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A diastereomer of methyl (1*R*,3′*S*)-1′,1″-dimethyl-2,2″-dioxo-2*H*-dispiro[acenaphthylene-1,2′-pyrrolidine-3′,3″-indoline]-4′-carboxylate

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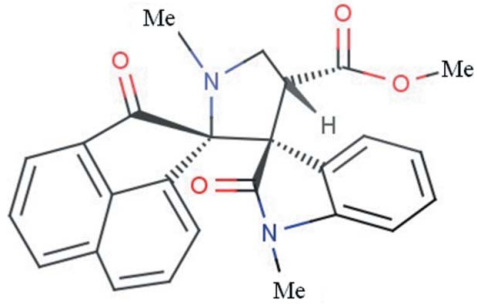
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.135; data-to-parameter ratio = 17.3.

In the title compound, $C_{26}H_{22}N_2O_4$, the central pyrrolidine ring adopts a twist conformation and the cyclopentane ring of the dihydroacenapthylene group adopts an envelope conformation with the spiro C atom as the flap. The naphthalene ring system of the dihydroacenaphthylene group forms dihedral angles of 83.4 (9) and 61.3 (7)°, respectively, with the mean planes of the pyrrolidine and indole rings. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds. The title compound is a diastereomer of a previously reported structure.

Related literature

For background literature and the previously reported diastereomer, see: Ganesh *et al.* (2013). For a related structure, see: Wei *et al.* (2012). For information on ring conformations, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{26}H_{22}N_2O_4$
M_r = 426.46
Orthorhombic, *Pbcn*
a = 27.2997 (15) Å
b = 9.7923 (6) Å
c = 15.8557 (10) Å
V = 4238.7 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.25 × 0.22 × 0.19 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.978, T_{max} = 0.983
23813 measured reflections
5039 independent reflections
3022 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.135
S = 1.02
5039 reflections
292 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···O3^{i}	0.96	2.48	3.299 (3)	143
C20—H20···O3^{ii}	0.93	2.59	3.403 (3)	146

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT*; data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

ASP thanks the University Grants Commission, India, for a Minor research Project.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6885).

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supporting information

Acta Cryst. (2013). E**69**, o441 [doi:10.1107/S1600536813004868]

A diastereomer of methyl (1*R*,3′*S*)-1′,1′′-dimethyl-2,2′′-dioxo-2*H*-dispiro[acenaphthylene-1,2′-pyrrolidine-3′,3′′-indoline]-4′-carboxylate

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S1. Comment

We have recently reported the structure of a diastereomer of the title compound (Ganesh *et al.*, 2013). Here we report the structural details of its diastereomer.

X–Ray analysis confirms the molecular structure and atom connectivity as illustrated in Fig. 1. The geometry of the acenaphthylene and pyrrolidine ring systems are comparable with the related structure (Wei *et al.*, 2012). The sum of the angles at N1 [339.5 (1)°] and N2 [359.8 (1)°] of the pyrrolidine rings are in accordance with sp^3 and sp^2 hybridization. The naphthalene ring system [C7–C16] of the dihydroacenaphthylene group forms dihedral angles of 83.4 (9) and 61.3 (7)° with the central pyrrolidine ring [N1/C2–C5] and the indole ring [N2/C4/C17–C23]. The central pyrrolidine also makes a dihedral angle of 87.6 (9)° with the indole which shows that these two rings are almost perpendicular with each other.

The pyrrolidine rings [N1/C2-C5] adopts a twist conformation, on C4 and C5 atoms with puckering parameters of q_2 = 0.470 (2) Å, φ = 128.1 (2) (Cremer & Pople, 1975). The cyclopentane ring [C5-C7/C12-C13] in the dihydroacenapthylene group adopts an envelope conformation [q_2 = 0.074 (9)(2) Å and φ = 173.3 (2)°], and with atom C5 deviating by 0.044 (2) Å from the least-squares plane passing through the remaining four atoms (C13/C12/C7/C6) of that ring. In the crystal, the molecules are linked by intermolecular C20-H20···O3 and C1-H1B···O3 hydrogen bonds Fig. 2.

