IUCrData

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2-(5-Methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-5-phenyl-1,3,4-oxadiazole

Gamal A. El-Hiti,[a]* Bakr F. Abdel-Wahab,[b,c] Mohamed S. Mostafa,[d] Rizk E. Khidre,[d,e] Amany S. Hegazy[f] and Benson M. Kariuki[f]‡

[a]Cornea Research Chair, Department of Optometry, College of Applied Medical Sciences, King Saud University, PO Box 10219, Riyadh 11433, Saudi Arabia, [b]Department of Chemistry, College of Science and Humanities, Shaqra University, Duwadimi, Saudi Arabia, [c]Applied Organic Chemistry Department, National Research Centre, Dokki, Giza, Egypt, [d]Chemistry Department, Faculty of Science, Jazan University, Jazan 2079, Saudi Arabia, [e]Chemical Industries Division, National Research Centre, Dokki 12622, Giza, Egypt, and [f]School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, UK. *Correspondence e-mail: gelhiti@ksu.edu.sa

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‡ Additional corresponding author, e-mail: kariukib@cardiff.ac.uk.

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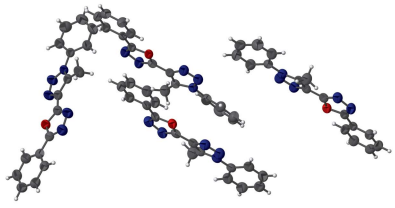
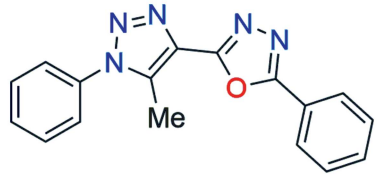
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{17}H_{13}N_5O$, comprises four independent molecules (*A*–*D*). The respective interplanar angles between the phenyl/oxadiazole/methyltriazole/phenyl rings for the four independent molecules are *A* 8.8 (2), 13.0 (2), 22.5 (2)°; *B* 6.3 (2), 8.9 (2), 29.0 (1)°; *C* 4.0 (2), 10.0 (2), 24.5 (2)°; *D* 3.5 (2), 10.1 (2), 27.2 (2)°. In the crystal, molecules form two separate stacks parallel to the *b*-axis direction: one consists of *A* and *D* molecules, and the other of *B* and *C* molecules. Aromatic π–π stacking is observed within each stack, with the shortest centroid–centroid separation being 3.552 (2) Å.

3D view



Chemical scheme



Structure description

The synthesis of heterocycles containing triazole and oxadiazole moieties is of interest because of their biological activities (Bonandi *et al.*, 2017; Kumar & Kaur, 2014; Li *et al.*, 2011; Rajak *et al.*, 2011). As part of our studies in this area, we now report the synthesis and structure of the title compound.

The asymmetric unit comprises four independent molecules [*A* (C1–C17), *B* (C18–C34), *C* (C35–C51), *D* (C52–C68)] of $C_{17}H_{13}N_5O$ (Fig. 1). The molecule consists of a phenyl/oxadiazole/methyltriazole/phenyl ring system. The respective dihedral angles between the rings for the four independent molecules are (*A*) 8.8 (2), 13.0 (2), 22.5 (2)°; (*B*) 6.3 (2), 8.9 (2), 29.0 (1)°; (*C*) 4.0 (2), 10.0 (2), 24.5 (2)°; (*D*) 3.5 (2), 10.1 (2), 27.2 (2)°.

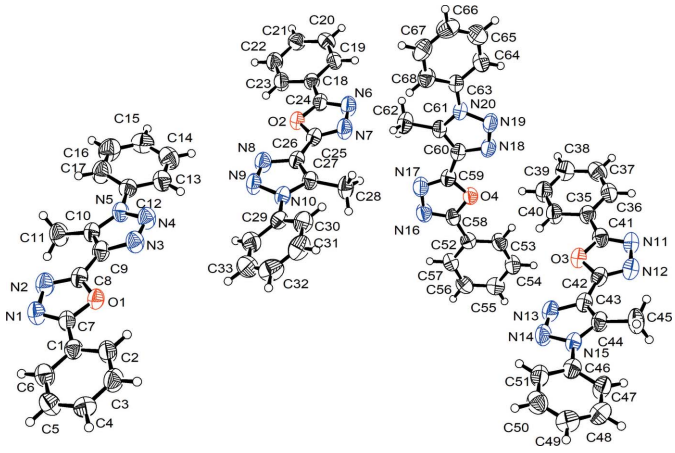


Figure 1
The molecular structure showing 50% probability.

