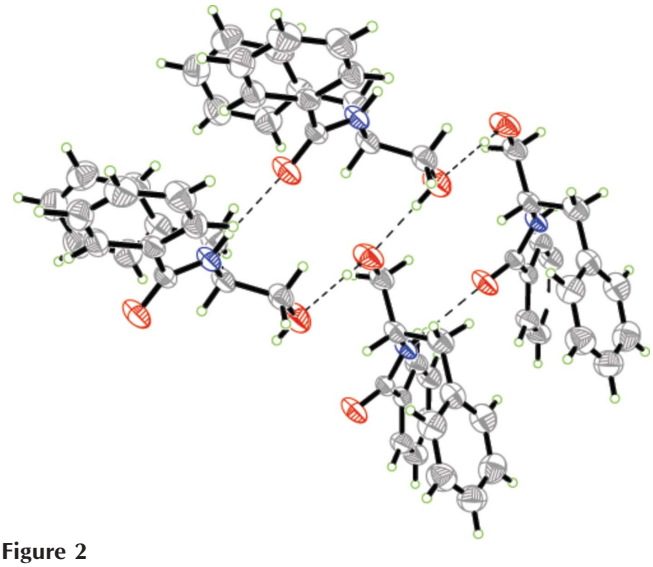


Figure 2
Packing diagram (Accelrys, 2001) of the title compound. Dashed lines indicate O—H···O and N—H···O hydrogen bonds.

Experimental

In an ice–water bath, a solution of (*S*)-2-amino-3-phenylpropan-1-ol (0.32 g, 2 mmol) and triethylamine (0.4 ml) in dichloromethane (10 ml) was added dropwise to a solution of benzoyl chloride (0.28 g, 2 mmol) in dichloromethane (25 ml) (Zeng, Liu, Cui *et al.*, 2002). The resulting solution was stirred at room temperature for 22 h, then water (10 ml) was added to the mixture in order to quench the reaction. The organic layer was separated and the aqueous layer was extracted with dichloromethane. The organic layers were combined, dried over anhydrous magnesium sulfate and filtered. The solvent was removed under reduced pressure, giving 0.43 g of a colorless liquid (yield 84.3%). Single crystals suitable for X-ray analysis were crystallized from the crude product by slow evaporation of an ethyl acetate–dichloromethane (2:1 *v*/*v*) solution.

Crystal data

$C_{16}H_{17}NO_2$
M_r = 255.31
Monoclinic, $P2_1$
a = 8.082 (3) Å
b = 5.0983 (16) Å
c = 16.034 (5) Å
β = 98.424 (5)°
V = 653.5 (4) Å^3
Z = 2
D_x = 1.297 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2983 reflections
θ = 2.6–28.1°
μ = 0.09 mm^{-1}
T = 273 (2) K
Irregular fragment, colorless
0.20 × 0.15 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.983, T_{max} = 0.992
4641 measured reflections
1286 independent reflections
1243 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 25.0°
$h = -9 \rightarrow 9$
$k = -6 \rightarrow 6$
$l = -19 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.089
S = 1.07
1286 reflections
172 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.0567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C4	1.325 (3)	C1—C2	1.511 (3)
N1—C2	1.434 (2)	C11—C4	1.478 (3)
O1—C3	1.403 (2)	C3—C2	1.502 (3)
C5—C1	1.484 (3)	O2—C4	1.217 (3)
C4—N1—C2	124.10 (17)	N1—C2—C3	108.42 (16)
C6—C5—C1	121.3 (2)	N1—C2—C1	110.92 (16)
C10—C5—C1	121.2 (2)	C3—C2—C1	112.14 (18)
C5—C1—C2	113.00 (18)	O2—C4—N1	122.96 (18)
C12—C11—C4	117.89 (19)	O2—C4—C11	120.55 (18)
C16—C11—C4	123.15 (18)	N1—C4—C11	116.49 (17)
O1—C3—C2	113.08 (18)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*C*···O1^{i}	0.82	1.90	2.7231 (13)	179
N1—H1*D*···O2^{ii}	0.86	2.14	2.907 (3)	148

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

The H atoms were positioned geometrically (C—H = 0.93, 0.98 or 0.97 Å for phenyl, tertiary or methylene H atoms, respectively, O—H = 0.82 Å and N—H = 0.86 Å) and were included in the refinement in the riding-model approximation. The isotropic displacement parameters were set at 1.2 times U_{eq} of the parent atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged; the absolute configuration was assigned on the basis of the known configuration of 2-amino-3-phenylpropan-1-ol.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *ViewerPro* (Accelrys, 2001); software used to prepare material for publication: *SHELXL97*.

