organic compounds

3-(*tert*-Butyliminomethyl)-1,1′-binaphthol ethanol solvate

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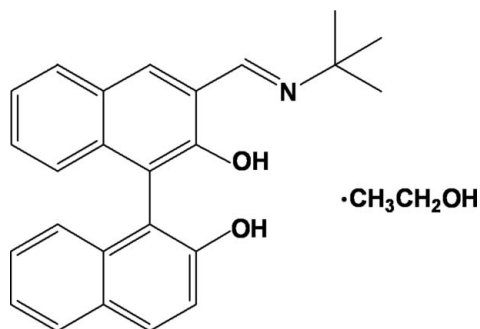Correspondence e-mail: sculiruixiang@163.com

The 1,1′-bi-2,2′-naphthol (BINOL) backbone of the title compound, $C_{25}H_{23}NO_2 \cdot C_2H_6O$, indicates that it has potential in asymmetric catalysis, with the two hydroxy and the imino groups providing sites for coordination with metal ions as an O/N heterotridentate ligand. There is an intramolecular O—H···N hydrogen bond which forms a ring, and intermolecular O—H···O hydrogen bonds to the ethanol solvent molecule, which link two ethanol molecules and two naphthol molecules around a centre of symmetry.

Related literature

For background on the application of salen complexes to asymmetric catalysis, see: Pu (1998). For details of the synthesis, see: Chin *et al.* (2004).

Experimental

Crystal data

$C_{25}H_{23}NO_2 \cdot C_2H_6O$	$\gamma = 81.66\ (3)°$
$M_r = 415.51$	$V = 1144.8\ (5)$ Å^3
Triclinic, $P\bar{1}$	$Z = 2$
$a = 10.538\ (2)$ Å	Mo $K\alpha$ radiation
$b = 10.883\ (2)$ Å	$\mu = 0.08$ mm^{-1}
$c = 11.628\ (2)$ Å	$T = 294\ (2)$ K
$\alpha = 74.27\ (3)°$	$0.38 \times 0.32 \times 0.23$ mm
$\beta = 63.15\ (3)°$	

Data collection

Enraf–Nonius CAD-4 diffractometer	1591 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{int} = 0.007$
4249 measured reflections	3 standard reflections
4243 independent reflections	every 300 reflections
	intensity decay: 0.9%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$	285 parameters
$wR(F^2) = 0.128$	H-atom parameters constrained
$S = 1.01$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
4243 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N	0.82	1.79	2.530 (3)	148
O2—H2···O3	0.82	1.87	2.684 (2)	170
O3—H3···O1^i	0.82	2.06	2.828 (2)	156

Symmetry code: (i) $-x + 1, -y + 1, -z$.

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

References

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Chin, J., Kim, D. C., Kim, H. J., Francis, B. P. & Kim, K. M. (2004). *Org. Lett.* **6**, 2591–2593.
Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
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supplementary materials

3-(*tert*-Butyliminomethyl)-1,1'-binaphthol ethanol solvate

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Comment

BINOL and its derivatives have been extensively used in chiral recognition and asymmetric catalysis (Pu, 1998). Herein we present the structure of the title compound, as a continuation of our previous studies.

As shown in Fig. 1, an intramolecular O—H···N hydrogen bond between the hydroxy and the imino groups forms a ring.

The molecules are connected by O—H···O hydrogen bonds to the ethanol, Fig. 2.

Experimental

The salen ligand, 3-((*p*-tolylimino)methyl)-di-1,1'-binaphthol was prepared by condensation of 3-carboxaldehyde-1,1'-binaphthol with *tert*-butylamine, which was prepared by reported methods (Chin *et al.*, 2004). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol–methylene chloride (1:5) solution of the compound.

Refinement

All the H atoms were placed in calculated positions and refined using the riding-model approximation.
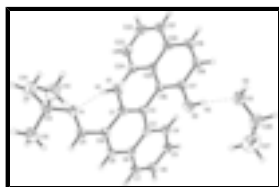
Figures

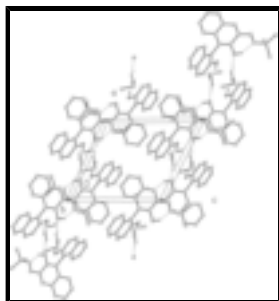Fig. 1. A perspective view of the title compound. Ellipsoids are drawn at the 30% probability level.