In the crystal, the molecules stack parallel to the *b*-axis direction (Fig. 2). Two types of stack are observed with each composed of two of the four independent molecules (*A* and *D* in one stack; *B* and *C* in the other stack). Aromatic π–π stacking is observed within each stack, with the shortest centroid–centroid separation being 3.552 (2) Å.

Synthesis and crystallization

The title compound was synthesized according to the literature procedure (Abdel-Wahab *et al.*, 2017) and recrystallized from dimethylformamide solution to give colourless needles.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. This structure has a strong *b*/2 subcell containing two molecules in the asymmetric unit but refinements based on this model led to unrealistic displacement parameters for the atoms of the phenyl ring bound to the triazole ring and much poorer residuals.

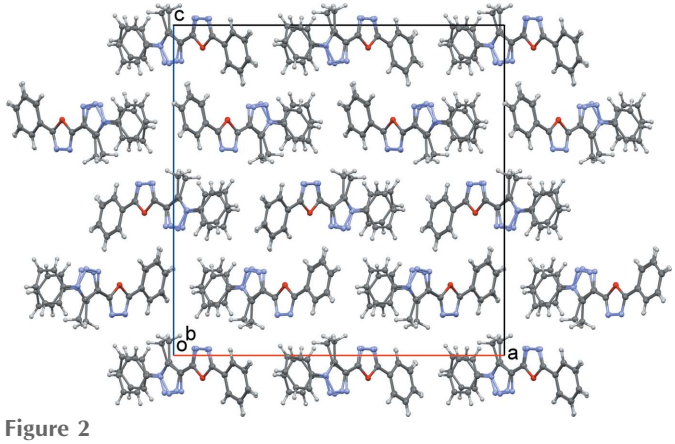


Figure 2
Crystal packing viewed down the *b* axis.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{13}N_5O$
M_r	303.32
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	296
a, *b*, *c* (Å)	23.5234 (10), 10.5928 (4), 23.4895 (13)
V (Å^3)	5853.1 (5)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.32 × 0.05 × 0.04
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.785, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30253, 13074, 8134
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.701
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.145, 1.06
No. of reflections	13074
No. of parameters	833
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.23

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

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full crystallographic data

IUCrData (2018). **3**, x180966 [https://doi.org/10.1107/S2414314618009665]

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2-(5-Methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-5-phenyl-1,3,4-oxadiazole

Crystal data

$C_{17}H_{13}N_5O$
M_r = 303.32
Orthorhombic, $Pca2_1$
a = 23.5234 (10) Å
b = 10.5928 (4) Å
c = 23.4895 (13) Å
V = 5853.1 (5) Å^3
Z = 16
$F(000)$ = 2528
D_x = 1.377 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5718 reflections
θ = 3.3–28.5°
μ = 0.09 mm^{-1}
T = 296 K
Needle, colourless
0.32 × 0.05 × 0.04 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.785, T_{max} = 1.000
30253 measured reflections
13074 independent reflections
8134 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 29.9°, θ_{min} = 1.7°
h = −24→32
k = −14→11
l = −29→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.145
S = 1.06
13074 reflections
833 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.057P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack x determined using 2598 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter: 0.8 (10)

