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1,2-Diphenyl-2-[(1-phenylethyl)amino]-ethanol

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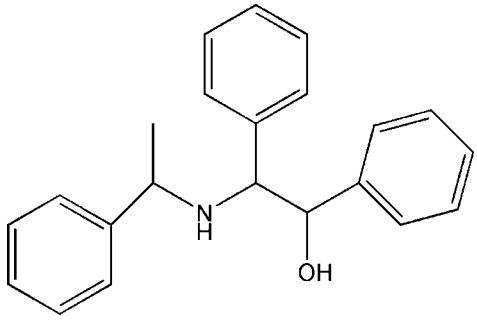
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.059; wR factor = 0.160; data-to-parameter ratio = 20.5.

In the molecule of the title compound, $C_{22}H_{23}NO$, there are two chiral atoms (R* for the C atom attached to the OH group and S* for the C atom attached to the phenyl ring). In the crystal, neighbouring molecules are connected into a chain along the b axis by N—H···O hydrogen bonds.

Related literature

For background to the synthesis of chiral organic compounds, see: Alcaide *et al.* (1981)



Experimental

Crystal data

$C_{22}H_{23}NO$
M_r = 317.41
Orthorhombic, $P2_12_12_1$
a = 6.307 (4) Å
b = 12.801 (7) Å
c = 22.490 (12) Å
V = 1815.7 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 K
0.50 × 0.29 × 0.21 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.966, T_{max} = 0.985
11619 measured reflections
4471 independent reflections
2660 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.160
S = 1.00
4471 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.90	2.04	2.908 (2)	160

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: DS2194).

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supplementary materials

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1,2-Diphenyl-2-[(1-phenylethyl)amino]ethanol

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Comment

In the molecule of chiral title compound 1,2-dipheny1-2-((1-phenylethyl)amino)ethanol,which derived from (R_p) phenylamine,accroding to the Cram rules and the molecular structure, two chiral atoms: C1(R*) and C8(S*) are observed. In the crystal structure, intermolecular N—H···O hydrogen bonds connect the same neighbour molecules into a one-dimensional chain,giving rise along b axis. The angle of C1-O1-H1,O1-N1-H1A, C8-N1-H1A and C15-N1-H1A are 109.47°, 160.4°, 108.11° and 108.19°. The torsion angle of O1-C1-C8-N1 is 56.46 (0.22)°. The arrangement between two neighbour molecules are same.

Experimental

Benzil (0.75 g, 3.6 mmol) was added to a stirred ethanol solution of *R*-phenylethylamine (0.87 g, 3.96 mmol) in a round-bottomed flask under a nitrogen atmosphere and heated until ethanol refluxed. This reaction took about 31 h. In the ice bath environment, sodium borohydride (0.27 g, 7.92 mmol) was added to the mixture in batches. Then drained ethanol, white solid was obtained. The crude product was extracted with dichloromethane three times. The organic phase was dried over anhydrous magnesium sulfate and then evaporated. The pure product was obtained after recrystallized with petroleum ether. Single crystal of the title compound suitable for *X*–ray diffraction were obtained by slow evaporation of petroleum ether solution of the title compound.

Refinement

All H atoms attached to C N O atoms were fixed geometrically and treated as riding with C—H = 0.93 - 0.98 Å, N—H = 0.90 Å, O—H = 0.820 Å with U_{iso}(H) = 1.5 U_{eq}(methyl) and U_{iso}(H) = 1.2 U_{eq}(C) for all other H atoms.In the absence of significant anomalous scattering, Friedel pairs were merged and the absolute structure was assigned arbitrarily.