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Zeng, Q., Liu, H., Mi, A. Q., Jiang, Y. Z., Li, X. S., Choi, M. C. & Chan, A. S. C. (2002). *Tetrahedron*, **58**, 8799–8803.

supporting information

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S1. Comment

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Bond lengths and angles in (I) are in agreement with the values reported in the literature (Allen, 2002). The crystal packing is stabilized by strong O—-H···O and N—H···O intermolecular hydrogen-bonding interactions (Table 2 and Fig. 2).

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In an ice–water bath, a solution of (*S*)-2-amino-3-phenylpropan-1-ol (0.32 g, 2 mmol) and triethylamine (0.4 ml) in dichloromethane (10 ml) was added dropwise to a solution of benzoyl chloride (0.28 g, 2 mmol) in dichloromethane (25 ml) (Zeng, Liu, Cui *et al.*, 2002). The resulting solution was stirred at room temperature for 22 h, then water (10 ml) was added to the mixture in order to quench the reaction. The organic layer was separated and the aqueous layer was extracted with dichloromethane. The organic layers were combined, dried over anhydrous magnesium sulfate and filtered. The solvent was removed under reduced pressure, giving 0.43 g of a colorless liquid (yield 84.3%). Single crystals suitable for X-ray analysis were crystallized from the crude product by slow evaporation of an ethyl acetate–dichloromethane (2:1 *v*/*v*) solution.

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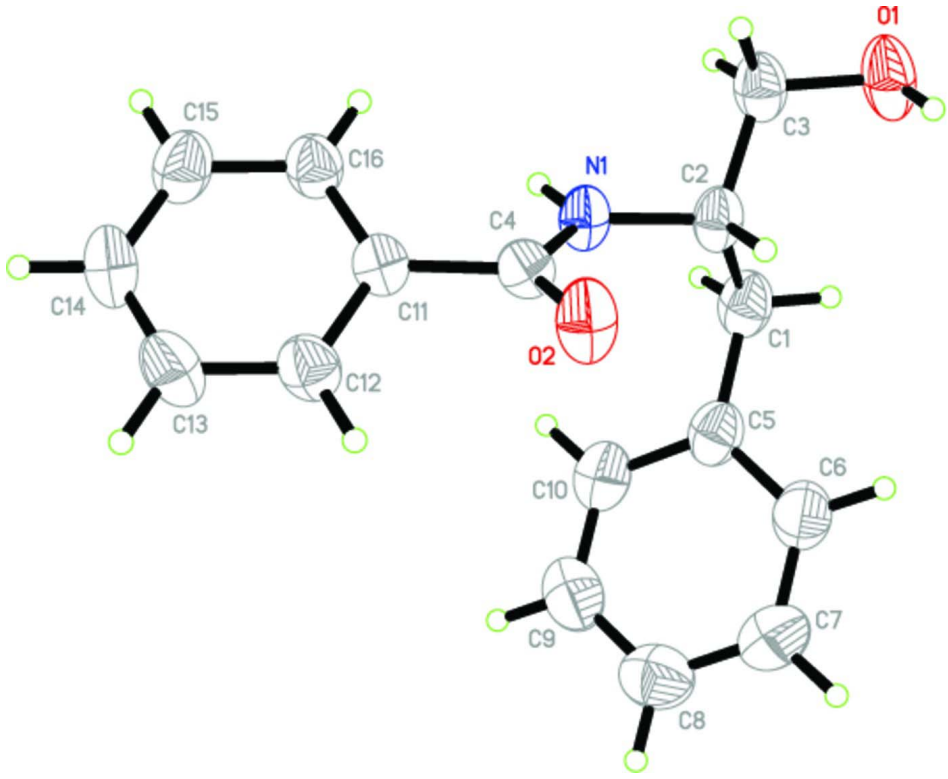
The H atoms were positioned geometrically (C—H = 0.93, 0.98 or 0.97 Å for phenyl, tertiary or methylene H atoms, respectively, O—H = 0.82 Å and N—H = 0.86 Å) and were included in the refinement in the riding-model approximation. The isotropic displacement parameters were set at 1.2 times U_{eq} of the parent atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged; the absolute configuration was assigned on the basis of the known configuration of 2-amino-3-phenylpropan-1-ol.