Fig. 2. A view down the *b* axis showing intermolecular hydrogen bonding in the crystal structure.

supplementary materials

3-(*tert*-Butyliminomethyl)-1,1'-binaphthol ethanol solvate

Crystal data

$C_{25}H_{23}NO_2 \cdot C_2H_6O$	$Z = 2$
$M_r = 415.51$	$F_{000} = 444$
Triclinic, $P\bar{1}$	$D_x = 1.205$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.538$ (2) Å	Cell parameters from 17 reflections
$b = 10.883$ (2) Å	$\theta = 4.6$–$7.4°$
$c = 11.628$ (2) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 74.27$ (3)°	$T = 294$ (2) K
$\beta = 63.15$ (3)°	Block, red
$\gamma = 81.66$ (3)°	$0.38 \times 0.32 \times 0.23$ mm
$V = 1144.8$ (5) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.007$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.5°$
Monochromator: graphite	$\theta_{min} = 1.9°$
$T = 294(2)$ K	$h = -12 \rightarrow 12$
$\omega/2\theta$ scans	$k = -5 \rightarrow 13$
Absorption correction: none	$l = -13 \rightarrow 14$
4249 measured reflections	3 standard reflections
4243 independent reflections	every 300 reflections
1591 reflections with $I > 2\sigma(I)$	intensity decay: 0.9%

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.060$	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.128$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
4243 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
285 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0106 (18)
Secondary atom site location: difference Fourier map	

Special details

Experimental. The data are rather weak, as indicated by the poor fraction of observed reflections. This could be caused by a combination of factors, including an old *x*-ray tube and a crystal consisting of C, H, O, N atoms only. Nevertheless, the structure is complete and the refinement was stable.

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*	$U_{iso}*/U_{eq}$
O1	0.23813 (14)	0.25295 (15)	0.00754 (14)	0.0714 (5)
H1	0.2308	0.2413	−0.0560	0.107*
O2	0.29138 (15)	0.51814 (14)	0.13021 (16)	0.0765 (5)
H2	0.3533	0.5671	0.1126	0.115*
N	0.11745 (18)	0.22122 (17)	−0.12695 (17)	0.0622 (6)
C1	0.1127 (2)	0.3002 (2)	0.0889 (2)	0.0531 (7)
C2	0.1015 (2)	0.32673 (19)	0.2017 (2)	0.0465 (6)
C3	−0.0321 (2)	0.36873 (19)	0.2912 (2)	0.0476 (6)
C4	−0.0533 (2)	0.38853 (19)	0.4145 (2)	0.0553 (7)
H4A	0.0235	0.3789	0.4355	0.066*
C5	−0.1833 (2)	0.4212 (2)	0.5020 (2)	0.0662 (7)
H5A	−0.1951	0.4316	0.5831	0.079*
C6	−0.3004 (2)	0.4397 (2)	0.4716 (2)	0.0749 (8)
H6A	−0.3892	0.4622	0.5323	0.090*
C7	−0.2834 (2)	0.4246 (2)	0.3531 (2)	0.0711 (8)
H7A	−0.3610	0.4389	0.3328	0.085*
C8	−0.1503 (2)	0.38757 (19)	0.2599 (2)	0.0517 (6)
C9	−0.1306 (2)	0.3642 (2)	0.1395 (2)	0.0584 (7)
H9A	−0.2062	0.3807	0.1164	0.070*
C10	−0.0050 (2)	0.3184 (2)	0.0554 (2)	0.0517 (6)
C11	0.0085 (2)	0.2836 (2)	−0.0631 (2)	0.0584 (7)
H11A	−0.0631	0.3073	−0.0914	0.070*
C12	0.1377 (3)	0.1757 (2)	−0.2426 (2)	0.0725 (8)
C13	0.2872 (3)	0.2117 (3)	−0.3442 (3)	0.1122 (12)
H13A	0.3527	0.1765	−0.3063	0.168*
H13B	0.2935	0.3030	−0.3707	0.168*
H13C	0.3106	0.1784	−0.4201	0.168*
C14	0.1281 (3)	0.0320 (2)	−0.1994 (3)	0.1163 (11)
H14A	0.0319	0.0092	−0.1381	0.175*

