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4,7-Bis(4-methoxyphenyl)-1,3,7-triphenyl-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 = 0.058
wR factor = 0.139
Data-to-parameter ratio = 16.3

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

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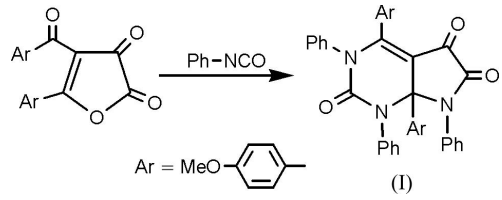
The synthesis of the title compound, $C_{38}H_{29}N_3O_5$, proceeds through a [4 + 2]-cycloaddition reaction. 4-(4-Methoxybenzoyl)-5-(4-methoxyphenyl)furan-2,3-dione was reacted with phenyl isocyanate to synthesize this new derivative of pyrrolo[2,3-*d*]pyrimidine in a low-temperature reaction. The molecule is composed of a pyrrolopyrimidine moiety with three phenyl and two *p*-methoxyphenyl substituents.

Comment

Some pyrrolo[2,3-*d*]pyrimidines are known to possess considerable antitumor, antiallergic, antiviral and anti-inflammatory activities (Hutzenlaub *et al.*, 1972; Smith *et al.*, 1972). As part of our interest in such compounds, we have synthesized and studied the single-crystal X-ray structure of the title compound, (I).



(I)

The molecular structure of (I) is illustrated in Fig. 1. Its structure is similar to that of 7,7a-dihydro-1,3-bis(4-methylphenyl)-4,7,7a-triphenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-2,5,6-(3*H*)-trione, (II) (Kollenz *et al.*, 1984). However, the substitution on the pyrrolopyrimidine moiety differs. In (I), the substituents on atoms N1 and N2 are phenyl, whereas in (II) they are *p*-tolyl. The substituents on atoms C1 and C6 in (I) are *p*-methoxyphenyl, whereas in (II) these substituents are phenyl. The bond lengths and angles for the pyrrolopyrimidine skeleton of (I) and (II) are comparable.

In the crystal structure of (I), there are intermolecular C—H···O hydrogen-bonding interactions (Table 1).

Experimental

A mixture of 4-(4-methoxybenzoyl)-5-(4-methoxyphenyl)furan-2,3-dione (1 g, 2.96 mmol) and phenyl isocyanate (1.05 g, 8.88 mmol) was heated at 333–338 K for 24 h without any solvent in a 25 ml round-bottomed flask equipped with a calcium chloride guard tube. After cooling to room temperature, the residue was treated with anhydrous diethyl ether and the crude product recrystallized from acetic acid and ethanol to give yellow crystals of (I) (yield: 1.26 g, 70%; m.p. 474 K). IR (KBr): ν 1730, 1686, 674 cm^{-1} (C═O), 1579 cm^{-1} (C═C). ^1H NMR ($CDCl_3$): δ 7.67–6.20 (*m*, 23H, Ph), 3.89, 3.76 (*s*, 6H, CH_3O); ^{13}C NMR ($CDCl_3$): δ 178.35, 165.37, 164.59 (C═O), 162.469–115.58 (C═C, aromatic and aliphatic), 81.36 (N—C—N), 57.53, 57.28

(CH_3O). Analysis calculated for $C_{38}H_{29}N_3O_5$: C 75.12, H 4.77, N 6.91%; found: C 74.75, H 4.83, N 7.01%.