S2. Experimental

A mixture of 1 eq of (*E*)-methyl 2-(1-methyl-2-oxoindolin-3-ylidene) acetate, 1 eq of isatin and 1.5 eq of acenaphthylene-1,2-dione were dissolved in acetonitrile. This reaction mixture was refluxed at 353K for 8 hours. The reaction mixture was monitored for completion by thin layer chromatography. Upon completion, the the product was dried and purified by coloumn chromatography using ethyl acetate and hexane (1:9) as an elutent to afforded pure dispiro oxindole. Yield (78%). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution of the title compound in ethyl acetate at room temperature.

S3. Refinement

All H atoms were fixed geometrically and allowed to ride on their parent C atoms, with C—H distances fixed in the range 0.93–0.98 Å with U_{iso}(H) = 1.5U_{eq}(C) for methyl H 1.2U_{eq}(C) for other H atoms.

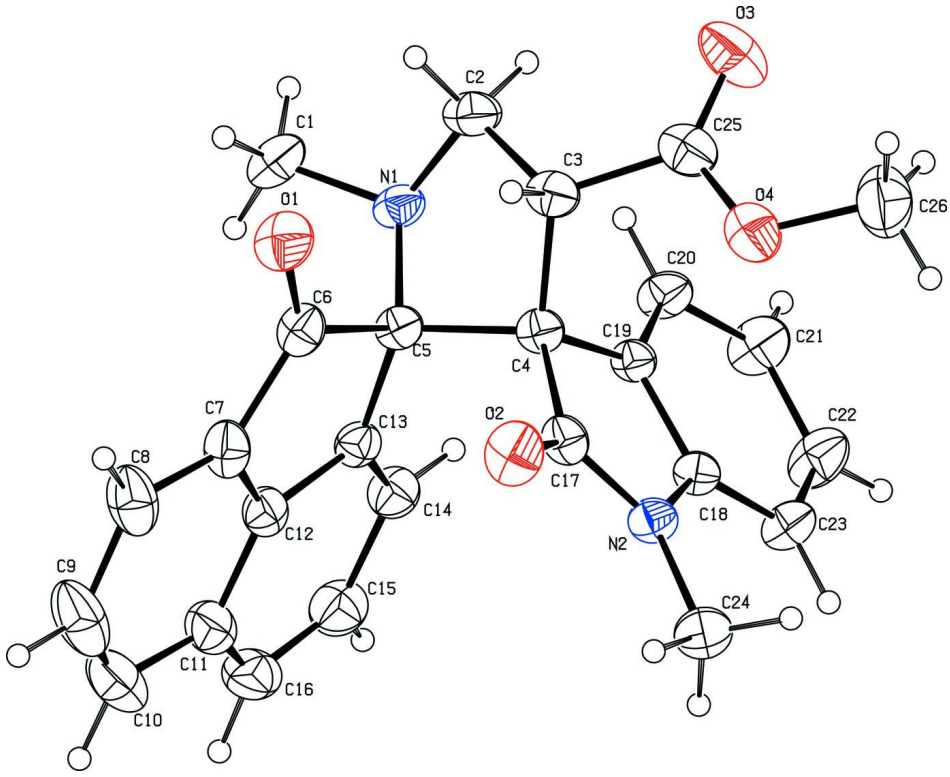

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as small spheres of arbitrary radius.

