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5-(4-Methoxyphenyl)-4-methyl-1-phenyl-3-*p*-tolyl-1*H*-pyrazole

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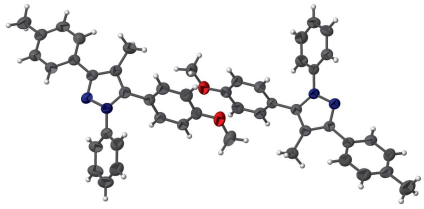
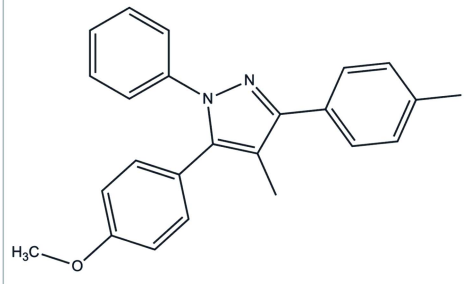
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{24}H_{22}N_2O$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The phenyl, *p*-tolyl and *p*-methoxyphenyl rings are inclined to the pyrazole ring by 42.5 (2), 17.68 (19) and 52.20 (19)°, respectively, in molecule *A*, and by 39.5 (2), 40.77 (19) and 59.76 (18)°, respectively, in molecule *B*. In the asymmetric unit, the pyrarole ring of molecule *A* makes a dihedral angle of 3.7 (2)° with that of molecule *B*. In the crystal, the two independent molecules are linked to each other by a C—H···O hydrogen bond.

3D view



Chemical scheme



Structure description

Trans-anethole {systematic name: 1-methoxy-4-[(*E*)-prop-1-en-1-yl]benzene} is an active ingredient of the essential oil of anise and the source of the aniseed scent. It has anti-genotoxic (Abraham *et al.*, 2001), gastroprotective and antioxidative (Freire *et al.*, 2005), and antimicrobial and antiviral (Astani *et al.*, 2010) properties. The molecule has a double bond in the aromatic portion, which confers some reactivity. In this work, we focused our efforts on the preparation of new pentagonal heterocyclic systems by the 1,3-dipolar cycloaddition reaction from *trans*-anethole and diarylnitrilimine.

The molecular structure of the title compound is illustrated in Fig. 1. The main geometric features are in good agreement with those observed in a similar compound (Loughzail *et al.*, 2014). In the crystal, the two crystallographically independent molecules are linked to each other into a dimer *via* a C—H···O hydrogen bond (C50—H50···O1^{i}; Table 1 and Fig. 2).

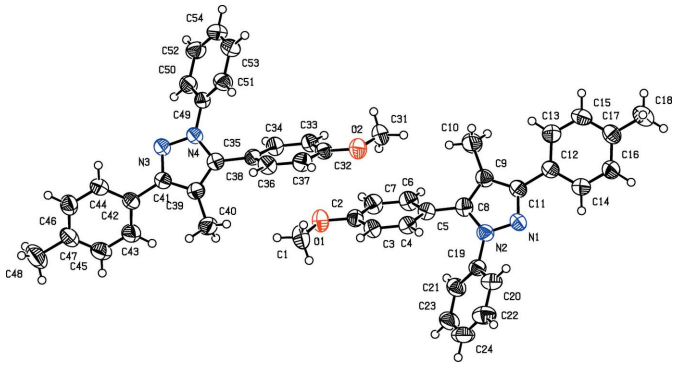


Figure 1
The asymmetric unit of the title compound with the atom-labelling scheme and 30% probability ellipsoids for non-H atoms.

Synthesis and crystallization

Triethylamine (9 mmol) dissolved in dichloromethane (5 ml) was added dropwise to a solution of anethole (6.74 mmol) and the precursor diarylnitrilimine (6.74 mmol) (Huisgen *et al.*, 1962) in dichloromethane (20 ml). After stirring for one day at room temperature, the mixture was washed several times with water (25 ml). The organic layers were separated, dried by anhydrous sodium sulfate, filtered and evaporated. The residue was purified in a silica gel column (eluent: hexane–ethyl acetate 2:98 *v*/*v*). We have isolated two products 1 and 2. Only the compound 2 is treated in this work. Single crystals of the title compound were obtained from a mixed solution of hexane and ethyl acetate (2:98 *v*/*v*) at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