H14B	0.1900	−0.0020	−0.1573	0.175*
H14C	0.1563	−0.0025	−0.2755	0.175*
C15	0.0337 (3)	0.2332 (3)	−0.3008 (3)	0.1185 (11)
H15A	−0.0605	0.2055	−0.2381	0.178*
H15B	0.0600	0.2059	−0.3807	0.178*
H15C	0.0357	0.3247	−0.3205	0.178*
C16	0.2282 (2)	0.3038 (2)	0.2312 (2)	0.0469 (6)
C17	0.3201 (2)	0.3998 (2)	0.1930 (2)	0.0540 (6)
C18	0.4422 (2)	0.3778 (2)	0.2172 (2)	0.0638 (7)
H18A	0.5024	0.4444	0.1923	0.077*
C19	0.4707 (2)	0.2594 (2)	0.2766 (2)	0.0671 (7)
H19A	0.5528	0.2450	0.2900	0.080*
C20	0.3808 (2)	0.1575 (2)	0.3187 (2)	0.0552 (7)
C21	0.4097 (3)	0.0347 (2)	0.3816 (2)	0.0747 (8)
H21A	0.4917	0.0199	0.3950	0.090*
C22	0.3207 (3)	−0.0630 (3)	0.4234 (3)	0.0834 (9)
H22A	0.3411	−0.1437	0.4656	0.100*
C23	0.1980 (3)	−0.0410 (2)	0.4022 (2)	0.0796 (9)
H23A	0.1365	−0.1075	0.4311	0.096*
C24	0.1670 (2)	0.0769 (2)	0.3398 (2)	0.0613 (7)
H24A	0.0853	0.0893	0.3261	0.074*
C25	0.2570 (2)	0.1797 (2)	0.2961 (2)	0.0513 (6)
O3	0.47214 (17)	0.68639 (16)	0.10162 (18)	0.0984 (7)
H3	0.5567	0.6966	0.0511	0.148*
C26	0.4083 (3)	0.8033 (3)	0.1328 (3)	0.1012 (11)
H26A	0.4742	0.8488	0.1426	0.121*
H26B	0.3242	0.7867	0.2168	0.121*
C27	0.3677 (4)	0.8845 (3)	0.0288 (3)	0.1396 (15)
H27A	0.3169	0.9596	0.0569	0.209*
H27B	0.3081	0.8374	0.0143	0.209*
H27C	0.4519	0.9089	−0.0521	0.209*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0537 (8)	0.1142 (12)	0.0639 (9)	0.0069 (9)	−0.0302 (7)	−0.0440 (9)
O2	0.0724 (9)	0.0695 (11)	0.1014 (11)	−0.0121 (9)	−0.0543 (9)	−0.0057 (9)
N	0.0721 (11)	0.0697 (13)	0.0620 (11)	0.0085 (10)	−0.0401 (10)	−0.0271 (10)
C1	0.0419 (12)	0.0615 (15)	0.0629 (14)	0.0039 (11)	−0.0250 (11)	−0.0238 (12)
C2	0.0440 (11)	0.0521 (13)	0.0491 (13)	−0.0024 (11)	−0.0232 (10)	−0.0146 (11)
C3	0.0488 (12)	0.0479 (13)	0.0532 (13)	−0.0003 (11)	−0.0262 (10)	−0.0159 (11)
C4	0.0499 (12)	0.0612 (15)	0.0614 (14)	−0.0012 (12)	−0.0266 (11)	−0.0201 (12)
C5	0.0610 (14)	0.0778 (16)	0.0662 (15)	0.0030 (13)	−0.0247 (12)	−0.0344 (13)
C6	0.0507 (14)	0.0947 (18)	0.0915 (17)	0.0131 (13)	−0.0292 (13)	−0.0511 (15)
C7	0.0539 (13)	0.0862 (17)	0.0958 (17)	0.0199 (13)	−0.0435 (13)	−0.0474 (14)
C8	0.0480 (12)	0.0494 (14)	0.0668 (14)	0.0016 (11)	−0.0285 (11)	−0.0226 (11)
C9	0.0525 (12)	0.0641 (15)	0.0822 (15)	0.0089 (12)	−0.0454 (11)	−0.0295 (12)
C10	0.0479 (12)	0.0601 (15)	0.0580 (14)	0.0013 (11)	−0.0314 (11)	−0.0165 (11)