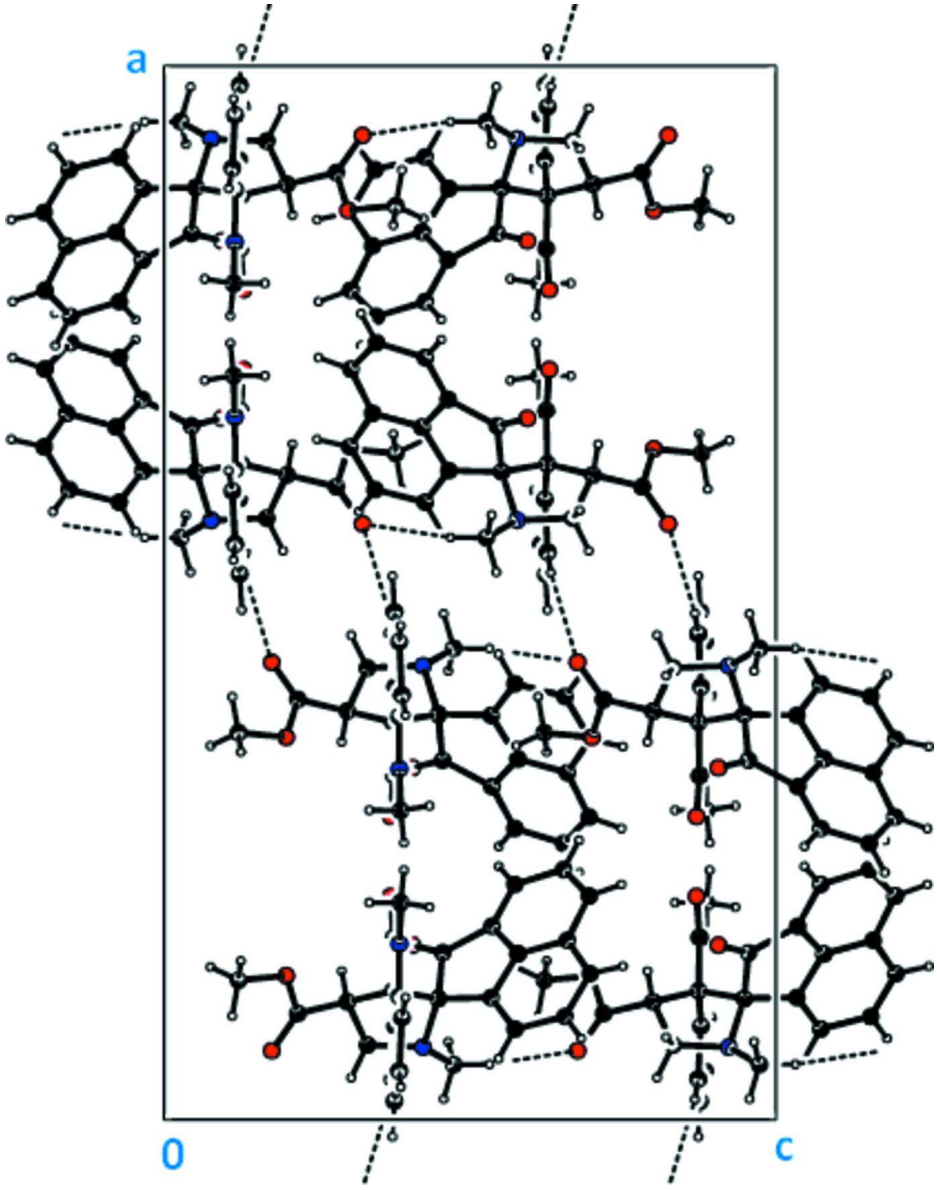

Figure 2

The molecular packing viewed down the *b* axis. Dashed lines shows the intermolecular C-H···O hydrogen bonds.

Methyl (1*R*,3′*S*)-1′,1′′-dimethyl-2,2′′-dioxo-2*H*-dispiro[acenaphthylene-1,2′-pyrrolidine-3′,3′′-indoline]-4′-carboxylate