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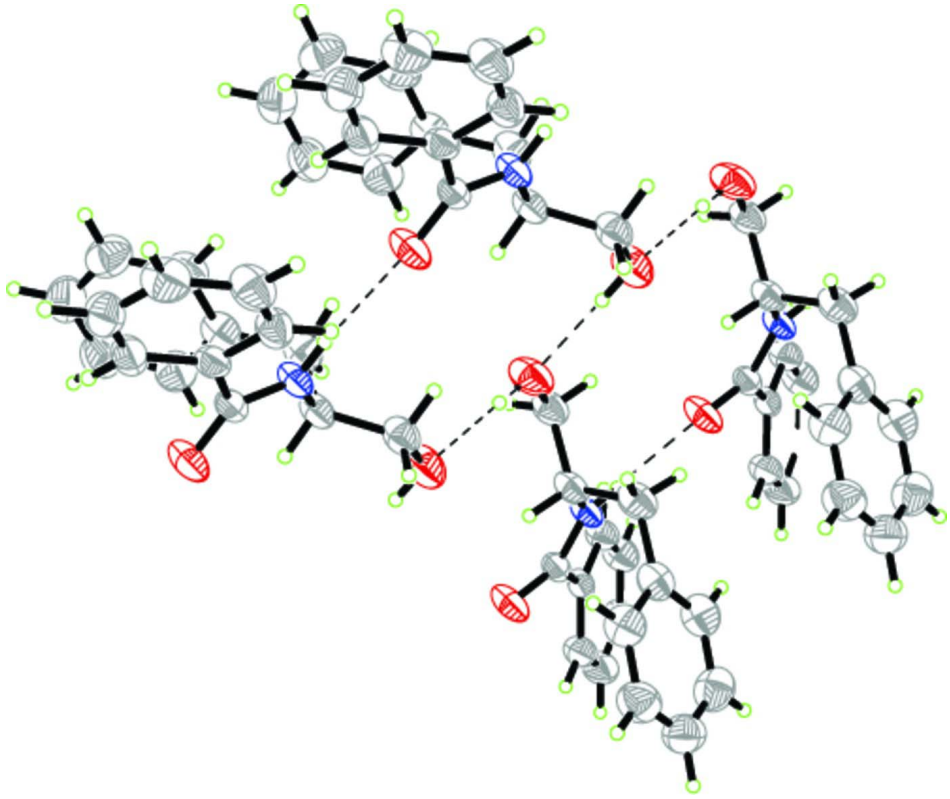

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Irregular fragment, colorless
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$h = -9\rightarrow9$
$k = -6\rightarrow6$
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Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.089$
$S = 1.07$
1286 reflections
172 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.0567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.3162 (2)	0.8638 (3)	0.25623 (10)	0.0363 (4)
H1D	0.3210	0.7143	0.2319	0.044*
O1	0.5104 (2)	0.7209 (3)	0.47135 (9)	0.0582 (5)
H1C	0.5054	0.8712	0.4890	0.087*
C9	−0.2092 (3)	1.0082 (6)	0.23908 (16)	0.0609 (7)
H9A	−0.2708	0.9741	0.1865	0.073*
C8	−0.2560 (3)	1.2081 (6)	0.28713 (17)	0.0606 (7)
H8A	−0.3481	1.3116	0.2673	0.073*
C14	0.2384 (3)	0.9824 (5)	−0.05569 (14)	0.0524 (6)
H14A	0.2245	0.9647	−0.1140	0.063*
C7	−0.1668 (3)	1.2544 (6)	0.36432 (17)	0.0597 (7)
H7A	−0.1988	1.3885	0.3979	0.072*
C6	−0.0312 (3)	1.1051 (6)	0.39251 (15)	0.0532 (6)
H6A	0.0289	1.1394	0.4454	0.064*
C5	0.0197 (3)	0.9046 (5)	0.34492 (13)	0.0446 (5)
C15	0.3353 (3)	0.8076 (5)	−0.00601 (14)	0.0503 (6)
H15A	0.3886	0.6726	−0.0307	0.060*
C13	0.1624 (3)	1.1815 (5)	−0.02042 (14)	0.0520 (6)
H13A	0.0961	1.3000	−0.0545	0.062*
C1	0.1734 (3)	0.7515 (5)	0.37435 (13)	0.0468 (6)
H1A	0.1586	0.5737	0.3530	0.056*
H1B	0.1892	0.7428	0.4354	0.056*
C10	−0.0732 (3)	0.8585 (6)	0.26740 (14)	0.0533 (6)
H10A	−0.0427	0.7231	0.2339	0.064*
C16	0.3545 (3)	0.8295 (5)	0.07955 (13)	0.0418 (5)