Computing details

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

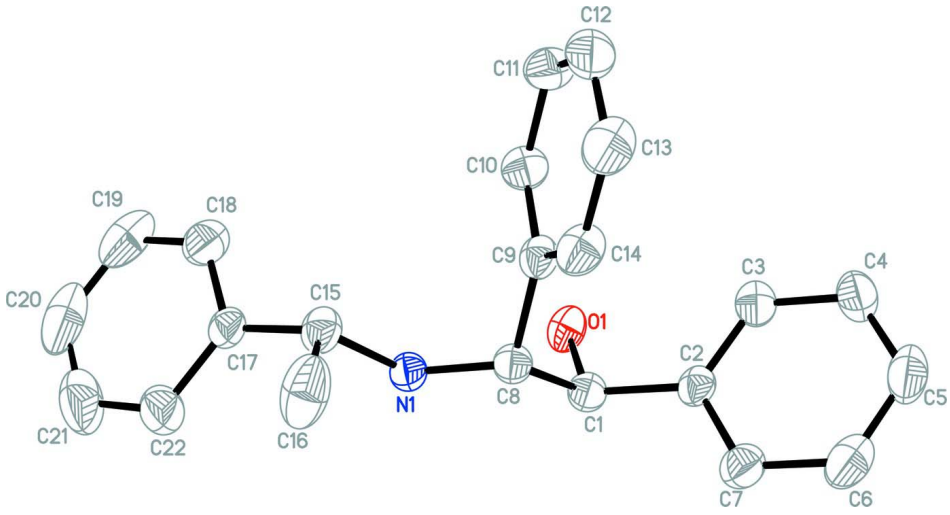

Figure 1

The molecular structure of the compound. Displacement ellipsoids are drawn at the 50% probability level.

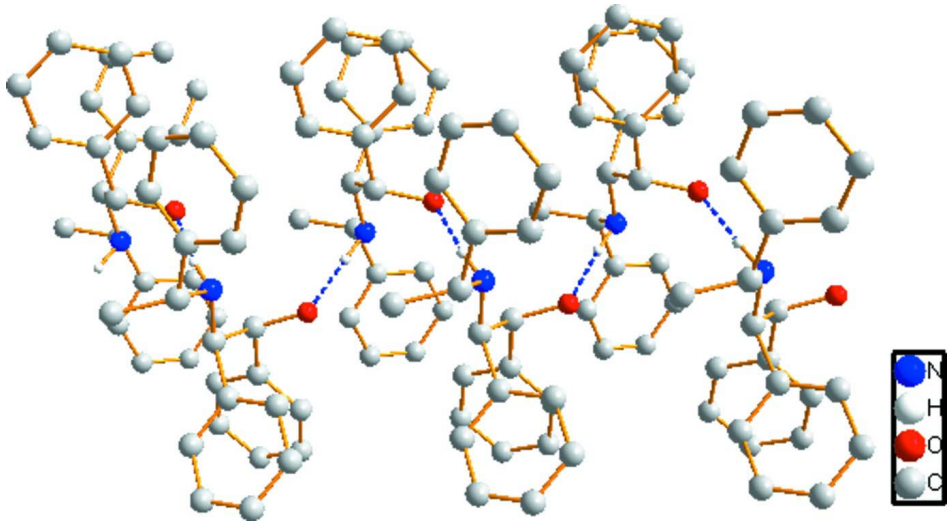

Figure 2

The one–dimensional chain, linked by N—H···O hydrogen bonds.

1,2-Diphenyl-2-[(1-phenylethyl)amino]ethanol

Crystal data

$C_{22}H_{23}NO$
$M_r = 317.41$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.307$ (4) Å
$b = 12.801$ (7) Å
$c = 22.490$ (12) Å
$V = 1815.7$ (17) Å^3
$Z = 4$

$F(000) = 680$
$D_x = 1.161$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3097 reflections
$\theta = 2.4$–$21.5°$
$\mu = 0.07$ mm^{-1}
$T = 298$ K
Needle, colourless
0.50 × 0.29 × 0.21 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.966, T_{max} = 0.985
11619 measured reflections
4471 independent reflections
2660 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 28.3°, θ_{min} = 2.4°
h = −8→8
k = −16→17
l = −29→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.160
S = 1.00
4471 reflections
218 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0777P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 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	0.1361 (3)	0.17083 (12)	0.92509 (8)	0.0483 (5)
H1A	0.2115	0.2278	0.9353	0.058*
O1	−0.1676 (3)	0.15306 (12)	1.01455 (7)	0.0583 (5)
H1	−0.1779	0.1634	0.9787	0.087*
C1	0.0499 (4)	0.13193 (16)	1.02933 (10)	0.0485 (5)
H1C	0.1173	0.1976	1.0414	0.058*
C2	0.0702 (4)	0.05485 (16)	1.07981 (10)	0.0470 (5)
C3	−0.0921 (5)	−0.01341 (18)	1.09504 (11)	0.0610 (7)
H3	−0.2206	−0.0099	1.0749	0.073*
C4	−0.0662 (6)	−0.0858 (2)	1.13920 (12)	0.0772 (8)
H4	−0.1770	−0.1307	1.1487	0.093*
C5	0.1249 (6)	−0.0928 (2)	1.17002 (12)	0.0811 (9)
H5	0.1427	−0.1424	1.1998	0.097*
C6	0.2869 (5)	−0.0255 (2)	1.15575 (12)	0.0775 (9)
H6	0.4153	−0.0295	1.1760	0.093*
C7	0.2594 (5)	0.04835 (19)	1.11128 (11)	0.0621 (7)
H7	0.3693	0.0942	1.1024	0.075*