Crystal data

$C_{26}H_{22}N_2O_4$
$M_r = 426.46$
Orthorhombic, *Pbcn*
Hall symbol: -P 2n 2ab
$a = 27.2997$ (15) Å
$b = 9.7923$ (6) Å
$c = 15.8557$ (10) Å
$V = 4238.7$ (4) Å^3
$Z = 8$
$F(000) = 1792$
$D_x = 1.337$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5039 reflections
$\theta = 1.5$–27.9°
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Block, colourless
0.25 × 0.22 × 0.19 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.978, T_{max} = 0.983
23813 measured reflections
5039 independent reflections
3022 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.9°, θ_{min} = 2.2°
h = −35→31
k = −12→11
l = −18→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.135
S = 1.02
5039 reflections
292 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
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 1.3523P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.55248 (7)	−0.08437 (18)	0.02663 (15)	0.0583 (6)
H1A	0.5740	−0.1607	0.0354	0.087*
H1B	0.5527	−0.0596	−0.0320	0.087*
H1C	0.5198	−0.1088	0.0432	0.087*
C2	0.57113 (7)	0.0054 (2)	0.16787 (14)	0.0543 (5)
H2A	0.5784	−0.0897	0.1794	0.065*
H2B	0.5402	0.0285	0.1943	0.065*
C3	0.61210 (7)	0.09760 (19)	0.20075 (12)	0.0463 (5)
H3	0.6412	0.0409	0.2098	0.056*
C4	0.62250 (6)	0.19357 (17)	0.12618 (11)	0.0380 (4)
C5	0.61516 (6)	0.09285 (16)	0.05178 (12)	0.0380 (4)
C6	0.65873 (6)	−0.01367 (18)	0.04464 (13)	0.0454 (5)
C7	0.68374 (6)	0.0100 (2)	−0.03587 (13)	0.0492 (5)
C8	0.72342 (7)	−0.0500 (2)	−0.07337 (16)	0.0672 (6)
H8	0.7404	−0.1202	−0.0469	0.081*
C9	0.73756 (9)	−0.0022 (3)	−0.15287 (18)	0.0842 (8)

H9	0.7652	−0.0399	−0.1781	0.101*
C10	0.71257 (9)	0.0973 (3)	−0.19492 (16)	0.0778 (7)
H10	0.7234	0.1258	−0.2477	0.093*
C11	0.67050 (8)	0.1574 (2)	−0.15918 (14)	0.0573 (5)
C12	0.65758 (7)	0.11197 (19)	−0.07840 (12)	0.0444 (4)
C13	0.61607 (6)	0.15884 (17)	−0.03457 (12)	0.0401 (4)
C14	0.58614 (7)	0.24994 (19)	−0.07357 (13)	0.0500 (5)
H14	0.5581	0.2818	−0.0467	0.060*
C15	0.59812 (9)	0.2955 (2)	−0.15527 (14)	0.0617 (6)
H15	0.5773	0.3571	−0.1819	0.074*
C16	0.63878 (9)	0.2529 (2)	−0.19651 (14)	0.0661 (6)
H16	0.6458	0.2872	−0.2499	0.079*
C17	0.67325 (6)	0.26047 (19)	0.12476 (12)	0.0413 (4)
C18	0.61710 (6)	0.43187 (17)	0.11591 (11)	0.0368 (4)
C19	0.58897 (6)	0.31498 (16)	0.12240 (11)	0.0359 (4)
C20	0.53874 (6)	0.32524 (19)	0.12696 (13)	0.0479 (5)
H20	0.5193	0.2477	0.1322	0.058*
C21	0.51788 (7)	0.4538 (2)	0.12360 (16)	0.0627 (6)
H21	0.4840	0.4627	0.1268	0.075*
C22	0.54625 (8)	0.5680 (2)	0.11568 (16)	0.0644 (6)
H22	0.5313	0.6532	0.1132	0.077*
C23	0.59676 (7)	0.55977 (19)	0.11128 (13)	0.0501 (5)
H23	0.6161	0.6374	0.1054	0.060*
C24	0.70630 (7)	0.4956 (2)	0.11344 (14)	0.0560 (5)
H24A	0.7370	0.4487	0.1084	0.084*
H24B	0.7060	0.5481	0.1646	0.084*
H24C	0.7020	0.5554	0.0660	0.084*
C25	0.60097 (8)	0.1700 (2)	0.28144 (14)	0.0548 (5)
C26	0.63246 (11)	0.3314 (3)	0.37857 (16)	0.0865 (8)
H26A	0.5988	0.3558	0.3876	0.130*
H26B	0.6520	0.4127	0.3756	0.130*
H26C	0.6436	0.2755	0.4245	0.130*
N1	0.56904 (5)	0.03024 (14)	0.07673 (10)	0.0434 (4)
N2	0.66700 (5)	0.39740 (15)	0.11545 (9)	0.0403 (4)
O1	0.66576 (5)	−0.10603 (14)	0.09387 (10)	0.0617 (4)
O2	0.71209 (5)	0.20188 (14)	0.12955 (10)	0.0625 (4)
O3	0.56571 (6)	0.1529 (2)	0.32417 (11)	0.0878 (6)
O4	0.63683 (6)	0.25647 (16)	0.30058 (10)	0.0693 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0490 (11)	0.0381 (10)	0.0879 (17)	−0.0046 (9)	−0.0040 (11)	0.0022 (10)
C2	0.0531 (12)	0.0480 (11)	0.0617 (14)	−0.0003 (10)	0.0105 (10)	0.0145 (10)
C3	0.0414 (10)	0.0462 (10)	0.0512 (12)	0.0086 (8)	0.0057 (9)	0.0108 (9)
C4	0.0278 (8)	0.0392 (9)	0.0470 (11)	0.0050 (7)	0.0022 (7)	0.0035 (8)
C5	0.0293 (8)	0.0356 (8)	0.0491 (11)	0.0030 (7)	0.0016 (8)	0.0035 (8)
C6	0.0369 (9)	0.0405 (10)	0.0588 (12)	0.0054 (8)	−0.0038 (9)	−0.0033 (9)