C11	0.0685 (13)	0.0624 (15)	0.0639 (14)	−0.0033 (12)	−0.0455 (12)	−0.0136 (12)
C12	0.0925 (17)	0.0819 (18)	0.0570 (14)	0.0030 (15)	−0.0403 (13)	−0.0261 (13)
C13	0.129 (2)	0.122 (2)	0.075 (2)	0.000 (2)	−0.0265 (19)	−0.0417 (18)
C14	0.192 (3)	0.077 (2)	0.103 (2)	−0.002 (2)	−0.082 (2)	−0.0257 (17)
C15	0.156 (2)	0.149 (3)	0.1035 (19)	0.034 (2)	−0.1005 (17)	−0.0517 (18)
C16	0.0381 (11)	0.0618 (14)	0.0489 (13)	0.0007 (11)	−0.0224 (10)	−0.0202 (11)
C17	0.0510 (12)	0.0637 (15)	0.0585 (14)	−0.0015 (12)	−0.0319 (11)	−0.0167 (12)
C18	0.0552 (13)	0.0801 (18)	0.0756 (15)	−0.0063 (13)	−0.0418 (12)	−0.0218 (13)
C19	0.0515 (13)	0.0961 (19)	0.0725 (15)	0.0053 (14)	−0.0393 (12)	−0.0301 (14)
C20	0.0502 (12)	0.0728 (16)	0.0509 (13)	0.0081 (12)	−0.0264 (11)	−0.0243 (12)
C21	0.0834 (16)	0.0813 (18)	0.0788 (16)	0.0238 (15)	−0.0507 (13)	−0.0339 (14)
C22	0.1048 (19)	0.0683 (18)	0.0862 (18)	0.0195 (16)	−0.0547 (16)	−0.0196 (15)
C23	0.0879 (18)	0.0596 (17)	0.0850 (19)	−0.0023 (15)	−0.0317 (16)	−0.0170 (15)
C24	0.0583 (13)	0.0584 (16)	0.0728 (16)	0.0023 (13)	−0.0336 (12)	−0.0164 (13)
C25	0.0471 (12)	0.0638 (15)	0.0496 (13)	0.0021 (12)	−0.0208 (11)	−0.0254 (12)
O3	0.0676 (11)	0.0905 (12)	0.1351 (15)	−0.0118 (10)	−0.0260 (11)	−0.0503 (11)
C26	0.0854 (19)	0.107 (2)	0.113 (2)	−0.0059 (18)	−0.0273 (18)	−0.0545 (19)
C27	0.171 (3)	0.126 (3)	0.111 (3)	0.006 (3)	−0.057 (2)	−0.022 (2)

Geometric parameters (Å, °)

O1—C1	1.358 (2)	C14—H14A	0.9600
O1—H1	0.8200	C14—H14B	0.9600
O2—C17	1.364 (3)	C14—H14C	0.9600
O2—H2	0.8200	C15—H15A	0.9600
N—C11	1.268 (3)	C15—H15B	0.9600
N—C12	1.473 (3)	C15—H15C	0.9600
C1—C2	1.368 (3)	C16—C17	1.371 (3)
C1—C10	1.433 (3)	C16—C25	1.421 (3)
C2—C3	1.422 (3)	C17—C18	1.411 (3)
C2—C16	1.494 (3)	C18—C19	1.350 (3)
C3—C4	1.419 (3)	C18—H18A	0.9300
C3—C8	1.422 (3)	C19—C20	1.400 (3)
C4—C5	1.354 (3)	C19—H19A	0.9300
C4—H4A	0.9300	C20—C21	1.402 (3)
C5—C6	1.404 (3)	C20—C25	1.419 (3)
C5—H5A	0.9300	C21—C22	1.358 (3)
C6—C7	1.361 (3)	C21—H21A	0.9300
C6—H6A	0.9300	C22—C23	1.398 (3)
C7—C8	1.416 (3)	C22—H22A	0.9300
C7—H7A	0.9300	C23—C24	1.366 (3)
C8—C9	1.408 (3)	C23—H23A	0.9300
C9—C10	1.364 (3)	C24—C25	1.404 (3)
C9—H9A	0.9300	C24—H24A	0.9300
C10—C11	1.468 (3)	O3—C26	1.409 (3)
C11—H11A	0.9300	O3—H3	0.8200
C12—C13	1.510 (3)	C26—C27	1.485 (4)
C12—C14	1.511 (3)	C26—H26A	0.9700
C12—C15	1.514 (3)	C26—H26B	0.9700