Crystal data

$C_{38}H_{29}N_3O_5$	D_x = 1.348 Mg m^{-3}
M_r = 607.64	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2924 reflections
a = 13.196 (2) Å	θ = 4.5–50.6°
b = 19.853 (3) Å	μ = 0.09 mm^{-1}
c = 11.9850 (19) Å	T = 150 (2) K
β = 107.470 (3)°	Block, yellow
V = 2995.0 (8) Å^3	0.47 × 0.29 × 0.29 mm
Z = 4	

Data collection

Bruker SMART1000 diffractometer	3696 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.092
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	θ_{max} = 27.5°
T_{min} = 0.959, T_{max} = 0.974	$h = -16 \rightarrow 17$
25141 measured reflections	$k = -25 \rightarrow 24$
6764 independent reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.2194P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.058	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.139	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
6764 reflections	
415 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···O2^{i}	0.95	2.32	3.163 (3)	148
C20—H20A···O4^{ii}	0.95	2.43	3.366 (3)	169

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

H atoms were positioned geometrically and refined with a riding model (including torsional freedom for methyl groups), with C—H = 0.95–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) [1.5U_{eq}(C) for methyl groups].

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

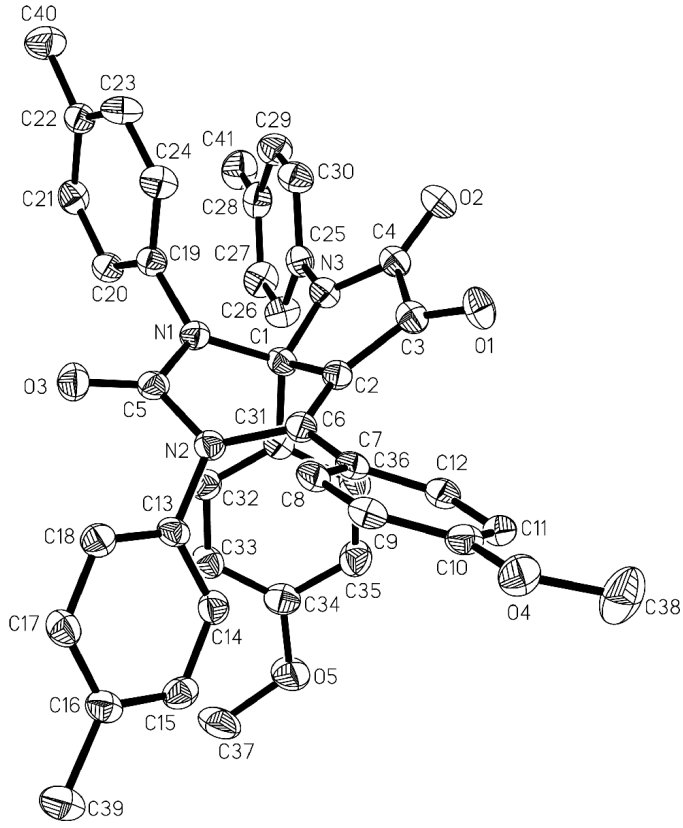


Figure 1
A view of the molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

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$h = -16 \rightarrow 17$
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Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.139$
$S = 1.01$
6764 reflections
415 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
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.2194P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ 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	0.22818 (15)	0.48148 (9)	0.61781 (15)	0.0209 (4)
N2	0.18582 (14)	0.38437 (9)	0.70492 (15)	0.0206 (4)
N3	0.35882 (14)	0.55639 (9)	0.74563 (16)	0.0235 (5)
O1	0.52084 (13)	0.43269 (9)	0.91803 (15)	0.0351 (5)
O2	0.54250 (13)	0.56121 (9)	0.81429 (15)	0.0334 (4)
O3	0.10243 (13)	0.40791 (8)	0.51149 (13)	0.0289 (4)
O4	0.43281 (15)	0.15394 (9)	1.05270 (17)	0.0510 (6)
O5	−0.04410 (13)	0.58606 (8)	0.94390 (13)	0.0293 (4)
C1	0.27425 (18)	0.50689 (11)	0.73901 (19)	0.0205 (5)
C2	0.33419 (18)	0.44833 (12)	0.80866 (19)	0.0219 (5)
C3	0.44564 (19)	0.46391 (12)	0.8553 (2)	0.0242 (6)
C4	0.45856 (19)	0.53296 (12)	0.8042 (2)	0.0259 (6)
C5	0.16730 (18)	0.42464 (11)	0.6028 (2)	0.0215 (5)
C6	0.28215 (18)	0.38811 (11)	0.79458 (19)	0.0217 (5)
C7	0.32216 (18)	0.32738 (11)	0.8633 (2)	0.0229 (5)
C8	0.31060 (19)	0.26354 (12)	0.8113 (2)	0.0288 (6)
H8A	0.2761	0.2593	0.7298	0.035*