C8	0.1619 (4)	0.09159 (15)	0.97284 (9)	0.0455 (5)
H8	0.3136	0.0881	0.9820	0.055*
C9	0.0926 (4)	−0.01903 (16)	0.95574 (9)	0.0478 (5)
C10	−0.1051 (4)	−0.03981 (18)	0.93349 (11)	0.0580 (6)
H10	−0.2015	0.0145	0.9285	0.070*
C11	−0.1636 (5)	−0.1413 (2)	0.91822 (12)	0.0695 (7)
H11	−0.2984	−0.1546	0.9032	0.083*
C12	−0.0218 (6)	−0.2215 (2)	0.92537 (13)	0.0787 (9)
H12	−0.0601	−0.2891	0.9148	0.094*
C13	0.1766 (6)	−0.2023 (2)	0.94810 (11)	0.0790 (9)
H13	0.2721	−0.2569	0.9535	0.095*
C14	0.2331 (5)	−0.10146 (18)	0.96280 (10)	0.0621 (7)
H14	0.3680	−0.0885	0.9777	0.075*
C15	0.2056 (4)	0.13711 (19)	0.86494 (10)	0.0557 (6)
H15	0.1306	0.0720	0.8558	0.067*
C16	0.4411 (5)	0.1131 (3)	0.86352 (13)	0.0943 (11)
H16A	0.5194	0.1738	0.8757	0.141*
H16B	0.4818	0.0939	0.8239	0.141*
H16C	0.4711	0.0563	0.8901	0.141*
C17	0.1383 (4)	0.21679 (17)	0.81918 (9)	0.0529 (6)
C18	−0.0514 (5)	0.2047 (2)	0.78936 (12)	0.0708 (7)
H18	−0.1364	0.1473	0.7982	0.085*
C19	−0.1189 (7)	0.2751 (3)	0.74684 (14)	0.1008 (12)
H19	−0.2490	0.2665	0.7280	0.121*
C20	0.0119 (11)	0.3595 (3)	0.73269 (16)	0.1194 (17)
H20	−0.0280	0.4064	0.7031	0.143*
C21	0.1949 (9)	0.3727 (3)	0.76188 (19)	0.1124 (15)
H21	0.2794	0.4302	0.7530	0.135*
C22	0.2613 (6)	0.3028 (2)	0.80495 (12)	0.0826 (9)
H22	0.3894	0.3136	0.8245	0.099*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0643 (13)	0.0404 (8)	0.0402 (9)	−0.0054 (8)	0.0012 (9)	−0.0029 (8)
O1	0.0641 (12)	0.0634 (9)	0.0473 (8)	0.0145 (8)	−0.0044 (8)	0.0033 (7)
C1	0.0546 (14)	0.0432 (11)	0.0478 (12)	0.0012 (10)	−0.0004 (11)	−0.0010 (10)
C2	0.0614 (14)	0.0433 (10)	0.0363 (10)	0.0026 (10)	0.0002 (11)	−0.0068 (9)
C3	0.0647 (16)	0.0626 (14)	0.0556 (14)	−0.0012 (13)	0.0005 (13)	0.0061 (12)
C4	0.106 (2)	0.0668 (16)	0.0587 (16)	−0.0146 (16)	0.0050 (18)	0.0115 (14)
C5	0.125 (3)	0.0666 (16)	0.0515 (15)	0.0088 (19)	−0.0084 (19)	0.0114 (13)
C6	0.094 (2)	0.0794 (17)	0.0587 (16)	0.0127 (18)	−0.0215 (17)	−0.0033 (15)
C7	0.0732 (18)	0.0578 (13)	0.0552 (14)	−0.0007 (13)	−0.0096 (14)	−0.0035 (12)
C8	0.0490 (12)	0.0431 (10)	0.0446 (11)	0.0008 (10)	0.0004 (10)	−0.0011 (9)
C9	0.0598 (15)	0.0451 (11)	0.0385 (11)	0.0054 (10)	0.0038 (11)	−0.0021 (9)
C10	0.0578 (16)	0.0548 (13)	0.0613 (14)	0.0041 (11)	−0.0007 (13)	−0.0060 (11)
C11	0.0788 (19)	0.0655 (15)	0.0643 (15)	−0.0126 (14)	−0.0010 (15)	−0.0126 (13)
C12	0.128 (3)	0.0460 (13)	0.0621 (16)	−0.0081 (16)	0.0044 (18)	−0.0076 (13)
C13	0.120 (3)	0.0516 (14)	0.0654 (16)	0.0206 (17)	−0.0123 (18)	−0.0053 (13)
C14	0.0788 (18)	0.0537 (12)	0.0540 (13)	0.0154 (12)	−0.0063 (14)	−0.0070 (11)

