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4,7a-Bis(4-methoxyphenyl)-1,3,7-tris(4-methylphenyl)-2,3,5,6,7,7a-hexahydro-1*H*-pyrrolo[2,3-*d*]pyrimidine-2,5,6-trione

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.129
Data-to-parameter ratio = 16.5

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

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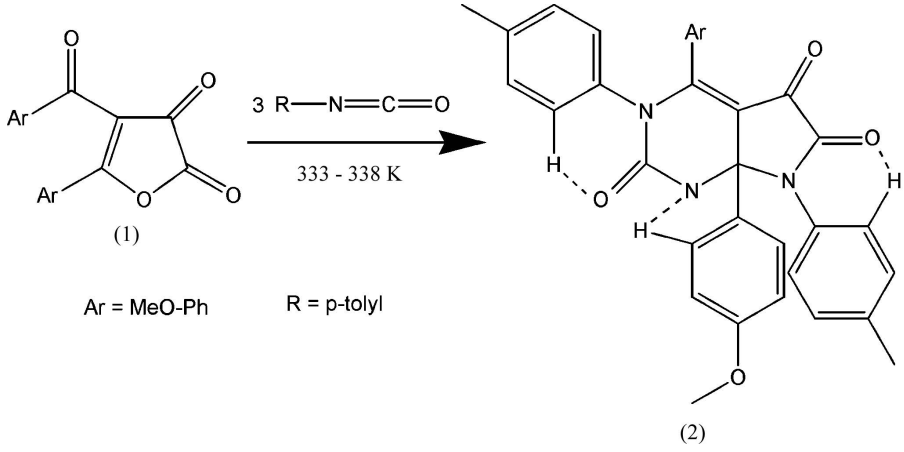
The structure of the title compound, $C_{41}H_{35}N_3O_5$, is stabilized by intra- and intermolecular C—H···O hydrogen bonds.

Comment

Pyrrolo[2,3]pyrimidines are an important class of compounds that are structurally and chemically related to nucleosides and some antibiotics (Ohgi *et al.*, 1979; Tolmann *et al.*, 1968). The well known biological activity of these compounds has led to intensive investigation of their use as antitumor, anti-allergic, antiviral and anti-inflammatory agents (Hutzenlaub *et al.*, 1972; Smith *et al.*, 1972).

In the light of this, we have synthesized and characterized the title compound, (2), and have determined its structure by X-ray analysis.



(1)

Ar = MeO-Ph R = p-tolyl

(2)

Fig. 1 shows the molecular structure of (2), with the atomic numbering scheme. The six-membered non-aromatic ring (C2/C1/N1/C5/N2/C6) has a total puckering amplitude of 0.532 (3) Å (Cremer & Pople, 1975) and a boat conformation [φ = 179.5 (4)° and θ = 105.0 (5)°]. The five-membered aromatic ring (C1–C4/N3) and the five benzene rings (C7–C12, C13–C18, C19–C24, C25–C30 and C31–C36) are each essentially planar, with r.m.s. deviations of 0.0296 (13), 0.0104 (14), 0.0069 (15), 0.0067 (15), 0.046 (16) and 0.126 (15) Å, respectively. The bond lengths and angles are in agreement with reported literature values (Allen *et al.*, 1987).

The structure is stabilized by intra- and intermolecular C—H···O hydrogen bonds (Table 1). In the crystal structure, the C—H···O intermolecular hydrogen bonds link the molecules into dimers which are stacked along the *b* axis (Fig. 2).

Experimental

Compound (1) was prepared from the cyclocondensation reaction that occurs between *p*,*p*′-dimethoxydibenzoylketene and oxalyl