C13—H13A	0.9600	C27—H27A	0.9600
C13—H13B	0.9600	C27—H27B	0.9600
C13—H13C	0.9600	C27—H27C	0.9600
C1—O1—H1	109.5	H14A—C14—H14C	109.5
C17—O2—H2	109.5	H14B—C14—H14C	109.5
C11—N—C12	124.3 (2)	C12—C15—H15A	109.5
O1—C1—C2	119.2 (2)	C12—C15—H15B	109.5
O1—C1—C10	118.9 (2)	H15A—C15—H15B	109.5
C2—C1—C10	121.89 (19)	C12—C15—H15C	109.5
C1—C2—C3	119.3 (2)	H15A—C15—H15C	109.5
C1—C2—C16	118.98 (18)	H15B—C15—H15C	109.5
C3—C2—C16	121.6 (2)	C17—C16—C25	119.2 (2)
C4—C3—C8	118.28 (19)	C17—C16—C2	121.1 (2)
C4—C3—C2	122.0 (2)	C25—C16—C2	119.73 (19)
C8—C3—C2	119.7 (2)	O2—C17—C16	118.4 (2)
C5—C4—C3	121.1 (2)	O2—C17—C18	120.2 (2)
C5—C4—H4A	119.4	C16—C17—C18	121.3 (2)
C3—C4—H4A	119.4	C19—C18—C17	119.4 (2)
C4—C5—C6	120.8 (2)	C19—C18—H18A	120.3
C4—C5—H5A	119.6	C17—C18—H18A	120.3
C6—C5—H5A	119.6	C18—C19—C20	122.1 (2)
C7—C6—C5	119.8 (2)	C18—C19—H19A	119.0
C7—C6—H6A	120.1	C20—C19—H19A	119.0
C5—C6—H6A	120.1	C19—C20—C21	122.1 (2)
C6—C7—C8	121.4 (2)	C19—C20—C25	118.6 (2)
C6—C7—H7A	119.3	C21—C20—C25	119.3 (2)
C8—C7—H7A	119.3	C22—C21—C20	121.5 (3)
C9—C8—C7	122.9 (2)	C22—C21—H21A	119.2
C9—C8—C3	118.41 (19)	C20—C21—H21A	119.2
C7—C8—C3	118.6 (2)	C21—C22—C23	119.3 (3)
C10—C9—C8	122.6 (2)	C21—C22—H22A	120.4
C10—C9—H9A	118.7	C23—C22—H22A	120.4
C8—C9—H9A	118.7	C24—C23—C22	121.0 (3)
C9—C10—C1	118.0 (2)	C24—C23—H23A	119.5
C9—C10—C11	121.3 (2)	C22—C23—H23A	119.5
C1—C10—C11	120.62 (19)	C23—C24—C25	120.9 (2)
N—C11—C10	120.1 (2)	C23—C24—H24A	119.5
N—C11—H11A	120.0	C25—C24—H24A	119.5
C10—C11—H11A	120.0	C24—C25—C20	118.0 (2)
N—C12—C13	105.0 (2)	C24—C25—C16	122.6 (2)
N—C12—C14	107.0 (2)	C20—C25—C16	119.4 (2)
C13—C12—C14	109.5 (2)	C26—O3—H3	109.5
N—C12—C15	114.6 (2)	O3—C26—C27	111.7 (3)
C13—C12—C15	109.7 (2)	O3—C26—H26A	109.3
C14—C12—C15	110.8 (2)	C27—C26—H26A	109.3
C12—C13—H13A	109.5	O3—C26—H26B	109.3
C12—C13—H13B	109.5	C27—C26—H26B	109.3
H13A—C13—H13B	109.5	H26A—C26—H26B	107.9
C12—C13—H13C	109.5	C26—C27—H27A	109.5