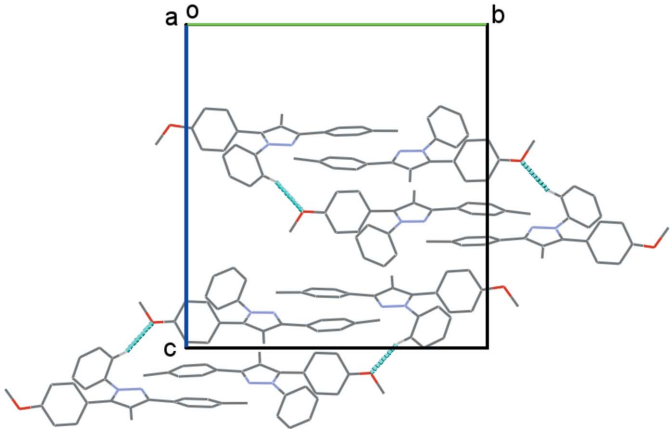


Figure 2
A partial packing diagram of the title compound viewed down the *a* axis, showing the C—H···O hydrogen bonds as blue lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C50—H50···O1^{i}	0.93	2.44	3.327 (4)	160

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{22}N_2O$
M_r	354.43
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	293
a, *b*, *c* (Å)	11.615 (5), 17.562 (4), 18.847 (8)
V (Å^3)	3844 (2)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.25 × 0.22
Data collection	
Diffractometer	Bruker X8 APEX
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.441, 0.981
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9494, 7577, 4885
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.117, 1.00
No. of reflections	7577
No. of parameters	494
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.17

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2017). **2**, x171626 [https://doi.org/10.1107/S2414314617016261]

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Crystal data

$C_{24}H_{22}N_2O$
M_r = 354.43
Orthorhombic, $P2_12_12_1$
a = 11.615 (5) Å
b = 17.562 (4) Å
c = 18.847 (8) Å
V = 3844 (2) Å^3
Z = 8
F(000) = 1504
D_x = 1.225 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7577 reflections
θ = 2.1–26.4°
μ = 0.08 mm^{-1}
T = 293 K
Box, white
0.30 × 0.25 × 0.22 mm

Data collection

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.441, T_{max} = 0.981
9494 measured reflections
7577 independent reflections
4885 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.4°, θ_{min} = 2.1°
h = −5→14
k = −21→16
l = −8→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.117
S = 1.00
7577 reflections
494 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2 + 0.0246P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: SHELXL2016 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0037 (7)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.3907 (2)	0.61275 (12)	0.07832 (13)	0.0600 (7)
O2	0.6071 (2)	0.44506 (13)	0.18934 (14)	0.0618 (7)
N1	0.1252 (2)	0.20939 (14)	0.10883 (13)	0.0459 (7)
N2	0.1370 (2)	0.28613 (14)	0.10968 (14)	0.0450 (7)
N3	0.8590 (2)	0.85027 (14)	0.12709 (13)	0.0436 (6)
N4	0.8512 (2)	0.77294 (13)	0.12969 (13)	0.0414 (6)
C1	0.3896 (4)	0.6563 (2)	0.1417 (2)	0.0702 (11)
H1A	0.417712	0.706600	0.131989	0.105*
H1B	0.437952	0.632338	0.176426	0.105*
H1C	0.312272	0.659319	0.159469	0.105*
C2	0.3526 (3)	0.53972 (17)	0.08170 (17)	0.0445 (8)
C3	0.3190 (3)	0.50307 (18)	0.14364 (16)	0.0451 (8)
H3	0.322648	0.528430	0.186900	0.054*
C4	0.2804 (3)	0.42947 (18)	0.14076 (16)	0.0443 (8)
H4	0.257938	0.405475	0.182511	0.053*
C5	0.2740 (3)	0.38955 (18)	0.07710 (16)	0.0437 (7)
C6	0.3081 (3)	0.42728 (19)	0.01563 (17)	0.0525 (9)
H6	0.304020	0.402153	−0.027736	0.063*
C7	0.3475 (3)	0.50075 (19)	0.01787 (17)	0.0535 (9)
H7	0.370943	0.524624	−0.023734	0.064*
C8	0.2350 (3)	0.30971 (18)	0.07626 (16)	0.0461 (8)
C9	0.2886 (3)	0.2449 (2)	0.05149 (17)	0.0487 (8)
C10	0.4015 (4)	0.2431 (2)	0.0128 (2)	0.0820 (14)
H10A	0.394819	0.210908	−0.028235	0.123*
H10B	0.460165	0.223427	0.043604	0.123*
H10C	0.421641	0.293692	−0.001873	0.123*
C11	0.2172 (3)	0.18364 (18)	0.07349 (16)	0.0440 (8)
C12	0.2317 (3)	0.10019 (18)	0.06841 (15)	0.0438 (8)
C13	0.3356 (3)	0.0659 (2)	0.05164 (19)	0.0574 (9)
H13	0.397459	0.095733	0.037359	0.069*
C14	0.1405 (3)	0.05216 (19)	0.08543 (19)	0.0549 (9)
H14	0.068522	0.073049	0.094795	0.066*
C15	0.3483 (3)	−0.0120 (2)	0.05586 (19)	0.0580 (9)
H15	0.419332	−0.033240	0.044624	0.070*
C16	0.1545 (3)	−0.0256 (2)	0.08871 (18)	0.0566 (9)
H16	0.091462	−0.055996	0.099709	0.068*
C17	0.2599 (3)	−0.05963 (19)	0.07607 (17)	0.0516 (9)
C18	0.2776 (4)	−0.1432 (2)	0.0865 (2)	0.0686 (11)
H18A	0.207149	−0.169697	0.076515	0.103*
H18B	0.300122	−0.152720	0.134700	0.103*
H18C	0.336832	−0.160790	0.055011	0.103*
C19	0.0522 (3)	0.32924 (18)	0.14675 (17)	0.0449 (8)
C20	0.0128 (3)	0.3022 (2)	0.21083 (17)	0.0551 (9)
H20	0.040889	0.256601	0.228984	0.066*
C21	0.0098 (3)	0.39652 (18)	0.11932 (19)	0.0551 (9)