chloride (Hökelek *et al.*, 2002). Compound (2) was obtained from (1) (1.0 g, 2.96 mmol) by reaction with an excess of *p*-tolyl isocyanate in a 25 ml round-bottomed flask equipped with a calcium chloride tube. The mixture was heated at 338 K for 24 h. After cooling to room temperature, the residue was triturated with anhydrous diethyl ether, and the crude product was recrystallized from ethanol (yield 1.26 g, 66%; m.p. 475 K). IR (KBr, cm^{-1}): υ 1727 (C3—O1), 1709 (C4—O2), 1684 (C5—O3); ^{1}H NMR ($CDCl_3$, p.p.m..): δ 7.64–6.04 (*m*, 20H, Ar—H), 3.88, 3.77 (*s*, 6H, CH_3O), 2.25, 2.18, 2.15 (*s*, 9H, Ar—CH_3); ^{13}C NMR ($CDCl_3$, p.p.m..): δ 178.51 (C3—O1), 165.58 (C4—O2), 164.47 (C5—O3), 162.35–115.52 (C=C, arom. and aliph.), 81.36 (N1—C1—N2), 57.50 (O4—C38), 57.28 (O5—C37), 23.00, 22.94, 22.92 (Ar—CH_3). Analysis calculated for $C_{41}H_{35}N_3O_5$: C 75.80, H 5.39, N 6.47%; found: C 76.02, H 5.69, N 6.22%.

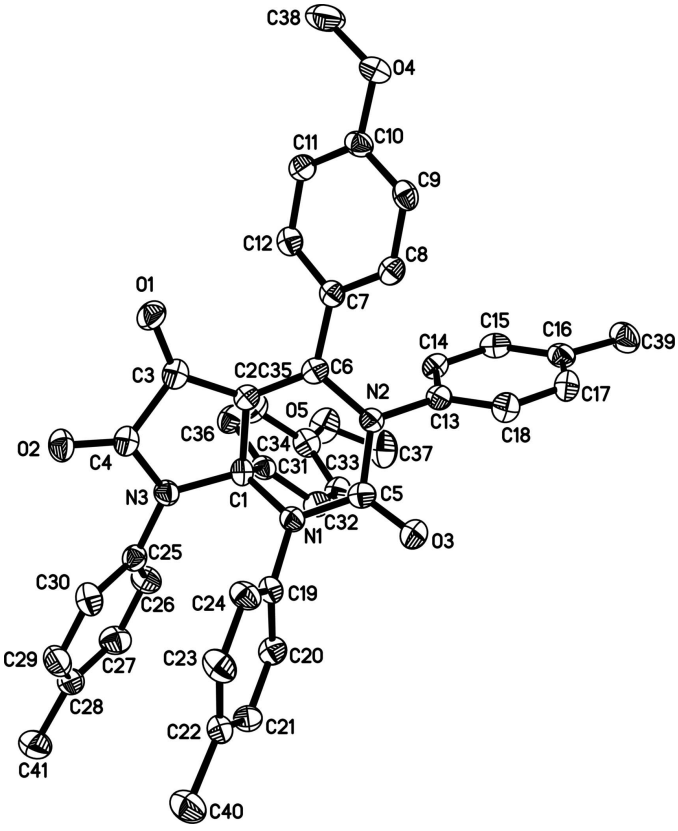


Figure 1
The molecular structure of (2), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted.

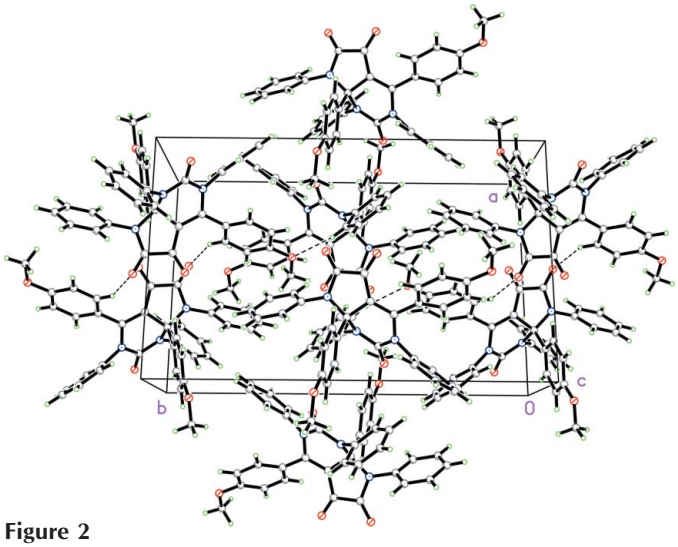


Figure 2
Packing diagram of (2); C—H···O hydrogen bonds are shown as dashed lines.