H16A	0.4186	0.7075	0.1132	0.050*
C11	0.2787 (2)	1.0333 (4)	0.11608 (12)	0.0340 (4)
C12	0.1829 (3)	1.2084 (5)	0.06504 (13)	0.0435 (5)
H12A	0.1314	1.3468	0.0890	0.052*
C3	0.4843 (3)	0.7233 (5)	0.38291 (13)	0.0441 (5)
H3A	0.4772	0.5440	0.3625	0.053*
H3B	0.5798	0.8050	0.3631	0.053*
O2	0.2971 (2)	1.2973 (3)	0.23677 (9)	0.0501 (5)
C2	0.3283 (3)	0.8676 (4)	0.34635 (11)	0.0382 (5)
H2A	0.3386	1.0503	0.3654	0.046*
C4	0.2982 (2)	1.0764 (4)	0.20817 (12)	0.0343 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0562 (10)	0.0215 (8)	0.0307 (8)	0.0010 (8)	0.0050 (7)	−0.0013 (7)
O1	0.0961 (12)	0.0390 (10)	0.0345 (8)	0.0057 (9)	−0.0075 (8)	0.0028 (7)
C9	0.0608 (15)	0.072 (2)	0.0481 (13)	−0.0070 (14)	0.0010 (11)	0.0024 (13)
C8	0.0548 (13)	0.0602 (17)	0.0672 (16)	0.0048 (13)	0.0103 (12)	0.0115 (14)
C14	0.0710 (15)	0.0544 (15)	0.0304 (10)	−0.0076 (13)	0.0026 (10)	0.0003 (11)
C7	0.0625 (14)	0.0534 (17)	0.0656 (15)	0.0073 (13)	0.0176 (12)	−0.0046 (13)
C6	0.0609 (13)	0.0553 (16)	0.0437 (12)	0.0008 (13)	0.0081 (10)	−0.0041 (12)
C5	0.0564 (12)	0.0412 (13)	0.0385 (10)	−0.0024 (11)	0.0142 (9)	0.0022 (10)
C15	0.0671 (14)	0.0434 (13)	0.0420 (11)	0.0028 (12)	0.0129 (10)	−0.0052 (11)
C13	0.0642 (14)	0.0452 (13)	0.0423 (12)	0.0021 (12)	−0.0067 (10)	0.0077 (11)
C1	0.0650 (14)	0.0404 (13)	0.0364 (11)	0.0018 (11)	0.0120 (10)	0.0053 (9)
C10	0.0642 (14)	0.0517 (15)	0.0451 (13)	−0.0036 (13)	0.0114 (10)	−0.0060 (12)
C16	0.0509 (11)	0.0368 (12)	0.0368 (10)	0.0030 (10)	0.0039 (8)	0.0012 (9)
C11	0.0400 (10)	0.0270 (11)	0.0343 (10)	−0.0050 (8)	0.0033 (8)	0.0014 (8)
C12	0.0527 (12)	0.0344 (12)	0.0418 (11)	0.0037 (10)	0.0008 (9)	0.0013 (10)
C3	0.0627 (12)	0.0345 (13)	0.0335 (10)	0.0016 (11)	0.0022 (9)	0.0019 (9)
O2	0.0859 (12)	0.0248 (8)	0.0381 (8)	0.0006 (8)	0.0036 (7)	−0.0006 (7)
C2	0.0583 (12)	0.0257 (10)	0.0304 (9)	0.0012 (10)	0.0055 (8)	−0.0014 (9)
C4	0.0404 (10)	0.0246 (10)	0.0368 (10)	−0.0005 (8)	0.0015 (8)	−0.0004 (9)

Geometric parameters (Å, º)

N1—C4	1.325 (3)	C15—C16	1.362 (3)
N1—C2	1.434 (2)	C15—H15A	0.9300
N1—H1D	0.8600	C13—C12	1.363 (3)
O1—C3	1.403 (2)	C13—H13A	0.9300
O1—H1C	0.8200	C1—C2	1.511 (3)
C9—C10	1.361 (4)	C1—H1A	0.9700
C9—C8	1.364 (4)	C1—H1B	0.9700
C9—H9A	0.9300	C10—H10A	0.9300
C8—C7	1.358 (4)	C16—C11	1.380 (3)
C8—H8A	0.9300	C16—H16A	0.9300
C14—C13	1.352 (4)	C11—C12	1.371 (3)