H21	0.035792	0.414732	0.075852	0.066*
C22	−0.0685 (3)	0.3431 (2)	0.2479 (2)	0.0675 (11)
H22	−0.094828	0.325044	0.291347	0.081*
C23	−0.0719 (3)	0.4363 (2)	0.1575 (2)	0.0664 (11)
H23	−0.100984	0.481672	0.139356	0.080*
C24	−0.1109 (3)	0.4100 (2)	0.2216 (2)	0.0713 (12)
H24	−0.165644	0.437435	0.247008	0.086*
C31	0.5970 (4)	0.39782 (19)	0.1281 (2)	0.0701 (11)
H31A	0.569242	0.348494	0.141874	0.105*
H31B	0.670928	0.392678	0.105867	0.105*
H31C	0.543837	0.420494	0.095265	0.105*
C32	0.6434 (3)	0.51809 (18)	0.17963 (17)	0.0466 (8)
C33	0.6633 (3)	0.55078 (17)	0.11367 (17)	0.0473 (8)
H33	0.652377	0.522615	0.072428	0.057*
C34	0.6995 (3)	0.62521 (17)	0.10999 (16)	0.0464 (8)
H34	0.711752	0.646939	0.065629	0.056*
C35	0.7185 (3)	0.66915 (17)	0.17020 (15)	0.0399 (7)
C36	0.6979 (3)	0.63489 (19)	0.23567 (16)	0.0501 (8)
H36	0.709410	0.662726	0.277048	0.060*
C37	0.6610 (3)	0.5608 (2)	0.24019 (18)	0.0534 (9)
H37	0.647678	0.539093	0.284466	0.064*
C38	0.7539 (3)	0.74977 (18)	0.16443 (15)	0.0416 (7)
C39	0.6965 (3)	0.81413 (19)	0.18527 (16)	0.0452 (8)
C40	0.5837 (3)	0.8173 (2)	0.2233 (2)	0.0630 (10)
H40A	0.581630	0.861504	0.253183	0.095*
H40B	0.574666	0.772371	0.251761	0.095*
H40C	0.522278	0.820008	0.189263	0.095*
C41	0.7656 (3)	0.87515 (17)	0.16080 (15)	0.0407 (7)
C42	0.7479 (3)	0.95839 (17)	0.16699 (15)	0.0429 (8)
C43	0.6422 (3)	0.9920 (2)	0.1569 (2)	0.0575 (9)
H43	0.578354	0.961348	0.148218	0.069*
C44	0.8406 (3)	1.00620 (19)	0.18066 (17)	0.0496 (8)
H44	0.913078	0.985398	0.188486	0.060*
C45	0.6285 (3)	1.0697 (2)	0.15938 (19)	0.0622 (10)
H45	0.555578	1.090348	0.152831	0.075*
C46	0.8263 (3)	1.0847 (2)	0.18279 (19)	0.0571 (10)
H46	0.889482	1.115594	0.192148	0.069*
C47	0.7200 (4)	1.1177 (2)	0.17129 (19)	0.0589 (10)
C48	0.7046 (5)	1.2031 (2)	0.1710 (3)	0.0912 (15)
H48A	0.743677	1.224671	0.211073	0.137*
H48B	0.624030	1.215025	0.173644	0.137*
H48C	0.736124	1.223728	0.128029	0.137*
C49	0.9395 (3)	0.72868 (17)	0.09685 (17)	0.0418 (8)
C50	0.9843 (3)	0.75376 (19)	0.03285 (17)	0.0503 (8)
H50	0.957752	0.798646	0.012419	0.060*
C51	0.9805 (3)	0.66320 (19)	0.12800 (19)	0.0548 (9)
H51	0.952290	0.647393	0.171771	0.066*
C52	1.0688 (3)	0.7114 (2)	−0.0003 (2)	0.0598 (10)