C7	0.0354 (9)	0.0547 (11)	0.0576 (13)	0.0022 (9)	−0.0015 (9)	−0.0152 (10)
C8	0.0456 (12)	0.0851 (16)	0.0708 (16)	0.0130 (11)	0.0014 (11)	−0.0249 (13)
C9	0.0501 (14)	0.130 (2)	0.0731 (18)	0.0053 (16)	0.0132 (13)	−0.0356 (18)
C10	0.0615 (15)	0.118 (2)	0.0535 (15)	−0.0135 (15)	0.0146 (12)	−0.0166 (15)
C11	0.0541 (12)	0.0691 (14)	0.0487 (13)	−0.0160 (11)	0.0033 (10)	−0.0122 (11)
C12	0.0383 (10)	0.0490 (10)	0.0460 (11)	−0.0077 (8)	−0.0008 (8)	−0.0098 (9)
C13	0.0346 (9)	0.0391 (9)	0.0465 (11)	−0.0042 (7)	−0.0007 (8)	−0.0018 (8)
C14	0.0522 (11)	0.0468 (10)	0.0510 (12)	0.0023 (9)	−0.0042 (9)	0.0033 (9)
C15	0.0739 (15)	0.0565 (12)	0.0546 (14)	−0.0030 (11)	−0.0114 (12)	0.0076 (10)
C16	0.0824 (16)	0.0717 (15)	0.0443 (13)	−0.0195 (14)	−0.0002 (12)	0.0046 (11)
C17	0.0298 (9)	0.0503 (10)	0.0439 (11)	0.0042 (8)	0.0005 (8)	−0.0039 (8)
C18	0.0312 (9)	0.0406 (9)	0.0388 (10)	0.0001 (7)	−0.0009 (7)	0.0022 (7)
C19	0.0302 (8)	0.0364 (9)	0.0410 (10)	0.0028 (7)	0.0035 (7)	0.0027 (7)
C20	0.0287 (9)	0.0435 (10)	0.0716 (14)	0.0002 (8)	0.0057 (9)	0.0043 (9)
C21	0.0327 (10)	0.0522 (12)	0.1033 (19)	0.0103 (9)	0.0043 (11)	0.0031 (12)
C22	0.0507 (12)	0.0411 (11)	0.1013 (19)	0.0123 (10)	−0.0040 (12)	0.0057 (11)
C23	0.0472 (11)	0.0385 (10)	0.0646 (14)	−0.0027 (8)	−0.0034 (10)	0.0049 (9)
C24	0.0359 (10)	0.0637 (12)	0.0684 (15)	−0.0142 (9)	0.0005 (10)	−0.0036 (11)
C25	0.0512 (12)	0.0612 (13)	0.0522 (13)	0.0139 (10)	0.0039 (10)	0.0137 (10)
C26	0.113 (2)	0.0783 (17)	0.0680 (17)	0.0095 (16)	0.0000 (16)	−0.0145 (14)
N1	0.0343 (8)	0.0364 (8)	0.0595 (10)	−0.0005 (6)	0.0051 (7)	0.0061 (7)
N2	0.0283 (7)	0.0451 (8)	0.0474 (9)	−0.0041 (6)	−0.0004 (6)	0.0007 (7)
O1	0.0559 (9)	0.0494 (8)	0.0797 (11)	0.0188 (7)	0.0000 (8)	0.0083 (8)
O2	0.0301 (7)	0.0664 (9)	0.0908 (12)	0.0120 (6)	−0.0030 (7)	−0.0080 (8)
O3	0.0700 (11)	0.1265 (15)	0.0668 (11)	0.0017 (10)	0.0238 (9)	−0.0047 (11)
O4	0.0766 (11)	0.0749 (10)	0.0566 (10)	−0.0028 (9)	0.0069 (8)	−0.0051 (8)