Crystal data

$C_{41}H_{35}N_3O_5$
M_r = 649.72
Triclinic, $P\overline{1}$
a = 10.1797 (12) Å
b = 12.5347 (14) Å
c = 13.6855 (16) Å
α = 107.999 (2)°
β = 99.985 (2)°
γ = 90.504 (2)°
V = 1632.0 (3) Å^3
Z = 2
D_x = 1.322 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3062 reflections
θ = 4.7–50.5°
μ = 0.09 mm^{-1}
T = 150 (2) K
Block, yellow
0.38 × 0.21 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.968, T_{max} = 0.991
18940 measured reflections
7331 independent reflections
4028 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 27.6°
$h = -13 \rightarrow 13$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.129
S = 0.98
7331 reflections
445 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.1342P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O1^{i}	0.95	2.55	3.409 (3)	150
C11—H11A···O2^{ii}	0.95	2.53	3.158 (3)	123
C18—H18A···O3	0.95	2.58	2.927 (3)	102
C30—H30A···O2	0.95	2.55	2.928 (3)	104
C32—H32A···N1	0.95	2.51	2.858 (3)	102
C39—H39C···O5^{iii}	0.98	2.48	3.422 (3)	160
C40—H40C···O4^{iv}	0.98	2.54	3.341 (3)	139

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y+1, -z$; (iii) $x-1, y, z$; (iv) $x+1, y, z+1$.

H atoms were positioned geometrically [0.95 (CH) and 0.98 Å (CH_3)] and constrained to ride on their parent atoms, with U_{iso}(H) values of 1.2 (1.5 for methyl) times U_{eq}.

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

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supporting information

Acta Cryst. (2005). E**61**, o3953–o3955 [https://doi.org/10.1107/S1600536805035191]

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$h = -13\rightarrow13$
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$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.129$
$S = 0.98$
7331 reflections
445 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
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.1342P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ 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	0.44303 (17)	0.76941 (14)	0.35720 (13)	0.0225 (4)
N2	0.26565 (17)	0.80260 (14)	0.23849 (13)	0.0224 (4)
N3	0.60522 (17)	0.64263 (14)	0.28048 (13)	0.0236 (4)
O1	0.38721 (15)	0.45850 (12)	0.06781 (12)	0.0318 (4)
O2	0.62192 (15)	0.45004 (12)	0.21556 (12)	0.0298 (4)
O3	0.27951 (15)	0.88193 (13)	0.41620 (12)	0.0318 (4)
O4	−0.11979 (15)	0.52626 (13)	−0.19218 (12)	0.0324 (4)
O5	0.66647 (17)	1.05878 (13)	0.09981 (13)	0.0406 (4)
C1	0.5081 (2)	0.72444 (17)	0.26482 (16)	0.0224 (5)
C2	0.4005 (2)	0.65493 (17)	0.17695 (16)	0.0213 (5)
C3	0.4375 (2)	0.54068 (18)	0.14025 (17)	0.0248 (5)
C4	0.5655 (2)	0.53540 (18)	0.21550 (17)	0.0242 (5)
C5	0.3282 (2)	0.82213 (17)	0.34428 (17)	0.0232 (5)
C6	0.2842 (2)	0.70480 (17)	0.16055 (16)	0.0226 (5)
C7	0.1781 (2)	0.66148 (16)	0.06802 (16)	0.0217 (5)
C8	0.0421 (2)	0.66904 (16)	0.07351 (17)	0.0233 (5)
H8A	0.0167	0.7060	0.1386	0.028*
C9	−0.0554 (2)	0.62364 (17)	−0.01428 (17)	0.0245 (5)
H9A	−0.1473	0.6279	−0.0096	0.029*
C10	−0.0170 (2)	0.57146 (17)	−0.10992 (17)	0.0249 (5)
C11	0.1167 (2)	0.56659 (17)	−0.11805 (17)	0.0242 (5)
H11A	0.1419	0.5330	−0.1839	0.029*
C12	0.2132 (2)	0.61127 (17)	−0.02897 (16)	0.0243 (5)
H12A	0.3050	0.6076	−0.0341	0.029*
C13	0.1911 (2)	0.89035 (17)	0.21112 (16)	0.0225 (5)
C14	0.2316 (2)	0.93196 (17)	0.13800 (16)	0.0247 (5)
H14A	0.3056	0.9027	0.1069	0.030*
C15	0.1637 (2)	1.01653 (18)	0.11028 (17)	0.0273 (5)
H15A	0.1908	1.0438	0.0589	0.033*
C16	0.0568 (2)	1.06241 (18)	0.15605 (17)	0.0267 (5)
C17	0.0171 (2)	1.01765 (18)	0.22822 (17)	0.0284 (5)
H17A	−0.0573	1.0462	0.2591	0.034*
C18	0.0831 (2)	0.93267 (18)	0.25615 (17)	0.0275 (5)
H18A	0.0545	0.9035	0.3059	0.033*
C19	0.4964 (2)	0.75896 (17)	0.45847 (16)	0.0225 (5)