H52	1.099358	0.727963	−0.043213	0.072*
C53	1.0642 (3)	0.6211 (2)	0.0934 (2)	0.0643 (10)
H53	1.090963	0.576157	0.113607	0.077*
C54	1.1081 (3)	0.6450 (2)	0.0298 (2)	0.0649 (11)
H54	1.164328	0.616321	0.006960	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0741 (16)	0.0462 (14)	0.0597 (14)	−0.0098 (13)	−0.0039 (14)	0.0067 (11)
O2	0.0678 (16)	0.0454 (14)	0.0721 (16)	−0.0050 (13)	0.0089 (14)	0.0112 (12)
N1	0.0503 (16)	0.0393 (16)	0.0480 (15)	0.0027 (13)	−0.0005 (14)	−0.0044 (12)
N2	0.0473 (17)	0.0444 (16)	0.0434 (15)	0.0020 (13)	0.0024 (13)	−0.0037 (12)
N3	0.0492 (16)	0.0400 (15)	0.0415 (14)	0.0016 (13)	0.0025 (13)	0.0003 (11)
N4	0.0463 (16)	0.0366 (15)	0.0412 (14)	0.0029 (12)	0.0019 (13)	0.0002 (11)
C1	0.086 (3)	0.046 (2)	0.078 (3)	−0.007 (2)	−0.008 (2)	−0.0056 (19)
C2	0.0439 (18)	0.0408 (19)	0.0489 (18)	0.0001 (15)	−0.0064 (16)	0.0034 (15)
C3	0.0548 (19)	0.0447 (19)	0.0358 (16)	−0.0002 (16)	−0.0025 (15)	−0.0022 (14)
C4	0.0505 (19)	0.0479 (19)	0.0346 (15)	−0.0001 (16)	0.0016 (15)	0.0025 (14)
C5	0.0467 (18)	0.0467 (18)	0.0378 (16)	−0.0006 (16)	−0.0011 (16)	0.0010 (14)
C6	0.065 (2)	0.056 (2)	0.0366 (17)	−0.0001 (19)	0.0025 (16)	−0.0025 (15)
C7	0.066 (2)	0.053 (2)	0.0418 (18)	−0.002 (2)	0.0053 (18)	0.0086 (15)
C8	0.056 (2)	0.0486 (19)	0.0340 (15)	−0.0028 (17)	0.0000 (16)	−0.0028 (14)
C9	0.055 (2)	0.048 (2)	0.0431 (17)	0.0005 (18)	0.0046 (17)	−0.0057 (15)
C10	0.086 (3)	0.062 (3)	0.098 (3)	−0.006 (2)	0.048 (3)	−0.012 (2)
C11	0.0502 (19)	0.0447 (18)	0.0372 (16)	0.0029 (17)	−0.0023 (16)	−0.0043 (14)
C12	0.0494 (19)	0.0464 (19)	0.0355 (16)	0.0019 (17)	0.0002 (16)	−0.0042 (13)
C13	0.054 (2)	0.056 (2)	0.062 (2)	−0.0011 (19)	0.0084 (19)	−0.0053 (18)
C14	0.049 (2)	0.053 (2)	0.062 (2)	0.0038 (17)	0.0077 (19)	−0.0031 (17)
C15	0.054 (2)	0.058 (2)	0.061 (2)	0.015 (2)	0.0041 (19)	−0.0093 (18)
C16	0.059 (2)	0.049 (2)	0.061 (2)	−0.0015 (18)	0.0105 (19)	−0.0041 (18)
C17	0.063 (2)	0.049 (2)	0.0431 (18)	0.004 (2)	−0.0049 (18)	−0.0082 (15)
C18	0.082 (3)	0.055 (2)	0.068 (2)	0.013 (2)	0.005 (2)	−0.004 (2)
C19	0.0393 (17)	0.047 (2)	0.0485 (19)	0.0030 (15)	−0.0057 (15)	−0.0079 (15)
C20	0.0467 (19)	0.066 (2)	0.052 (2)	0.0113 (19)	0.0012 (18)	−0.0035 (18)
C21	0.055 (2)	0.052 (2)	0.059 (2)	0.0073 (18)	−0.0079 (19)	−0.0030 (17)
C22	0.057 (2)	0.089 (3)	0.057 (2)	0.010 (2)	0.005 (2)	−0.010 (2)
C23	0.054 (2)	0.054 (2)	0.091 (3)	0.0135 (19)	−0.013 (2)	−0.009 (2)
C24	0.045 (2)	0.085 (3)	0.083 (3)	0.015 (2)	0.000 (2)	−0.024 (2)
C31	0.071 (3)	0.042 (2)	0.098 (3)	−0.0032 (19)	0.010 (2)	−0.002 (2)
C32	0.0457 (19)	0.0405 (19)	0.0535 (19)	0.0045 (16)	0.0050 (17)	0.0078 (16)
C33	0.054 (2)	0.0426 (19)	0.0457 (18)	−0.0001 (16)	0.0017 (16)	0.0001 (14)
C34	0.056 (2)	0.047 (2)	0.0360 (17)	−0.0026 (16)	0.0025 (15)	0.0023 (14)
C35	0.0389 (17)	0.0427 (19)	0.0379 (16)	−0.0009 (15)	0.0009 (14)	0.0014 (13)
C36	0.061 (2)	0.052 (2)	0.0368 (17)	0.0026 (18)	0.0015 (16)	0.0007 (15)
C37	0.060 (2)	0.058 (2)	0.0428 (17)	0.0002 (19)	0.0076 (17)	0.0102 (16)
C38	0.0443 (18)	0.0461 (18)	0.0345 (16)	−0.0003 (17)	−0.0035 (14)	−0.0010 (14)
C39	0.0431 (18)	0.053 (2)	0.0391 (16)	−0.0016 (17)	−0.0024 (15)	−0.0105 (15)