Geometric parameters (Å, º)

C1—N1	1.447 (2)	C13—C14	1.359 (2)
C1—H1A	0.9600	C14—C15	1.408 (3)
C1—H1B	0.9600	C14—H14	0.9300
C1—H1C	0.9600	C15—C16	1.354 (3)
C2—N1	1.467 (3)	C15—H15	0.9300
C2—C3	1.529 (3)	C16—H16	0.9300
C2—H2A	0.9700	C17—O2	1.208 (2)
C2—H2B	0.9700	C17—N2	1.360 (2)
C3—C25	1.494 (3)	C18—C23	1.372 (2)
C3—C4	1.537 (2)	C18—C19	1.382 (2)
C3—H3	0.9800	C18—N2	1.403 (2)
C4—C19	1.502 (2)	C19—C20	1.377 (2)
C4—C17	1.533 (2)	C20—C21	1.383 (3)
C4—C5	1.551 (2)	C20—H20	0.9300
C5—N1	1.455 (2)	C21—C22	1.366 (3)
C5—C13	1.514 (2)	C21—H21	0.9300
C5—C6	1.586 (2)	C22—C23	1.383 (3)
C6—O1	1.210 (2)	C22—H22	0.9300
C6—C7	1.466 (3)	C23—H23	0.9300

C7—C8	1.368 (3)	C24—N2	1.441 (2)
C7—C12	1.401 (3)	C24—H24A	0.9600
C8—C9	1.399 (4)	C24—H24B	0.9600
C8—H8	0.9300	C24—H24C	0.9600
C9—C10	1.364 (4)	C25—O3	1.189 (2)
C9—H9	0.9300	C25—O4	1.330 (3)
C10—C11	1.410 (3)	C26—O4	1.443 (3)
C10—H10	0.9300	C26—H26A	0.9600
C11—C12	1.401 (3)	C26—H26B	0.9600
C11—C16	1.406 (3)	C26—H26C	0.9600
C12—C13	1.406 (2)		