C9	0.3485 (2)	0.20700 (13)	0.8765 (2)	0.0358 (7)
H9A	0.3415	0.1641	0.8400	0.043*
C10	0.3971 (2)	0.21303 (13)	0.9963 (2)	0.0336 (6)
C11	0.40979 (19)	0.27547 (13)	1.0502 (2)	0.0301 (6)
H11A	0.4436	0.2794	1.1320	0.036*
C12	0.37216 (18)	0.33236 (12)	0.9828 (2)	0.0252 (6)
H12A	0.3809	0.3754	1.0191	0.030*
C13	0.10620 (18)	0.33701 (11)	0.71430 (19)	0.0210 (5)
C14	0.07666 (18)	0.33935 (12)	0.8151 (2)	0.0261 (6)
H14A	0.1012	0.3747	0.8700	0.031*
C15	0.0107 (2)	0.28965 (13)	0.8357 (2)	0.0326 (6)
H15A	−0.0096	0.2907	0.9053	0.039*
C16	−0.0254 (2)	0.23872 (13)	0.7553 (2)	0.0343 (7)
H16A	−0.0673	0.2032	0.7713	0.041*
C17	−0.0003 (2)	0.23956 (12)	0.6513 (2)	0.0324 (6)
H17A	−0.0292	0.2063	0.5936	0.039*
C18	0.06626 (18)	0.28826 (12)	0.6305 (2)	0.0254 (6)
H18A	0.0844	0.2883	0.5596	0.030*

C19	0.23359 (18)	0.51563 (11)	0.51332 (19)	0.0216 (5)
C20	0.3053 (2)	0.49193 (12)	0.4600 (2)	0.0291 (6)
H20A	0.3492	0.4544	0.4918	0.035*
C21	0.3133 (2)	0.52310 (14)	0.3594 (2)	0.0373 (7)
H21A	0.3624	0.5070	0.3216	0.045*
C22	0.2491 (2)	0.57799 (14)	0.3144 (2)	0.0388 (7)
H22A	0.2550	0.6000	0.2463	0.047*
C23	0.1769 (2)	0.60060 (14)	0.3679 (2)	0.0384 (7)
H23A	0.1329	0.6381	0.3364	0.046*
C24	0.16810 (19)	0.56921 (12)	0.4669 (2)	0.0299 (6)
H24A	0.1172	0.5844	0.5030	0.036*
C25	0.34291 (18)	0.62442 (12)	0.7013 (2)	0.0258 (6)
C26	0.3860 (2)	0.64385 (13)	0.6147 (2)	0.0316 (6)
H26A	0.4268	0.6128	0.5858	0.038*
C27	0.3697 (2)	0.70842 (14)	0.5699 (2)	0.0398 (7)
H27A	0.3994	0.7217	0.5103	0.048*
C28	0.3107 (2)	0.75343 (14)	0.6113 (3)	0.0472 (8)
H28A	0.2978	0.7974	0.5790	0.057*
C29	0.2706 (2)	0.73459 (14)	0.6994 (3)	0.0527 (9)
H29A	0.2312	0.7661	0.7294	0.063*
C30	0.2867 (2)	0.67022 (13)	0.7453 (3)	0.0412 (7)
H30A	0.2590	0.6577	0.8070	0.049*
C31	0.18631 (17)	0.53146 (11)	0.78843 (19)	0.0192 (5)
C32	0.21130 (19)	0.54413 (11)	0.9084 (2)	0.0240 (6)
H32A	0.2828	0.5402	0.9567	0.029*
C33	0.13332 (19)	0.56213 (12)	0.9569 (2)	0.0265 (6)
H33A	0.1514	0.5711	1.0384	0.032*
C34	0.02751 (18)	0.56739 (11)	0.8875 (2)	0.0235 (5)
C35	0.00152 (19)	0.55514 (11)	0.7685 (2)	0.0246 (6)
H35A	−0.0699	0.5590	0.7202	0.029*
C36	0.08152 (18)	0.53710 (11)	0.7208 (2)	0.0235 (5)
H36A	0.0636	0.5284	0.6392	0.028*
C37	−0.15281 (19)	0.59270 (15)	0.8737 (2)	0.0400 (7)
H37A	−0.1963	0.6061	0.9234	0.060*
H37B	−0.1783	0.5495	0.8362	0.060*
H37C	−0.1581	0.6270	0.8134	0.060*
C38	0.4979 (2)	0.15750 (15)	1.1707 (2)	0.0466 (8)
H38A	0.5182	0.1119	1.2003	0.070*
H38B	0.4585	0.1794	1.2182	0.070*
H38C	0.5619	0.1837	1.1750	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0240 (11)	0.0196 (11)	0.0178 (10)	−0.0037 (9)	0.0043 (8)	−0.0029 (8)
N2	0.0208 (11)	0.0209 (11)	0.0171 (10)	−0.0027 (8)	0.0015 (8)	−0.0013 (8)
N3	0.0190 (11)	0.0227 (11)	0.0286 (12)	−0.0033 (9)	0.0071 (9)	−0.0055 (9)
O1	0.0243 (10)	0.0377 (11)	0.0358 (11)	0.0055 (8)	−0.0022 (8)	−0.0069 (8)