C40	0.052 (2)	0.065 (2)	0.072 (2)	−0.006 (2)	0.012 (2)	−0.021 (2)
C41	0.0440 (18)	0.0439 (19)	0.0342 (15)	0.0019 (16)	−0.0043 (15)	−0.0039 (13)
C42	0.0502 (19)	0.0434 (19)	0.0352 (16)	0.0036 (16)	0.0014 (15)	−0.0048 (13)
C43	0.051 (2)	0.055 (2)	0.066 (2)	0.0045 (19)	−0.0041 (19)	−0.0040 (17)
C44	0.051 (2)	0.048 (2)	0.0499 (19)	0.0069 (17)	0.0033 (17)	−0.0034 (15)
C45	0.059 (2)	0.058 (2)	0.070 (2)	0.015 (2)	0.002 (2)	0.0017 (19)
C46	0.067 (2)	0.048 (2)	0.057 (2)	−0.0054 (19)	0.002 (2)	−0.0076 (17)
C47	0.076 (3)	0.043 (2)	0.057 (2)	0.009 (2)	0.011 (2)	−0.0014 (16)
C48	0.118 (4)	0.047 (2)	0.109 (4)	0.013 (3)	0.017 (3)	−0.001 (2)
C49	0.0397 (17)	0.0391 (18)	0.0465 (18)	−0.0001 (14)	−0.0010 (15)	−0.0040 (14)
C50	0.055 (2)	0.0459 (19)	0.0504 (19)	0.0017 (18)	0.0050 (18)	−0.0004 (16)
C51	0.053 (2)	0.050 (2)	0.062 (2)	0.0086 (18)	0.0002 (19)	0.0055 (17)
C52	0.051 (2)	0.068 (3)	0.060 (2)	−0.001 (2)	0.0128 (19)	−0.0093 (19)
C53	0.054 (2)	0.050 (2)	0.089 (3)	0.0123 (19)	−0.001 (2)	0.003 (2)
C54	0.048 (2)	0.062 (2)	0.085 (3)	0.009 (2)	0.010 (2)	−0.014 (2)

Geometric parameters (Å, º)

O1—C1	1.418 (4)	C22—H22	0.9300
O1—C2	1.358 (4)	C23—C24	1.371 (5)
O2—C31	1.427 (4)	C23—H23	0.9300
O2—C32	1.362 (4)	C24—H24	0.9300
N1—C11	1.337 (4)	C31—H31A	0.9600
N2—N1	1.355 (3)	C31—H31B	0.9600
N2—C8	1.365 (4)	C31—H31C	0.9600
N4—N3	1.362 (3)	C32—C37	1.381 (5)
N4—C38	1.367 (4)	C32—C33	1.389 (4)
C1—H1A	0.9600	C33—H33	0.9300
C1—H1B	0.9600	C34—C33	1.375 (4)
C1—H1C	0.9600	C34—C35	1.390 (4)
C3—C4	1.369 (4)	C34—H34	0.9300
C3—C2	1.389 (4)	C35—C38	1.478 (4)
C3—H3	0.9300	C36—C37	1.374 (5)
C4—C5	1.392 (4)	C36—C35	1.393 (4)
C4—H4	0.9300	C36—H36	0.9300
C5—C6	1.392 (4)	C37—H37	0.9300
C6—H6	0.9300	C38—C39	1.370 (4)
C7—C2	1.385 (4)	C39—C40	1.494 (5)
C7—C6	1.370 (4)	C40—H40A	0.9600
C7—H7	0.9300	C40—H40B	0.9600
C8—C5	1.473 (4)	C40—H40C	0.9600
C8—C9	1.379 (4)	C41—N3	1.331 (4)
C9—C10	1.501 (5)	C41—C39	1.416 (4)
C10—H10A	0.9600	C42—C43	1.376 (5)
C10—H10B	0.9600	C42—C44	1.389 (5)
C10—H10C	0.9600	C42—C41	1.481 (4)
C11—C9	1.420 (5)	C43—C45	1.375 (5)
C12—C13	1.385 (5)	C43—H43	0.9300