C15	0.0649 (16)	0.0579 (12)	0.0443 (12)	0.0038 (12)	0.0067 (11)	−0.0047 (11)
C16	0.077 (2)	0.144 (3)	0.0618 (18)	0.038 (2)	0.0151 (16)	0.011 (2)
C17	0.0719 (17)	0.0502 (11)	0.0368 (11)	−0.0049 (12)	0.0050 (12)	−0.0075 (10)
C18	0.079 (2)	0.0720 (16)	0.0615 (15)	−0.0004 (15)	−0.0066 (15)	−0.0065 (15)
C19	0.130 (3)	0.107 (3)	0.0654 (19)	0.032 (2)	−0.031 (2)	−0.016 (2)
C20	0.214 (6)	0.091 (3)	0.053 (2)	0.040 (3)	0.006 (3)	0.0041 (19)
C21	0.183 (5)	0.0677 (19)	0.086 (2)	−0.012 (3)	0.035 (3)	0.0164 (19)
C22	0.116 (3)	0.0656 (15)	0.0658 (15)	−0.0227 (17)	0.0110 (17)	−0.0010 (14)

Geometric parameters (Å, º)

N1—C8	1.486 (3)	C11—C12	1.371 (4)
N1—C15	1.486 (3)	C11—H11	0.9300
N1—H1A	0.9000	C12—C13	1.374 (4)
O1—C1	1.437 (3)	C12—H12	0.9300
O1—H1	0.8200	C13—C14	1.380 (4)
C1—C2	1.510 (3)	C13—H13	0.9300
C1—C8	1.543 (3)	C14—H14	0.9300
C1—H1C	0.9800	C15—C17	1.510 (3)
C2—C3	1.389 (4)	C15—C16	1.517 (4)
C2—C7	1.390 (4)	C15—H15	0.9800
C3—C4	1.368 (3)	C16—H16A	0.9600
C3—H3	0.9300	C16—H16B	0.9600
C4—C5	1.393 (5)	C16—H16C	0.9600
C4—H4	0.9300	C17—C18	1.380 (4)
C5—C6	1.375 (4)	C17—C22	1.384 (4)
C5—H5	0.9300	C18—C19	1.382 (4)
C6—C7	1.387 (4)	C18—H18	0.9300
C6—H6	0.9300	C19—C20	1.396 (6)
C7—H7	0.9300	C19—H19	0.9300
C8—C9	1.531 (3)	C20—C21	1.339 (6)
C8—H8	0.9800	C20—H20	0.9300
C9—C10	1.370 (4)	C21—C22	1.384 (5)
C9—C14	1.387 (3)	C21—H21	0.9300
C10—C11	1.394 (4)	C22—H22	0.9300
C10—H10	0.9300		

C8—N1—C15	115.29 (17)	C12—C11—H11	120.1
C8—N1—H1A	108.1	C10—C11—H11	120.1
C15—N1—H1A	108.1	C11—C12—C13	120.3 (3)
C1—O1—H1	109.5	C11—C12—H12	119.9
O1—C1—C2	112.21 (19)	C13—C12—H12	119.9
O1—C1—C8	108.02 (18)	C12—C13—C14	119.4 (3)
C2—C1—C8	111.21 (17)	C12—C13—H13	120.3
O1—C1—H1C	108.4	C14—C13—H13	120.3
C2—C1—H1C	108.4	C13—C14—C9	121.3 (3)
C8—C1—H1C	108.4	C13—C14—H14	119.3
C3—C2—C7	118.0 (2)	C9—C14—H14	119.3
C3—C2—C1	122.3 (2)	N1—C15—C17	109.95 (18)
C7—C2—C1	119.7 (2)	N1—C15—C16	111.5 (2)