H13A—C13—H13C	109.5	C26—C27—H27B	109.5
H13B—C13—H13C	109.5	H27A—C27—H27B	109.5
C12—C14—H14A	109.5	C26—C27—H27C	109.5
C12—C14—H14B	109.5	H27A—C27—H27C	109.5
H14A—C14—H14B	109.5	H27B—C27—H27C	109.5
C12—C14—H14C	109.5		
O1—C1—C2—C3	−176.13 (18)	C11—N—C12—C14	−110.2 (3)
C10—C1—C2—C3	2.5 (3)	C11—N—C12—C15	13.0 (3)
O1—C1—C2—C16	0.5 (3)	C1—C2—C16—C17	93.7 (3)
C10—C1—C2—C16	179.18 (19)	C3—C2—C16—C17	−89.7 (3)
C1—C2—C3—C4	175.2 (2)	C1—C2—C16—C25	−84.2 (3)
C16—C2—C3—C4	−1.4 (3)	C3—C2—C16—C25	92.3 (3)
C1—C2—C3—C8	−2.6 (3)	C25—C16—C17—O2	179.68 (19)
C16—C2—C3—C8	−179.11 (19)	C2—C16—C17—O2	1.7 (3)
C8—C3—C4—C5	1.7 (3)	C25—C16—C17—C18	−0.2 (3)
C2—C3—C4—C5	−176.0 (2)	C2—C16—C17—C18	−178.1 (2)
C3—C4—C5—C6	−1.6 (3)	O2—C17—C18—C19	−178.4 (2)
C4—C5—C6—C7	0.0 (4)	C16—C17—C18—C19	1.4 (3)
C5—C6—C7—C8	1.4 (4)	C17—C18—C19—C20	−1.8 (4)
C6—C7—C8—C9	176.4 (2)	C18—C19—C20—C21	−179.4 (2)
C6—C7—C8—C3	−1.3 (3)	C18—C19—C20—C25	1.0 (3)
C4—C3—C8—C9	−178.08 (19)	C19—C20—C21—C22	179.2 (2)
C2—C3—C8—C9	−0.3 (3)	C25—C20—C21—C22	−1.1 (4)
C4—C3—C8—C7	−0.2 (3)	C20—C21—C22—C23	0.5 (4)
C2—C3—C8—C7	177.57 (19)	C21—C22—C23—C24	0.3 (4)
C7—C8—C9—C10	−174.4 (2)	C22—C23—C24—C25	−0.6 (4)
C3—C8—C9—C10	3.3 (3)	C23—C24—C25—C20	0.0 (3)
C8—C9—C10—C1	−3.4 (3)	C23—C24—C25—C16	−179.8 (2)
C8—C9—C10—C11	174.17 (19)	C19—C20—C25—C24	−179.5 (2)
O1—C1—C10—C9	179.05 (19)	C21—C20—C25—C24	0.8 (3)
C2—C1—C10—C9	0.4 (3)	C19—C20—C25—C16	0.3 (3)
O1—C1—C10—C11	1.5 (3)	C21—C20—C25—C16	−179.4 (2)
C2—C1—C10—C11	−177.19 (19)	C17—C16—C25—C24	179.1 (2)
C12—N—C11—C10	176.56 (19)	C2—C16—C25—C24	−2.9 (3)
C9—C10—C11—N	−167.9 (2)	C17—C16—C25—C20	−0.7 (3)
C1—C10—C11—N	9.6 (3)	C2—C16—C25—C20	177.34 (19)
C11—N—C12—C13	133.5 (2)		

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N	0.82	1.79	2.530 (3)	148
O2—H2···O3	0.82	1.87	2.684 (2)	170
O3—H3···O1[i]	0.82	2.06	2.828 (2)	156

Symmetry codes: (i) −x+1, −y+1, −z.

Fig. 1

Fig. 2