C12—C14	1.391 (5)	C44—C46	1.389 (5)
C12—C11	1.478 (4)	C44—H44	0.9300
C13—C15	1.377 (5)	C45—C47	1.375 (5)
C13—H13	0.9300	C45—H45	0.9300
C14—C16	1.376 (5)	C46—C47	1.380 (5)
C14—H14	0.9300	C46—H46	0.9300
C15—C17	1.378 (5)	C47—C48	1.510 (5)
C15—H15	0.9300	C48—H48A	0.9600
C16—C17	1.383 (5)	C48—H48B	0.9600
C16—H16	0.9300	C48—H48C	0.9600
C17—C18	1.495 (5)	C49—C51	1.376 (4)
C18—H18A	0.9600	C49—C50	1.386 (4)
C18—H18B	0.9600	C49—N4	1.428 (4)
C18—H18C	0.9600	C50—C52	1.380 (5)
C19—C20	1.376 (4)	C50—H50	0.9300
C19—C21	1.381 (4)	C51—C53	1.385 (5)
C19—N2	1.426 (4)	C51—H51	0.9300
C20—C22	1.377 (5)	C52—C54	1.376 (5)
C20—H20	0.9300	C52—H52	0.9300
C21—C23	1.380 (5)	C53—C54	1.368 (5)
C21—H21	0.9300	C53—H53	0.9300
C22—C24	1.367 (5)	C54—H54	0.9300

C2—O1—C1	117.8 (3)	C24—C23—H23	119.5
C41—N3—N4	104.8 (3)	C21—C23—H23	119.5
C32—O2—C31	117.7 (3)	C22—C24—C23	119.3 (4)
C11—N1—N2	105.2 (3)	C22—C24—H24	120.3
N1—N2—C8	112.4 (3)	C23—C24—H24	120.3
N1—N2—C19	117.6 (3)	O2—C31—H31A	109.5
N3—N4—C38	111.7 (2)	O2—C31—H31B	109.5
N3—N4—C49	118.6 (3)	H31A—C31—H31B	109.5
C38—N4—C49	129.7 (2)	O2—C31—H31C	109.5
C8—N2—C19	129.9 (3)	H31A—C31—H31C	109.5
O1—C1—H1A	109.5	H31B—C31—H31C	109.5
O1—C1—H1B	109.5	O2—C32—C37	116.5 (3)
O1—C1—H1C	109.5	O2—C32—C33	124.1 (3)
H1A—C1—H1B	109.5	C37—C32—C33	119.4 (3)
H1A—C1—H1C	109.5	C34—C33—C32	119.3 (3)
H1B—C1—H1C	109.5	C34—C33—H33	120.4
O1—C2—C7	116.1 (3)	C32—C33—H33	120.4
O1—C2—C3	124.7 (3)	C33—C34—C35	122.4 (3)
C7—C2—C3	119.2 (3)	C33—C34—H34	118.8
C4—C3—C2	119.7 (3)	C35—C34—H34	118.8
C4—C3—H3	120.1	C34—C35—C36	117.1 (3)
C2—C3—H3	120.1	C34—C35—C38	121.0 (3)
C3—C4—C5	121.8 (3)	C36—C35—C38	121.8 (3)
C3—C4—H4	119.1	C37—C36—C35	121.2 (3)
C5—C4—H4	119.1	C37—C36—H36	119.4