C20	0.5933 (2)	0.83576 (18)	0.52888 (17)	0.0260 (5)
H20A	0.6232	0.8994	0.5129	0.031*
C21	0.6467 (2)	0.81931 (18)	0.62289 (17)	0.0274 (5)
H21A	0.7139	0.8719	0.6708	0.033*
C22	0.6039 (2)	0.72734 (18)	0.64869 (17)	0.0259 (5)
C23	0.5041 (2)	0.65289 (19)	0.57750 (18)	0.0314 (6)
H23A	0.4719	0.5904	0.5939	0.038*
C24	0.4509 (2)	0.66830 (18)	0.48307 (17)	0.0273 (5)
H24A	0.3830	0.6164	0.4352	0.033*
C25	0.7300 (2)	0.66768 (18)	0.35408 (17)	0.0238 (5)
C26	0.8186 (2)	0.75658 (19)	0.36299 (17)	0.0302 (5)
H26A	0.7978	0.8031	0.3199	0.036*
C27	0.9381 (2)	0.7774 (2)	0.43537 (18)	0.0338 (6)
H27A	0.9972	0.8393	0.4420	0.041*
C28	0.9725 (2)	0.7101 (2)	0.49759 (18)	0.0311 (6)
C29	0.8827 (2)	0.6213 (2)	0.48674 (18)	0.0336 (6)
H29A	0.9043	0.5738	0.5286	0.040*
C30	0.7630 (2)	0.60021 (19)	0.41695 (18)	0.0305 (6)
H30A	0.7031	0.5394	0.4119	0.037*
C31	0.5647 (2)	0.81932 (17)	0.23188 (16)	0.0226 (5)
C32	0.5630 (2)	0.93195 (18)	0.28642 (17)	0.0257 (5)
H32A	0.5371	0.9533	0.3529	0.031*
C33	0.5985 (2)	1.01516 (18)	0.24588 (18)	0.0288 (5)
H33A	0.5966	1.0923	0.2845	0.035*
C34	0.6365 (2)	0.98506 (19)	0.14950 (18)	0.0300 (5)
C35	0.6441 (2)	0.87138 (19)	0.09558 (18)	0.0334 (6)
H35A	0.6742	0.8502	0.0307	0.040*
C36	0.6081 (2)	0.79005 (18)	0.13603 (18)	0.0294 (5)
H36A	0.6128	0.7130	0.0984	0.035*
C37	0.6344 (3)	1.1725 (2)	0.1420 (2)	0.0442 (7)
H37A	0.6609	1.2169	0.1000	0.066*
H37B	0.6823	1.2038	0.2143	0.066*
H37C	0.5379	1.1750	0.1406	0.066*
C38	−0.0837 (3)	0.4640 (2)	−0.28888 (19)	0.0488 (7)
H38A	−0.1647	0.4356	−0.3418	0.073*
H38B	−0.0328	0.4006	−0.2797	0.073*
H38C	−0.0286	0.5129	−0.3116	0.073*
C39	−0.0105 (2)	1.15993 (19)	0.13091 (19)	0.0367 (6)
H39A	0.0251	1.1752	0.0741	0.055*
H39B	0.0066	1.2267	0.1931	0.055*
H39C	−0.1071	1.1413	0.1092	0.055*
C40	0.6651 (3)	0.7067 (2)	0.74888 (18)	0.0388 (6)
H40A	0.6011	0.6616	0.7682	0.058*
H40B	0.6880	0.7788	0.8045	0.058*
H40C	0.7462	0.6662	0.7392	0.058*
C41	1.1049 (2)	0.7299 (2)	0.57156 (19)	0.0424 (7)
H41A	1.1536	0.7965	0.5691	0.064*
H41B	1.1576	0.6643	0.5509	0.064*