C4—C3—C2	121.1 (3)	C17—C15—C16	113.5 (2)
C4—C3—H3	119.4	N1—C15—H15	107.2
C2—C3—H3	119.4	C17—C15—H15	107.2
C3—C4—C5	120.5 (3)	C16—C15—H15	107.2
C3—C4—H4	119.7	C15—C16—H16A	109.5
C5—C4—H4	119.7	C15—C16—H16B	109.5
C6—C5—C4	119.1 (3)	H16A—C16—H16B	109.5
C6—C5—H5	120.5	C15—C16—H16C	109.5
C4—C5—H5	120.5	H16A—C16—H16C	109.5
C5—C6—C7	120.2 (3)	H16B—C16—H16C	109.5
C5—C6—H6	119.9	C18—C17—C22	117.6 (3)
C7—C6—H6	119.9	C18—C17—C15	119.9 (2)
C6—C7—C2	121.0 (3)	C22—C17—C15	122.5 (3)
C6—C7—H7	119.5	C17—C18—C19	122.0 (3)
C2—C7—H7	119.5	C17—C18—H18	119.0
N1—C8—C9	114.75 (17)	C19—C18—H18	119.0
N1—C8—C1	108.46 (16)	C18—C19—C20	118.8 (4)
C9—C8—C1	112.69 (18)	C18—C19—H19	120.6
N1—C8—H8	106.8	C20—C19—H19	120.6
C9—C8—H8	106.8	C21—C20—C19	119.7 (4)
C1—C8—H8	106.8	C21—C20—H20	120.2
C10—C9—C14	118.4 (2)	C19—C20—H20	120.2
C10—C9—C8	122.1 (2)	C20—C21—C22	121.5 (4)
C14—C9—C8	119.5 (2)	C20—C21—H21	119.2
C9—C10—C11	120.8 (2)	C22—C21—H21	119.2
C9—C10—H10	119.6	C21—C22—C17	120.4 (4)
C11—C10—H10	119.6	C21—C22—H22	119.8
C12—C11—C10	119.8 (3)	C17—C22—H22	119.8

O1—C1—C2—C3	21.1 (3)	C14—C9—C10—C11	−0.1 (4)
C8—C1—C2—C3	−100.0 (3)	C8—C9—C10—C11	179.9 (2)
O1—C1—C2—C7	−161.18 (19)	C9—C10—C11—C12	−0.1 (4)
C8—C1—C2—C7	77.7 (3)	C10—C11—C12—C13	0.7 (4)
C7—C2—C3—C4	−0.8 (3)	C11—C12—C13—C14	−1.0 (4)
C1—C2—C3—C4	177.0 (2)	C12—C13—C14—C9	0.8 (4)
C2—C3—C4—C5	−0.1 (4)	C10—C9—C14—C13	−0.2 (4)
C3—C4—C5—C6	0.4 (4)	C8—C9—C14—C13	179.8 (2)
C4—C5—C6—C7	0.1 (4)	C8—N1—C15—C17	170.64 (18)
C5—C6—C7—C2	−1.0 (4)	C8—N1—C15—C16	−62.6 (3)
C3—C2—C7—C6	1.3 (3)	N1—C15—C17—C18	−93.4 (2)
C1—C2—C7—C6	−176.5 (2)	C16—C15—C17—C18	140.9 (3)
C15—N1—C8—C9	−43.9 (3)	N1—C15—C17—C22	87.2 (3)
C15—N1—C8—C1	−170.87 (19)	C16—C15—C17—C22	−38.4 (3)
O1—C1—C8—N1	56.5 (2)	C22—C17—C18—C19	−0.2 (4)
C2—C1—C8—N1	−179.96 (17)	C15—C17—C18—C19	−179.5 (2)
O1—C1—C8—C9	−71.7 (2)	C17—C18—C19—C20	1.7 (5)
C2—C1—C8—C9	51.9 (3)	C18—C19—C20—C21	−2.5 (5)
N1—C8—C9—C10	−53.9 (3)	C19—C20—C21—C22	1.8 (6)
C1—C8—C9—C10	70.9 (3)	C20—C21—C22—C17	−0.2 (5)

N1—C8—C9—C14	126.1 (2)	C18—C17—C22—C21	−0.6 (4)
C1—C8—C9—C14	−109.1 (2)	C15—C17—C22—C21	178.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.90	2.04	2.908 (2)	160

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