C4—C5—C6	117.5 (3)	C35—C36—H36	119.4
C4—C5—C8	120.3 (3)	C36—C37—C32	120.6 (3)
C6—C5—C8	122.1 (3)	C36—C37—H37	119.7
C7—C6—C5	121.2 (3)	C32—C37—H37	119.7
C7—C6—H6	119.4	N4—C38—C39	107.1 (3)
C5—C6—H6	119.4	N4—C38—C35	123.4 (3)
C6—C7—C2	120.4 (3)	C39—C38—C35	129.3 (3)
C6—C7—H7	119.8	C38—C39—C41	104.8 (3)
C2—C7—H7	119.8	C38—C39—C40	126.5 (3)
N2—C8—C9	106.4 (3)	C41—C39—C40	128.7 (3)
N2—C8—C5	122.7 (3)	C39—C40—H40A	109.5
C9—C8—C5	130.6 (3)	C39—C40—H40B	109.5
C8—C9—C11	105.3 (3)	H40A—C40—H40B	109.5
C8—C9—C10	125.2 (3)	C39—C40—H40C	109.5
C11—C9—C10	129.5 (3)	H40A—C40—H40C	109.5
C9—C10—H10A	109.5	H40B—C40—H40C	109.5
C9—C10—H10B	109.5	N3—C41—C39	111.7 (3)
H10A—C10—H10B	109.5	N3—C41—C42	118.3 (3)
C9—C10—H10C	109.5	C39—C41—C42	130.0 (3)
H10A—C10—H10C	109.5	C43—C42—C44	117.3 (3)
H10B—C10—H10C	109.5	C43—C42—C41	122.4 (3)
N1—C11—C9	110.8 (3)	C44—C42—C41	120.3 (3)
N1—C11—C12	117.3 (3)	C45—C43—C42	121.6 (3)
C9—C11—C12	131.7 (3)	C45—C43—H43	119.2
C13—C12—C14	116.8 (3)	C42—C43—H43	119.2
C13—C12—C11	123.1 (3)	C42—C44—C46	120.9 (3)
C14—C12—C11	119.9 (3)	C42—C44—H44	119.6
C15—C13—C12	120.8 (4)	C46—C44—H44	119.6
C15—C13—H13	119.6	C47—C45—C43	121.7 (4)
C12—C13—H13	119.6	C47—C45—H45	119.2
C16—C14—C12	121.5 (3)	C43—C45—H45	119.2
C16—C14—H14	119.3	C47—C46—C44	121.3 (4)
C12—C14—H14	119.3	C47—C46—H46	119.4
C13—C15—C17	122.6 (3)	C44—C46—H46	119.4
C13—C15—H15	118.7	C45—C47—C46	117.4 (3)
C17—C15—H15	118.7	C45—C47—C48	121.1 (4)
C14—C16—C17	121.7 (4)	C46—C47—C48	121.6 (4)
C14—C16—H16	119.1	C47—C48—H48A	109.5
C17—C16—H16	119.1	C47—C48—H48B	109.5
C15—C17—C16	116.4 (3)	H48A—C48—H48B	109.5
C15—C17—C18	122.0 (3)	C47—C48—H48C	109.5
C16—C17—C18	121.6 (4)	H48A—C48—H48C	109.5
C17—C18—H18A	109.5	H48B—C48—H48C	109.5
C17—C18—H18B	109.5	C51—C49—C50	120.5 (3)
H18A—C18—H18B	109.5	C51—C49—N4	121.2 (3)
C17—C18—H18C	109.5	C50—C49—N4	118.3 (3)
H18A—C18—H18C	109.5	C52—C50—C49	119.3 (3)
H18B—C18—H18C	109.5	C52—C50—H50	120.3

C20—C19—C21	120.4 (3)	C49—C50—H50	120.3
C20—C19—N2	118.5 (3)	C49—C51—C53	119.2 (3)
C21—C19—N2	121.2 (3)	C49—C51—H51	120.4
C19—C20—C22	119.5 (3)	C53—C51—H51	120.4
C19—C20—H20	120.2	C54—C52—C50	120.4 (4)
C22—C20—H20	120.2	C54—C52—H52	119.8
C23—C21—C19	118.9 (4)	C50—C52—H52	119.8
C23—C21—H21	120.5	C54—C53—C51	120.7 (4)
C19—C21—H21	120.5	C54—C53—H53	119.6
C24—C22—C20	120.8 (4)	C51—C53—H53	119.6
C24—C22—H22	119.6	C53—C54—C52	119.8 (4)
C20—C22—H22	119.6	C53—C54—H54	120.1
C24—C23—C21	121.0 (4)	C52—C54—H54	120.1