O2	0.0208 (9)	0.0374 (11)	0.0416 (11)	−0.0076 (8)	0.0086 (8)	−0.0135 (9)
O3	0.0333 (10)	0.0281 (10)	0.0187 (9)	−0.0080 (8)	−0.0022 (8)	0.0001 (7)
O4	0.0461 (12)	0.0344 (12)	0.0568 (13)	0.0014 (9)	−0.0083 (10)	0.0196 (10)
O5	0.0256 (10)	0.0405 (11)	0.0231 (9)	0.0030 (8)	0.0093 (8)	−0.0046 (8)
C1	0.0209 (12)	0.0187 (13)	0.0194 (12)	−0.0048 (10)	0.0023 (10)	−0.0047 (10)
C2	0.0211 (13)	0.0246 (14)	0.0180 (12)	0.0014 (10)	0.0029 (10)	−0.0043 (10)
C3	0.0223 (14)	0.0256 (14)	0.0230 (13)	0.0027 (11)	0.0042 (11)	−0.0081 (11)
C4	0.0222 (14)	0.0285 (14)	0.0254 (13)	−0.0014 (11)	0.0046 (11)	−0.0129 (11)
C5	0.0247 (13)	0.0212 (13)	0.0188 (13)	0.0000 (10)	0.0070 (11)	−0.0032 (10)
C6	0.0236 (13)	0.0246 (14)	0.0161 (12)	0.0038 (10)	0.0049 (10)	−0.0042 (10)
C7	0.0199 (13)	0.0231 (13)	0.0243 (13)	0.0002 (10)	0.0044 (10)	−0.0014 (10)
C8	0.0259 (14)	0.0271 (14)	0.0276 (14)	0.0019 (11)	−0.0008 (11)	−0.0044 (11)
C9	0.0282 (15)	0.0253 (15)	0.0447 (17)	0.0019 (12)	−0.0030 (13)	−0.0026 (13)
C10	0.0269 (15)	0.0273 (15)	0.0403 (16)	−0.0004 (12)	0.0005 (12)	0.0085 (13)
C11	0.0238 (14)	0.0391 (17)	0.0245 (13)	0.0016 (12)	0.0031 (11)	0.0064 (12)
C12	0.0228 (13)	0.0268 (14)	0.0245 (13)	0.0035 (11)	0.0047 (11)	−0.0019 (11)
C13	0.0217 (13)	0.0222 (13)	0.0177 (12)	0.0001 (10)	0.0036 (10)	0.0025 (10)
C14	0.0253 (14)	0.0308 (15)	0.0205 (13)	0.0028 (11)	0.0041 (11)	−0.0008 (11)
C15	0.0329 (16)	0.0391 (17)	0.0285 (14)	0.0060 (13)	0.0134 (12)	0.0097 (13)
C16	0.0317 (16)	0.0272 (15)	0.0472 (18)	0.0002 (12)	0.0166 (14)	0.0109 (13)
C17	0.0363 (16)	0.0249 (15)	0.0358 (16)	−0.0079 (12)	0.0103 (13)	−0.0041 (12)