H41C	1.0897	0.7417	0.6428	0.064*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0229 (10)	0.0235 (10)	0.0218 (10)	0.0032 (8)	0.0037 (8)	0.0084 (8)
N2	0.0232 (10)	0.0216 (9)	0.0215 (10)	0.0029 (8)	0.0017 (8)	0.0068 (8)
N3	0.0215 (10)	0.0218 (10)	0.0258 (10)	0.0008 (8)	0.0017 (8)	0.0067 (8)
O1	0.0299 (9)	0.0230 (8)	0.0345 (10)	−0.0005 (7)	0.0029 (7)	−0.0008 (7)
O2	0.0276 (9)	0.0221 (8)	0.0397 (10)	0.0039 (7)	0.0053 (7)	0.0102 (7)
O3	0.0335 (9)	0.0336 (9)	0.0274 (9)	0.0088 (7)	0.0084 (7)	0.0068 (7)
O4	0.0280 (9)	0.0376 (10)	0.0274 (9)	0.0028 (7)	−0.0040 (7)	0.0091 (7)
O5	0.0518 (11)	0.0304 (10)	0.0498 (11)	0.0014 (8)	0.0225 (9)	0.0202 (8)
C1	0.0218 (12)	0.0204 (11)	0.0266 (12)	0.0040 (9)	0.0065 (10)	0.0087 (9)
C2	0.0223 (12)	0.0193 (11)	0.0227 (12)	−0.0008 (9)	0.0048 (9)	0.0069 (9)
C3	0.0225 (12)	0.0222 (12)	0.0309 (13)	−0.0003 (9)	0.0090 (10)	0.0081 (10)
C4	0.0220 (12)	0.0216 (12)	0.0307 (13)	0.0011 (9)	0.0089 (10)	0.0084 (10)
C5	0.0271 (13)	0.0195 (11)	0.0233 (12)	−0.0020 (9)	0.0036 (10)	0.0078 (9)
C6	0.0248 (12)	0.0198 (11)	0.0237 (12)	−0.0016 (9)	0.0053 (10)	0.0074 (9)
C7	0.0236 (12)	0.0166 (11)	0.0261 (12)	0.0001 (9)	0.0031 (10)	0.0093 (9)
C8	0.0286 (13)	0.0157 (11)	0.0268 (12)	0.0003 (9)	0.0063 (10)	0.0079 (9)
C9	0.0221 (12)	0.0215 (11)	0.0325 (13)	0.0027 (9)	0.0041 (10)	0.0129 (10)
C10	0.0266 (13)	0.0229 (12)	0.0253 (12)	0.0003 (10)	−0.0016 (10)	0.0110 (10)
C11	0.0295 (13)	0.0222 (12)	0.0222 (12)	0.0018 (10)	0.0044 (10)	0.0089 (9)
C12	0.0241 (12)	0.0205 (11)	0.0304 (13)	0.0006 (9)	0.0057 (10)	0.0110 (10)
C13	0.0250 (12)	0.0166 (11)	0.0248 (12)	−0.0009 (9)	0.0014 (10)	0.0066 (9)
C14	0.0269 (13)	0.0222 (12)	0.0239 (12)	0.0001 (9)	0.0064 (10)	0.0047 (10)
C15	0.0327 (14)	0.0256 (12)	0.0237 (12)	−0.0050 (10)	0.0023 (10)	0.0095 (10)
C16	0.0285 (13)	0.0203 (11)	0.0276 (13)	−0.0015 (10)	−0.0031 (10)	0.0069 (10)
C17	0.0267 (13)	0.0255 (12)	0.0343 (14)	0.0050 (10)	0.0098 (11)	0.0088 (10)
C18	0.0297 (13)	0.0270 (12)	0.0289 (13)	0.0022 (10)	0.0092 (11)	0.0113 (10)
C19	0.0197 (12)	0.0233 (12)	0.0253 (12)	0.0032 (9)	0.0040 (10)	0.0087 (10)
C20	0.0294 (13)	0.0210 (12)	0.0279 (13)	−0.0010 (10)	0.0056 (10)	0.0079 (10)
C21	0.0258 (13)	0.0250 (12)	0.0257 (13)	−0.0010 (10)	−0.0009 (10)	0.0029 (10)
C22	0.0258 (12)	0.0265 (12)	0.0262 (13)	0.0066 (10)	0.0043 (10)	0.0094 (10)
C23	0.0310 (14)	0.0293 (13)	0.0383 (15)	−0.0022 (11)	0.0013 (11)	0.0200 (11)
C24	0.0217 (12)	0.0258 (12)	0.0315 (13)	−0.0051 (10)	−0.0031 (10)	0.0094 (10)
C25	0.0207 (12)	0.0232 (11)	0.0260 (12)	0.0017 (9)	0.0051 (10)	0.0050 (9)
C26	0.0277 (13)	0.0333 (13)	0.0306 (13)	−0.0017 (11)	0.0024 (11)	0.0131 (11)
C27	0.0275 (13)	0.0364 (14)	0.0339 (14)	−0.0052 (11)	0.0023 (11)	0.0080 (11)
C28	0.0231 (13)	0.0381 (14)	0.0273 (13)	0.0066 (11)	0.0027 (10)	0.0043 (11)
C29	0.0314 (14)	0.0365 (14)	0.0353 (14)	0.0088 (11)	0.0042 (11)	0.0157 (11)
C30	0.0254 (13)	0.0297 (13)	0.0395 (15)	0.0042 (10)	0.0071 (11)	0.0146 (11)
C31	0.0187 (11)	0.0227 (11)	0.0247 (12)	−0.0009 (9)	0.0011 (9)	0.0066 (9)
C32	0.0274 (13)	0.0259 (12)	0.0244 (12)	−0.0006 (10)	0.0060 (10)	0.0082 (10)
C33	0.0297 (13)	0.0226 (12)	0.0338 (14)	−0.0006 (10)	0.0073 (11)	0.0076 (10)
C34	0.0269 (13)	0.0289 (13)	0.0369 (14)	−0.0014 (10)	0.0059 (11)	0.0142 (11)
C35	0.0366 (15)	0.0330 (14)	0.0323 (14)	−0.0004 (11)	0.0144 (11)	0.0083 (11)