C1—O1—C2—C3	−4.0 (5)	C20—C22—C24—C23	0.1 (5)
C1—O1—C2—C7	175.7 (3)	C21—C23—C24—C22	−0.3 (5)
C11—N1—N2—C8	−0.6 (3)	C41—N3—N4—C38	0.2 (3)
C11—N1—N2—C19	−177.7 (3)	C41—N3—N4—C49	179.3 (3)
N2—N1—C11—C9	0.0 (3)	N4—N3—C41—C39	−0.2 (3)
N2—N1—C11—C12	175.9 (3)	N4—N3—C41—C42	−179.7 (3)
N1—N2—C8—C5	−172.8 (3)	N3—N4—C38—C35	174.9 (3)
N1—N2—C8—C9	1.0 (3)	N3—N4—C38—C39	−0.1 (3)
C19—N2—C8—C5	3.8 (5)	C49—N4—C38—C35	−4.1 (5)
C19—N2—C8—C9	177.6 (3)	C49—N4—C38—C39	−179.1 (3)
N1—N2—C19—C20	41.0 (4)	N3—N4—C49—C50	−39.0 (4)
N1—N2—C19—C21	−138.9 (3)	N3—N4—C49—C51	140.3 (3)
C8—N2—C19—C20	−135.5 (3)	C38—N4—C49—C50	140.0 (3)
C8—N2—C19—C21	44.7 (5)	C38—N4—C49—C51	−40.8 (5)
O1—C2—C3—C4	179.1 (3)	O2—C32—C33—C34	179.8 (3)
C7—C2—C3—C4	−0.6 (5)	C37—C32—C33—C34	−0.4 (5)
O1—C2—C7—C6	−178.7 (3)	O2—C32—C37—C36	179.8 (3)
C3—C2—C7—C6	1.0 (5)	C33—C32—C37—C36	−0.1 (5)
C31—O2—C32—C37	−175.1 (3)	C32—C33—C34—C35	0.8 (5)
C31—O2—C32—C33	4.7 (5)	C33—C34—C35—C36	−0.8 (5)
C2—C3—C4—C5	0.2 (5)	C33—C34—C35—C38	−178.1 (3)
C3—C4—C5—C6	−0.2 (5)	C34—C35—C36—C37	0.3 (5)
C3—C4—C5—C8	178.3 (3)	C38—C35—C36—C37	177.6 (3)
C8—C5—C6—C7	−177.9 (3)	C34—C35—C38—N4	−58.1 (5)
C4—C5—C8—N2	49.4 (5)	C34—C35—C38—C39	115.8 (4)
C6—C5—C8—N2	−132.2 (3)	C36—C35—C38—N4	124.7 (3)
C6—C5—C8—C9	55.7 (5)	C36—C35—C38—C39	−61.4 (5)
C4—C5—C8—C9	−122.8 (4)	C35—C36—C37—C32	0.1 (5)
C4—C5—C6—C7	0.6 (5)	N4—C38—C39—C40	178.2 (3)
C5—C6—C7—C2	−1.0 (5)	N4—C38—C39—C41	0.0 (3)
C5—C8—C9—C10	−5.2 (6)	C35—C38—C39—C40	3.5 (5)
C5—C8—C9—C11	172.2 (3)	C35—C38—C39—C41	−174.7 (3)
N2—C8—C9—C11	−0.9 (3)	C38—C39—C41—N3	0.1 (4)
N2—C8—C9—C10	−178.3 (3)	C38—C39—C41—C42	179.6 (3)

C8—C9—C11—N1	0.6 (4)	C40—C39—C41—N3	−178.0 (3)
C10—C9—C11—C12	2.7 (6)	C40—C39—C41—C42	1.5 (6)
C8—C9—C11—C12	−174.5 (3)	N3—C41—C42—C43	137.5 (3)
C10—C9—C11—N1	177.9 (3)	N3—C41—C42—C44	−39.8 (4)
C9—C11—C12—C13	13.4 (5)	C39—C41—C42—C43	−41.9 (5)
C9—C11—C12—C14	−171.0 (3)	C39—C41—C42—C44	140.7 (3)
N1—C11—C12—C13	−161.5 (3)	C41—C42—C43—C45	−176.7 (3)
N1—C11—C12—C14	14.2 (4)	C44—C42—C43—C45	0.7 (5)
C11—C12—C14—C16	−172.9 (3)	C41—C42—C44—C46	176.5 (3)
C11—C12—C13—C15	172.2 (3)	C43—C42—C44—C46	−1.0 (5)
C14—C12—C13—C15	−3.6 (5)	C42—C43—C45—C47	0.7 (6)
C13—C12—C14—C16	3.0 (5)	C42—C44—C46—C47	−0.1 (5)
C12—C13—C15—C17	0.5 (5)	C43—C45—C47—C46	−1.8 (5)
C12—C14—C16—C17	0.7 (5)	C43—C45—C47—C48	177.6 (4)
C13—C15—C17—C18	−174.6 (3)	C44—C46—C47—C45	1.5 (5)
C13—C15—C17—C16	3.2 (5)	C44—C46—C47—C48	−177.8 (4)
C14—C16—C17—C15	−3.8 (5)	N4—C49—C50—C52	−179.2 (3)
C14—C16—C17—C18	174.0 (3)	C51—C49—C50—C52	1.5 (5)
N2—C19—C20—C22	179.5 (3)	N4—C49—C51—C53	178.4 (3)
C20—C19—C21—C23	0.5 (5)	C50—C49—C51—C53	−2.3 (5)
C21—C19—C20—C22	−0.7 (5)	C49—C50—C52—C54	0.0 (5)
N2—C19—C21—C23	−179.7 (3)	C49—C51—C53—C54	1.6 (5)
C19—C20—C22—C24	0.3 (5)	C50—C52—C54—C53	−0.7 (5)
C19—C21—C23—C24	0.0 (5)	C51—C53—C54—C52	−0.1 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C50—H50···O1^{i}	0.93	2.44	3.327 (4)	160

Symmetry code: (i) *x*+1/2, −*y*+3/2, −*z*.