C18	0.0284 (14)	0.0250 (14)	0.0235 (13)	−0.0039 (11)	0.0086 (11)	−0.0026 (11)
C19	0.0233 (13)	0.0204 (13)	0.0193 (12)	−0.0033 (10)	0.0037 (10)	−0.0016 (10)
C20	0.0345 (15)	0.0198 (14)	0.0333 (15)	−0.0022 (11)	0.0106 (12)	−0.0017 (11)
C21	0.0475 (18)	0.0362 (16)	0.0354 (16)	−0.0127 (14)	0.0232 (14)	−0.0096 (13)
C22	0.0461 (18)	0.0396 (18)	0.0261 (15)	−0.0167 (14)	0.0037 (13)	0.0065 (13)
C23	0.0314 (16)	0.0337 (16)	0.0431 (17)	−0.0072 (13)	0.0005 (14)	0.0136 (13)
C24	0.0237 (14)	0.0251 (14)	0.0396 (16)	−0.0030 (11)	0.0074 (12)	0.0041 (12)
C25	0.0219 (14)	0.0185 (13)	0.0350 (15)	−0.0054 (10)	0.0057 (11)	−0.0094 (11)
C26	0.0347 (16)	0.0271 (15)	0.0369 (15)	−0.0066 (12)	0.0167 (13)	−0.0087 (12)
C27	0.0373 (17)	0.0373 (17)	0.0471 (18)	−0.0098 (13)	0.0164 (14)	0.0020 (14)
C28	0.0390 (18)	0.0292 (17)	0.077 (2)	−0.0010 (13)	0.0229 (17)	0.0088 (16)
C29	0.050 (2)	0.0229 (16)	0.102 (3)	0.0020 (14)	0.049 (2)	−0.0017 (16)
C30	0.0417 (17)	0.0249 (16)	0.069 (2)	−0.0046 (13)	0.0340 (16)	−0.0061 (14)
C31	0.0210 (13)	0.0147 (12)	0.0208 (13)	0.0000 (9)	0.0046 (10)	−0.0018 (9)
C32	0.0208 (13)	0.0234 (14)	0.0232 (13)	−0.0018 (10)	−0.0003 (11)	−0.0030 (10)
C33	0.0298 (15)	0.0275 (14)	0.0196 (13)	−0.0025 (11)	0.0035 (11)	−0.0050 (11)
C34	0.0269 (14)	0.0197 (13)	0.0260 (14)	−0.0005 (10)	0.0112 (11)	−0.0012 (11)
C35	0.0216 (13)	0.0276 (14)	0.0219 (13)	0.0004 (11)	0.0025 (11)	−0.0007 (11)
C36	0.0248 (14)	0.0250 (13)	0.0190 (12)	0.0005 (10)	0.0038 (11)	−0.0020 (10)
C37	0.0232 (15)	0.0610 (19)	0.0370 (16)	0.0024 (14)	0.0109 (13)	−0.0118 (14)
C38	0.0417 (18)	0.055 (2)	0.0455 (18)	0.0189 (15)	0.0165 (15)	0.0284 (15)