C36	0.0306 (13)	0.0224 (12)	0.0329 (14)	−0.0016 (10)	0.0077 (11)	0.0046 (10)
C37	0.0514 (18)	0.0315 (14)	0.0617 (19)	0.0095 (12)	0.0194 (14)	0.0269 (13)
C38	0.0387 (16)	0.069 (2)	0.0269 (15)	0.0036 (14)	−0.0053 (12)	0.0046 (14)
C39	0.0378 (15)	0.0307 (14)	0.0419 (15)	0.0048 (11)	−0.0007 (12)	0.0162 (12)
C40	0.0410 (16)	0.0408 (15)	0.0368 (15)	0.0034 (12)	0.0000 (12)	0.0195 (12)
C41	0.0346 (15)	0.0514 (17)	0.0348 (15)	0.0056 (12)	−0.0027 (12)	0.0093 (13)

Geometric parameters (Å, º)

N1—C5	1.360 (3)	C20—C21	1.384 (3)
N1—C19	1.444 (3)	C20—H20A	0.9500
N1—C1	1.487 (3)	C21—C22	1.392 (3)
N2—C6	1.393 (3)	C21—H21A	0.9500
N2—C5	1.421 (3)	C22—C23	1.389 (3)
N2—C13	1.448 (3)	C22—C40	1.504 (3)
N3—C4	1.374 (3)	C23—C24	1.384 (3)
N3—C25	1.442 (3)	C23—H23A	0.9500
N3—C1	1.468 (3)	C24—H24A	0.9500
O1—C3	1.220 (2)	C25—C30	1.387 (3)
O2—C4	1.219 (2)	C25—C26	1.389 (3)
O3—C5	1.223 (2)	C26—C27	1.395 (3)
O4—C10	1.368 (2)	C26—H26A	0.9500
O4—C38	1.425 (3)	C27—C28	1.380 (3)
O5—C34	1.365 (3)	C27—H27A	0.9500
O5—C37	1.427 (3)	C28—C29	1.389 (3)
C1—C2	1.511 (3)	C28—C41	1.506 (3)
C1—C31	1.536 (3)	C29—C30	1.379 (3)
C2—C6	1.360 (3)	C29—H29A	0.9500
C2—C3	1.441 (3)	C30—H30A	0.9500
C3—C4	1.530 (3)	C31—C32	1.380 (3)
C6—C7	1.468 (3)	C31—C36	1.399 (3)
C7—C12	1.392 (3)	C32—C33	1.395 (3)
C7—C8	1.402 (3)	C32—H32A	0.9500
C8—C9	1.381 (3)	C33—C34	1.380 (3)
C8—H8A	0.9500	C33—H33A	0.9500
C9—C10	1.395 (3)	C34—C35	1.397 (3)
C9—H9A	0.9500	C35—C36	1.376 (3)
C10—C11	1.385 (3)	C35—H35A	0.9500
C11—C12	1.385 (3)	C36—H36A	0.9500
C11—H11A	0.9500	C37—H37A	0.9800
C12—H12A	0.9500	C37—H37B	0.9800
C13—C14	1.380 (3)	C37—H37C	0.9800
C13—C18	1.383 (3)	C38—H38A	0.9800
C14—C15	1.384 (3)	C38—H38B	0.9800
C14—H14A	0.9500	C38—H38C	0.9800
C15—C16	1.391 (3)	C39—H39A	0.9800
C15—H15A	0.9500	C39—H39B	0.9800
C16—C17	1.389 (3)	C39—H39C	0.9800

C16—C39	1.508 (3)	C40—H40A	0.9800
C17—C18	1.381 (3)	C40—H40B	0.9800