N1—C1—H1A	109.5	C12—C13—C5	108.70 (15)
N1—C1—H1B	109.5	C13—C14—C15	119.1 (2)
H1A—C1—H1B	109.5	C13—C14—H14	120.4
N1—C1—H1C	109.5	C15—C14—H14	120.4
H1A—C1—H1C	109.5	C16—C15—C14	122.5 (2)
H1B—C1—H1C	109.5	C16—C15—H15	118.8
N1—C2—C3	105.47 (15)	C14—C15—H15	118.8
N1—C2—H2A	110.6	C15—C16—C11	120.4 (2)
C3—C2—H2A	110.6	C15—C16—H16	119.8
N1—C2—H2B	110.6	C11—C16—H16	119.8
C3—C2—H2B	110.6	O2—C17—N2	125.81 (17)
H2A—C2—H2B	108.8	O2—C17—C4	126.13 (17)
C25—C3—C2	115.06 (17)	N2—C17—C4	108.05 (14)
C25—C3—C4	113.98 (16)	C23—C18—C19	122.33 (16)
C2—C3—C4	103.53 (15)	C23—C18—N2	127.75 (16)
C25—C3—H3	108.0	C19—C18—N2	109.91 (14)
C2—C3—H3	108.0	C20—C19—C18	119.80 (15)
C4—C3—H3	108.0	C20—C19—C4	131.52 (15)
C19—C4—C17	102.25 (13)	C18—C19—C4	108.64 (14)
C19—C4—C3	113.70 (14)	C19—C20—C21	118.33 (17)
C17—C4—C3	116.09 (15)	C19—C20—H20	120.8
C19—C4—C5	113.23 (14)	C21—C20—H20	120.8
C17—C4—C5	112.19 (14)	C22—C21—C20	121.03 (18)
C3—C4—C5	99.93 (13)	C22—C21—H21	119.5
N1—C5—C13	116.08 (14)	C20—C21—H21	119.5
N1—C5—C4	99.96 (13)	C21—C22—C23	121.47 (18)
C13—C5—C4	114.48 (13)	C21—C22—H22	119.3
N1—C5—C6	113.03 (13)	C23—C22—H22	119.3
C13—C5—C6	101.76 (14)	C18—C23—C22	117.02 (18)
C4—C5—C6	112.06 (14)	C18—C23—H23	121.5
O1—C6—C7	127.30 (17)	C22—C23—H23	121.5
O1—C6—C5	124.36 (17)	N2—C24—H24A	109.5
C7—C6—C5	107.91 (15)	N2—C24—H24B	109.5
C8—C7—C12	120.0 (2)	H24A—C24—H24B	109.5
C8—C7—C6	132.8 (2)	N2—C24—H24C	109.5
C12—C7—C6	107.11 (16)	H24A—C24—H24C	109.5

C7—C8—C9	117.8 (2)	H24B—C24—H24C	109.5
C7—C8—H8	121.1	O3—C25—O4	123.7 (2)
C9—C8—H8	121.1	O3—C25—C3	125.9 (2)
C10—C9—C8	122.8 (2)	O4—C25—C3	110.38 (17)
C10—C9—H9	118.6	O4—C26—H26A	109.5
C8—C9—H9	118.6	O4—C26—H26B	109.5
C9—C10—C11	120.6 (2)	H26A—C26—H26B	109.5
C9—C10—H10	119.7	O4—C26—H26C	109.5
C11—C10—H10	119.7	H26A—C26—H26C	109.5
C12—C11—C16	116.18 (19)	H26B—C26—H26C	109.5
C12—C11—C10	116.1 (2)	C1—N1—C5	116.59 (15)
C16—C11—C10	127.6 (2)	C1—N1—C2	115.12 (15)
C7—C12—C11	122.55 (18)	C5—N1—C2	107.69 (14)
C7—C12—C13	113.93 (18)	C17—N2—C18	111.00 (14)
C11—C12—C13	123.44 (19)	C17—N2—C24	124.54 (15)
C14—C13—C12	118.29 (18)	C18—N2—C24	124.22 (15)
C14—C13—C5	133.00 (17)	C25—O4—C26	117.31 (19)