C14—C15	1.364 (4)	C11—C4	1.478 (3)
C14—H14A	0.9300	C12—H12A	0.9300
C7—C6	1.356 (4)	C3—C2	1.502 (3)
C7—H7A	0.9300	C3—H3A	0.9700
C6—C5	1.374 (4)	C3—H3B	0.9700
C6—H6A	0.9300	O2—C4	1.217 (3)
C5—C10	1.375 (3)	C2—H2A	0.9800
C5—C1	1.484 (3)		

C4—N1—C2	124.10 (17)	C5—C1—H1B	109.0
C4—N1—H1D	118.0	C2—C1—H1B	109.0
C2—N1—H1D	118.0	H1A—C1—H1B	107.8
C3—O1—H1C	109.5	C9—C10—C5	120.9 (3)
C10—C9—C8	120.5 (2)	C9—C10—H10A	119.6
C10—C9—H9A	119.7	C5—C10—H10A	119.6
C8—C9—H9A	119.7	C15—C16—C11	119.8 (2)
C7—C8—C9	119.4 (3)	C15—C16—H16A	120.1
C7—C8—H8A	120.3	C11—C16—H16A	120.1
C9—C8—H8A	120.3	C12—C11—C16	118.95 (19)
C13—C14—C15	120.2 (2)	C12—C11—C4	117.89 (19)
C13—C14—H14A	119.9	C16—C11—C4	123.15 (18)
C15—C14—H14A	119.9	C13—C12—C11	120.6 (2)
C6—C7—C8	120.1 (3)	C13—C12—H12A	119.7
C6—C7—H7A	120.0	C11—C12—H12A	119.7
C8—C7—H7A	120.0	O1—C3—C2	113.08 (18)
C7—C6—C5	121.7 (2)	O1—C3—H3A	109.0
C7—C6—H6A	119.2	C2—C3—H3A	109.0
C5—C6—H6A	119.2	O1—C3—H3B	109.0
C6—C5—C10	117.4 (2)	C2—C3—H3B	109.0
C6—C5—C1	121.3 (2)	H3A—C3—H3B	107.8
C10—C5—C1	121.2 (2)	N1—C2—C3	108.42 (16)
C16—C15—C14	120.3 (2)	N1—C2—C1	110.92 (16)
C16—C15—H15A	119.8	C3—C2—C1	112.14 (18)
C14—C15—H15A	119.8	N1—C2—H2A	108.4
C14—C13—C12	120.0 (2)	C3—C2—H2A	108.4
C14—C13—H13A	120.0	C1—C2—H2A	108.4
C12—C13—H13A	120.0	O2—C4—N1	122.96 (18)
C5—C1—C2	113.00 (18)	O2—C4—C11	120.55 (18)
C5—C1—H1A	109.0	N1—C4—C11	116.49 (17)
C2—C1—H1A	109.0		

C10—C9—C8—C7	−0.9 (4)	C14—C13—C12—C11	−0.8 (3)
C9—C8—C7—C6	0.9 (4)	C16—C11—C12—C13	0.2 (3)
C8—C7—C6—C5	−0.2 (4)	C4—C11—C12—C13	179.0 (2)
C7—C6—C5—C10	−0.6 (4)	C4—N1—C2—C3	−126.2 (2)
C7—C6—C5—C1	176.7 (2)	C4—N1—C2—C1	110.2 (2)
C13—C14—C15—C16	1.0 (4)	O1—C3—C2—N1	178.52 (18)
C15—C14—C13—C12	0.2 (4)	O1—C3—C2—C1	−58.7 (2)

C6—C5—C1—C2	−89.9 (3)	C5—C1—C2—N1	−63.5 (2)
C10—C5—C1—C2	87.3 (3)	C5—C1—C2—C3	175.08 (18)
C8—C9—C10—C5	0.1 (4)	C2—N1—C4—O2	3.1 (3)
C6—C5—C10—C9	0.6 (4)	C2—N1—C4—C11	−176.76 (16)
C1—C5—C10—C9	−176.7 (2)	C12—C11—C4—O2	−31.3 (3)
C14—C15—C16—C11	−1.5 (4)	C16—C11—C4—O2	147.4 (2)
C15—C16—C11—C12	0.9 (3)	C12—C11—C4—N1	148.6 (2)
C15—C16—C11—C4	−177.8 (2)	C16—C11—C4—N1	−32.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*C*···O1^{i}	0.82	1.90	2.7231 (13)	179
N1—H1*D*···O2^{ii}	0.86	2.14	2.907 (3)	149

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