Geometric parameters (Å, º)

N1—C5	1.366 (3)	C17—H17A	0.9500
N1—C19	1.445 (3)	C18—H18A	0.9500
N1—C1	1.484 (3)	C19—C20	1.375 (3)

N2—C6	1.399 (3)	C19—C24	1.378 (3)
N2—C5	1.420 (3)	C20—C21	1.387 (3)
N2—C13	1.439 (3)	C20—H20A	0.9500
N3—C4	1.374 (3)	C21—C22	1.387 (4)
N3—C25	1.444 (3)	C21—H21A	0.9500
N3—C1	1.471 (3)	C22—C23	1.373 (4)
O1—C3	1.219 (3)	C22—H22A	0.9500
O2—C4	1.215 (3)	C23—C24	1.375 (4)
O3—C5	1.216 (3)	C23—H23A	0.9500
O4—C10	1.365 (3)	C24—H24A	0.9500
O4—C38	1.418 (3)	C25—C30	1.375 (3)
O5—C34	1.368 (3)	C25—C26	1.379 (3)
O5—C37	1.435 (3)	C26—C27	1.381 (4)
C1—C2	1.509 (3)	C26—H26A	0.9500
C1—C31	1.532 (3)	C27—C28	1.372 (4)
C2—C6	1.364 (3)	C27—H27A	0.9500
C2—C3	1.441 (3)	C28—C29	1.368 (4)
C3—C4	1.532 (3)	C28—H28A	0.9500
C6—C7	1.466 (3)	C29—C30	1.382 (4)
C7—C12	1.388 (3)	C29—H29A	0.9500
C7—C8	1.400 (3)	C30—H30A	0.9500
C8—C9	1.373 (3)	C31—C36	1.382 (3)
C8—H8A	0.9500	C31—C32	1.399 (3)
C9—C10	1.391 (3)	C32—C33	1.372 (3)
C9—H9A	0.9500	C32—H32A	0.9500
C10—C11	1.385 (3)	C33—C34	1.398 (3)
C11—C12	1.391 (3)	C33—H33A	0.9500
C11—H11A	0.9500	C34—C35	1.384 (3)
C12—H12A	0.9500	C35—C36	1.390 (3)
C13—C14	1.377 (3)	C35—H35A	0.9500
C13—C18	1.380 (3)	C36—H36A	0.9500
C14—C15	1.386 (3)	C37—H37A	0.9800
C14—H14A	0.9500	C37—H37B	0.9800
C15—C16	1.379 (4)	C37—H37C	0.9800
C15—H15A	0.9500	C38—H38A	0.9800
C16—C17	1.382 (3)	C38—H38B	0.9800
C16—H16A	0.9500	C38—H38C	0.9800
C17—C18	1.379 (3)		

C5—N1—C19	116.98 (18)	C13—C18—H18A	120.5
C5—N1—C1	117.51 (18)	C20—C19—C24	120.8 (2)
C19—N1—C1	125.20 (18)	C20—C19—N1	117.6 (2)
C6—N2—C5	120.92 (19)	C24—C19—N1	121.6 (2)
C6—N2—C13	119.42 (18)	C19—C20—C21	119.6 (2)
C5—N2—C13	119.62 (18)	C19—C20—H20A	120.2
C4—N3—C25	121.07 (19)	C21—C20—H20A	120.2
C4—N3—C1	113.35 (19)	C22—C21—C20	119.4 (3)
C25—N3—C1	125.52 (18)	C22—C21—H21A	120.3