N1—C2—C3—C25	137.57 (16)	C12—C13—C14—C15	−1.0 (3)
N1—C2—C3—C4	12.55 (18)	C5—C13—C14—C15	178.08 (18)
C25—C3—C4—C19	−41.3 (2)	C13—C14—C15—C16	−0.7 (3)
C2—C3—C4—C19	84.45 (18)	C14—C15—C16—C11	1.5 (3)
C25—C3—C4—C17	77.0 (2)	C12—C11—C16—C15	−0.6 (3)
C2—C3—C4—C17	−157.33 (15)	C10—C11—C16—C15	176.3 (2)
C25—C3—C4—C5	−162.21 (15)	C19—C4—C17—O2	177.45 (19)
C2—C3—C4—C5	−36.50 (16)	C3—C4—C17—O2	53.1 (3)
C19—C4—C5—N1	−73.87 (16)	C5—C4—C17—O2	−60.9 (2)
C17—C4—C5—N1	171.02 (13)	C19—C4—C17—N2	−3.77 (19)
C3—C4—C5—N1	47.41 (14)	C3—C4—C17—N2	−128.12 (16)
C19—C4—C5—C13	50.91 (19)	C5—C4—C17—N2	117.86 (16)
C17—C4—C5—C13	−64.20 (18)	C23—C18—C19—C20	−2.0 (3)
C3—C4—C5—C13	172.20 (14)	N2—C18—C19—C20	177.74 (17)
C19—C4—C5—C6	166.14 (14)	C23—C18—C19—C4	−179.96 (17)
C17—C4—C5—C6	51.03 (19)	N2—C18—C19—C4	−0.3 (2)
C3—C4—C5—C6	−72.58 (16)	C17—C4—C19—C20	−175.3 (2)
N1—C5—C6—O1	−40.9 (3)	C3—C4—C19—C20	−49.4 (3)
C13—C5—C6—O1	−166.14 (18)	C5—C4—C19—C20	63.8 (3)
C4—C5—C6—O1	71.1 (2)	C17—C4—C19—C18	2.39 (18)
N1—C5—C6—C7	131.98 (16)	C3—C4—C19—C18	128.31 (16)
C13—C5—C6—C7	6.77 (17)	C5—C4—C19—C18	−118.52 (16)
C4—C5—C6—C7	−115.98 (16)	C18—C19—C20—C21	0.9 (3)
O1—C6—C7—C8	−8.3 (4)	C4—C19—C20—C21	178.4 (2)
C5—C6—C7—C8	179.0 (2)	C19—C20—C21—C22	0.2 (3)
O1—C6—C7—C12	168.86 (19)	C20—C21—C22—C23	−0.4 (4)
C5—C6—C7—C12	−3.79 (19)	C19—C18—C23—C22	1.7 (3)
C12—C7—C8—C9	2.4 (3)	N2—C18—C23—C22	−177.93 (19)
C6—C7—C8—C9	179.3 (2)	C21—C22—C23—C18	−0.5 (3)
C7—C8—C9—C10	−2.3 (4)	C2—C3—C25—O3	6.7 (3)

C8—C9—C10—C11	0.0 (4)	C4—C3—C25—O3	126.1 (2)
C9—C10—C11—C12	2.0 (3)	C2—C3—C25—O4	−174.36 (16)
C9—C10—C11—C16	−174.9 (2)	C4—C3—C25—O4	−55.0 (2)
C8—C7—C12—C11	−0.4 (3)	C13—C5—N1—C1	63.6 (2)
C6—C7—C12—C11	−178.03 (17)	C4—C5—N1—C1	−172.74 (14)
C8—C7—C12—C13	176.48 (17)	C6—C5—N1—C1	−53.5 (2)
C6—C7—C12—C13	−1.1 (2)	C13—C5—N1—C2	−165.25 (15)
C16—C11—C12—C7	175.42 (18)	C4—C5—N1—C2	−41.59 (16)
C10—C11—C12—C7	−1.8 (3)	C6—C5—N1—C2	77.70 (18)
C16—C11—C12—C13	−1.2 (3)	C3—C2—N1—C1	150.60 (15)
C10—C11—C12—C13	−178.42 (18)	C3—C2—N1—C5	18.64 (18)
C7—C12—C13—C14	−174.87 (16)	O2—C17—N2—C18	−177.33 (18)
C11—C12—C13—C14	2.0 (3)	C4—C17—N2—C18	3.9 (2)
C7—C12—C13—C5	5.8 (2)	O2—C17—N2—C24	−2.8 (3)
C11—C12—C13—C5	−177.31 (16)	C4—C17—N2—C24	178.40 (16)
N1—C5—C13—C14	50.3 (3)	C23—C18—N2—C17	177.32 (19)
C4—C5—C13—C14	−65.5 (2)	C19—C18—N2—C17	−2.4 (2)
C6—C5—C13—C14	173.43 (19)	C23—C18—N2—C24	2.8 (3)
N1—C5—C13—C12	−130.55 (15)	C19—C18—N2—C24	−176.90 (17)
C4—C5—C13—C12	113.69 (15)	O3—C25—O4—C26	1.0 (3)
C6—C5—C13—C12	−7.40 (17)	C3—C25—O4—C26	−177.94 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···O3^{i}	0.96	2.48	3.299 (3)	143
C20—H20···O3^{ii}	0.93	2.59	3.403 (3)	146

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