C17—H17A	0.9500	C40—H40C	0.9800
C18—H18A	0.9500	C41—H41A	0.9800
C19—C24	1.379 (3)	C41—H41B	0.9800
C19—C20	1.382 (3)	C41—H41C	0.9800

C5—N1—C19	119.39 (17)	C22—C21—H21A	119.3
C5—N1—C1	117.75 (17)	C23—C22—C21	117.8 (2)
C19—N1—C1	122.85 (16)	C23—C22—C40	120.5 (2)
C6—N2—C5	120.94 (17)	C21—C22—C40	121.6 (2)
C6—N2—C13	120.02 (17)	C24—C23—C22	121.1 (2)
C5—N2—C13	118.84 (16)	C24—C23—H23A	119.5
C4—N3—C25	121.79 (17)	C22—C23—H23A	119.5
C4—N3—C1	112.47 (17)	C19—C24—C23	120.0 (2)
C25—N3—C1	125.74 (17)	C19—C24—H24A	120.0
C10—O4—C38	116.51 (18)	C23—C24—H24A	120.0
C34—O5—C37	117.17 (18)	C30—C25—C26	119.1 (2)
N3—C1—N1	111.55 (16)	C30—C25—N3	118.95 (19)
N3—C1—C2	103.72 (16)	C26—C25—N3	121.9 (2)
N1—C1—C2	106.37 (16)	C25—C26—C27	119.8 (2)
N3—C1—C31	114.00 (17)	C25—C26—H26A	120.1
N1—C1—C31	111.61 (16)	C27—C26—H26A	120.1
C2—C1—C31	108.97 (17)	C28—C27—C26	121.6 (2)
C6—C2—C3	133.0 (2)	C28—C27—H27A	119.2
C6—C2—C1	116.01 (18)	C26—C27—H27A	119.2
C3—C2—C1	109.98 (18)	C27—C28—C29	117.5 (2)
O1—C3—C2	133.0 (2)	C27—C28—C41	121.1 (2)
O1—C3—C4	121.84 (19)	C29—C28—C41	121.4 (2)
C2—C3—C4	105.16 (18)	C30—C29—C28	121.9 (2)
O2—C4—N3	126.8 (2)	C30—C29—H29A	119.0
O2—C4—C3	125.02 (19)	C28—C29—H29A	119.0
N3—C4—C3	108.17 (17)	C29—C30—C25	120.1 (2)
O3—C5—N1	124.2 (2)	C29—C30—H30A	120.0
O3—C5—N2	121.0 (2)	C25—C30—H30A	120.0
N1—C5—N2	114.75 (18)	C32—C31—C36	118.3 (2)
C2—C6—N2	116.79 (18)	C32—C31—C1	123.56 (19)
C2—C6—C7	124.41 (19)	C36—C31—C1	117.84 (18)
N2—C6—C7	118.80 (18)	C31—C32—C33	121.3 (2)
C12—C7—C8	118.53 (19)	C31—C32—H32A	119.4
C12—C7—C6	119.09 (19)	C33—C32—H32A	119.4
C8—C7—C6	122.38 (19)	C34—C33—C32	119.8 (2)
C9—C8—C7	121.0 (2)	C34—C33—H33A	120.1
C9—C8—H8A	119.5	C32—C33—H33A	120.1
C7—C8—H8A	119.5	O5—C34—C33	124.9 (2)
C8—C9—C10	119.1 (2)	O5—C34—C35	115.7 (2)
C8—C9—H9A	120.5	C33—C34—C35	119.4 (2)
C10—C9—H9A	120.5	C36—C35—C34	120.3 (2)