C10—O4—C38	117.8 (2)	C20—C21—H21A	120.3
C34—O5—C37	116.89 (18)	C23—C22—C21	120.3 (2)
N3—C1—N1	111.16 (18)	C23—C22—H22A	119.8
N3—C1—C2	102.81 (18)	C21—C22—H22A	119.8
N1—C1—C2	105.80 (17)	C22—C23—C24	120.3 (3)
N3—C1—C31	114.64 (17)	C22—C23—H23A	119.9
N1—C1—C31	110.55 (17)	C24—C23—H23A	119.9
C2—C1—C31	111.30 (18)	C23—C24—C19	119.5 (3)
C6—C2—C3	130.8 (2)	C23—C24—H24A	120.2
C6—C2—C1	116.5 (2)	C19—C24—H24A	120.2
C3—C2—C1	110.7 (2)	C30—C25—C26	119.7 (2)
O1—C3—C2	132.6 (2)	C30—C25—N3	120.8 (2)
O1—C3—C4	122.3 (2)	C26—C25—N3	119.4 (2)
C2—C3—C4	105.1 (2)	C25—C26—C27	120.0 (2)
O2—C4—N3	126.8 (2)	C25—C26—H26A	120.0
O2—C4—C3	125.5 (2)	C27—C26—H26A	120.0
N3—C4—C3	107.6 (2)	C28—C27—C26	120.2 (3)
O3—C5—N1	124.9 (2)	C28—C27—H27A	119.9
O3—C5—N2	121.0 (2)	C26—C27—H27A	119.9
N1—C5—N2	114.16 (19)	C29—C28—C27	119.6 (3)
C2—C6—N2	116.7 (2)	C29—C28—H28A	120.2
C2—C6—C7	124.6 (2)	C27—C28—H28A	120.2
N2—C6—C7	118.6 (2)	C28—C29—C30	120.8 (3)
C12—C7—C8	118.6 (2)	C28—C29—H29A	119.6
C12—C7—C6	120.0 (2)	C30—C29—H29A	119.6
C8—C7—C6	121.4 (2)	C25—C30—C29	119.6 (3)
C9—C8—C7	120.9 (2)	C25—C30—H30A	120.2
C9—C8—H8A	119.5	C29—C30—H30A	120.2
C7—C8—H8A	119.5	C36—C31—C32	118.3 (2)
C8—C9—C10	119.6 (2)	C36—C31—C1	122.7 (2)
C8—C9—H9A	120.2	C32—C31—C1	118.86 (19)
C10—C9—H9A	120.2	C33—C32—C31	120.5 (2)
O4—C10—C11	124.2 (2)	C33—C32—H32A	119.8
O4—C10—C9	114.9 (2)	C31—C32—H32A	119.8
C11—C10—C9	120.8 (2)	C32—C33—C34	120.6 (2)
C10—C11—C12	118.9 (2)	C32—C33—H33A	119.7
C10—C11—H11A	120.6	C34—C33—H33A	119.7
C12—C11—H11A	120.6	O5—C34—C35	124.2 (2)
C7—C12—C11	121.2 (2)	O5—C34—C33	116.1 (2)
C7—C12—H12A	119.4	C35—C34—C33	119.6 (2)
C11—C12—H12A	119.4	C34—C35—C36	119.0 (2)
C14—C13—C18	121.0 (2)	C34—C35—H35A	120.5
C14—C13—N2	116.9 (2)	C36—C35—H35A	120.5
C18—C13—N2	122.0 (2)	C31—C36—C35	121.9 (2)
C13—C14—C15	119.4 (2)	C31—C36—H36A	119.0
C13—C14—H14A	120.3	C35—C36—H36A	119.0
C15—C14—H14A	120.3	O5—C37—H37A	109.5
C16—C15—C14	120.1 (2)	O5—C37—H37B	109.5

C16—C15—H15A	120.0	H37A—C37—H37B	109.5
C14—C15—H15A	120.0	O5—C37—H37C	109.5
C15—C16—C17	119.7 (2)	H37A—C37—H37C	109.5
C15—C16—H16A	120.2	H37B—C37—H37C	109.5
C17—C16—H16A	120.2	O4—C38—H38A	109.5
C18—C17—C16	120.6 (2)	O4—C38—H38B	109.5
C18—C17—H17A	119.7	H38A—C38—H38B	109.5
C16—C17—H17A	119.7	O4—C38—H38C	109.5
C17—C18—C13	119.0 (2)	H38A—C38—H38C	109.5
C17—C18—H18A	120.5	H38B—C38—H38C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*A*···O2^{i}	0.95	2.32	3.163 (3)	148
C18—H18*A*···O3	0.95	2.47	2.883 (3)	106
C20—H20*A*···O4^{ii}	0.95	2.43	3.366 (3)	169
C36—H36*A*···N1	0.95	2.45	2.815 (3)	103

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