O4—C10—C11	123.8 (2)	C36—C35—H35A	119.9
O4—C10—C9	115.23 (19)	C34—C35—H35A	119.9
C11—C10—C9	121.0 (2)	C35—C36—C31	120.9 (2)
C12—C11—C10	119.1 (2)	C35—C36—H36A	119.6
C12—C11—H11A	120.4	C31—C36—H36A	119.6
C10—C11—H11A	120.4	O5—C37—H37A	109.5
C11—C12—C7	121.2 (2)	O5—C37—H37B	109.5
C11—C12—H12A	119.4	H37A—C37—H37B	109.5
C7—C12—H12A	119.4	O5—C37—H37C	109.5
C14—C13—C18	120.2 (2)	H37A—C37—H37C	109.5
C14—C13—N2	117.77 (19)	H37B—C37—H37C	109.5
C18—C13—N2	122.04 (19)	O4—C38—H38A	109.5
C13—C14—C15	119.6 (2)	O4—C38—H38B	109.5
C13—C14—H14A	120.2	H38A—C38—H38B	109.5
C15—C14—H14A	120.2	O4—C38—H38C	109.5
C14—C15—C16	121.4 (2)	H38A—C38—H38C	109.5
C14—C15—H15A	119.3	H38B—C38—H38C	109.5
C16—C15—H15A	119.3	C16—C39—H39A	109.5
C15—C16—C17	117.6 (2)	C16—C39—H39B	109.5
C15—C16—C39	121.1 (2)	H39A—C39—H39B	109.5
C17—C16—C39	121.3 (2)	C16—C39—H39C	109.5
C18—C17—C16	121.6 (2)	H39A—C39—H39C	109.5
C18—C17—H17A	119.2	H39B—C39—H39C	109.5
C16—C17—H17A	119.2	C22—C40—H40A	109.5
C17—C18—C13	119.5 (2)	C22—C40—H40B	109.5
C17—C18—H18A	120.3	H40A—C40—H40B	109.5
C13—C18—H18A	120.3	C22—C40—H40C	109.5
C24—C19—C20	120.1 (2)	H40A—C40—H40C	109.5
C24—C19—N1	118.46 (19)	H40B—C40—H40C	109.5
C20—C19—N1	121.44 (19)	C28—C41—H41A	109.5
C19—C20—C21	119.5 (2)	C28—C41—H41B	109.5
C19—C20—H20A	120.3	H41A—C41—H41B	109.5
C21—C20—H20A	120.3	C28—C41—H41C	109.5
C20—C21—C22	121.4 (2)	H41A—C41—H41C	109.5
C20—C21—H21A	119.3	H41B—C41—H41C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···O1^{i}	0.95	2.55	3.409 (3)	150
C11—H11*A*···O2^{ii}	0.95	2.53	3.158 (3)	123
C18—H18*A*···O3	0.95	2.58	2.927 (3)	102
C30—H30*A*···O2	0.95	2.55	2.928 (3)	104
C32—H32*A*···N1	0.95	2.51	2.858 (3)	102
C39—H39*C*···O5^{iii}	0.98	2.48	3.422 (3)	160
C40—H40*C*···O4^{iv}	0.98	2.54	3.341 (3)	139

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