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}
C1	−0.15453 (13)	0.9158 (3)	0.44268 (15)	0.0452 (8)
C2	−0.16709 (15)	0.9197 (3)	0.38489 (16)	0.0547 (9)
H2	−0.151530	0.859749	0.360531	0.066*
C3	−0.20253 (19)	1.0122 (3)	0.3634 (3)	0.0600 (13)
H3	−0.211075	1.013623	0.324750	0.072*
C4	−0.22509 (15)	1.1015 (3)	0.39882 (18)	0.0578 (9)
H4	−0.248149	1.164948	0.384129	0.069*
C5	−0.21360 (16)	1.0975 (3)	0.45629 (17)	0.0598 (10)
H5	−0.229731	1.156862	0.480557	0.072*
C6	−0.17805 (19)	1.0049 (3)	0.4780 (3)	0.0520 (12)
H6	−0.170054	1.003184	0.516739	0.062*
C7	−0.11797 (13)	0.8203 (3)	0.46695 (16)	0.0461 (8)
C8	−0.05922 (13)	0.6669 (3)	0.46898 (15)	0.0451 (7)
C9	−0.02246 (14)	0.5691 (3)	0.44694 (15)	0.0464 (8)
C10	0.01729 (19)	0.4988 (3)	0.4756 (2)	0.0432 (10)
C11	0.03517 (17)	0.5073 (3)	0.5365 (2)	0.0631 (12)
H11A	0.018379	0.439200	0.557623	0.095*
H11B	0.022787	0.586372	0.552160	0.095*
H11C	0.075833	0.501714	0.538945	0.095*
C12	0.08230 (13)	0.3268 (3)	0.43811 (16)	0.0467 (8)
C13	0.10952 (15)	0.2921 (4)	0.38813 (19)	0.0600 (9)
H13	0.100051	0.330946	0.353901	0.072*
C14	0.15079 (16)	0.1995 (3)	0.3896 (2)	0.0693 (11)
H14	0.168674	0.175119	0.356072	0.083*
C15	0.16581 (16)	0.1428 (3)	0.4403 (2)	0.0687 (11)
H15	0.194143	0.081573	0.441225	0.082*
C16	0.13844 (17)	0.1778 (4)	0.4889 (2)	0.0724 (11)
H16	0.148621	0.140462	0.523204	0.087*
C17	0.09617 (17)	0.2671 (3)	0.48822 (19)	0.0648 (10)
H17	0.076932	0.287109	0.521600	0.078*
C18	0.40400 (13)	−0.1692 (3)	0.20211 (15)	0.0434 (8)
C19	0.42839 (19)	−0.2608 (3)	0.1662 (3)	0.0513 (12)
H19	0.420783	−0.260492	0.127397	0.062*
C20	0.46340 (15)	−0.3502 (3)	0.18924 (17)	0.0543 (9)
H20	0.479259	−0.411422	0.165706	0.065*
C21	0.47569 (14)	−0.3516 (3)	0.24661 (17)	0.0546 (9)
H21	0.499462	−0.413387	0.261587	0.066*
C22	0.4525 (2)	−0.2605 (3)	0.2817 (2)	0.0576 (13)
H22	0.460911	−0.260455	0.320412	0.069*

C23	0.41690 (15)	−0.1700 (3)	0.25959 (16)	0.0528 (8)
H23	0.401407	−0.108855	0.283399	0.063*
C24	0.36559 (14)	−0.0761 (3)	0.17737 (16)	0.0449 (7)
C25	0.30607 (13)	0.0736 (3)	0.17456 (15)	0.0451 (8)
C26	0.26856 (13)	0.1719 (3)	0.19583 (14)	0.0434 (7)
C27	0.23683 (18)	0.2559 (3)	0.1644 (2)	0.0426 (10)
C28	0.23507 (17)	0.2785 (3)	0.10223 (19)	0.0587 (10)
H28A	0.201965	0.238774	0.086421	0.088*
H28B	0.268553	0.243737	0.084900	0.088*
H28C	0.233563	0.367661	0.095059	0.088*
C29	0.16562 (13)	0.4180 (3)	0.20044 (15)	0.0455 (8)
C30	0.13170 (14)	0.4274 (3)	0.15289 (18)	0.0597 (9)
H30	0.134869	0.368892	0.123532	0.072*
C31	0.09275 (16)	0.5253 (4)	0.1494 (2)	0.0708 (11)
H31	0.070642	0.534388	0.116813	0.085*
C32	0.08655 (17)	0.6091 (4)	0.1937 (2)	0.0732 (13)
H32	0.059830	0.673663	0.191541	0.088*
C33	0.11999 (16)	0.5965 (4)	0.2406 (2)	0.0730 (11)
H33	0.115726	0.652850	0.270706	0.088*
C34	0.15999 (17)	0.5019 (3)	0.2445 (2)	0.0603 (11)
H34	0.182889	0.495059	0.276671	0.072*
C35	0.40286 (13)	0.3321 (3)	0.20455 (16)	0.0481 (8)
C36	0.4292 (2)	0.2426 (3)	0.1694 (3)	0.0595 (13)
H36	0.423127	0.243846	0.130261	0.071*
C37	0.46404 (17)	0.1534 (3)	0.19299 (18)	0.0618 (10)
H37	0.481498	0.093860	0.169739	0.074*
C38	0.47345 (15)	0.1508 (3)	0.25056 (18)	0.0607 (9)
H38	0.496711	0.088968	0.266259	0.073*
C39	0.4484 (2)	0.2399 (4)	0.2851 (3)	0.0622 (13)
H39	0.455325	0.238668	0.324106	0.075*
C40	0.41348 (16)	0.3305 (3)	0.26249 (17)	0.0590 (9)
H40	0.396907	0.390682	0.286034	0.071*
C41	0.36506 (14)	0.4259 (3)	0.17931 (16)	0.0484 (8)
C42	0.30688 (14)	0.5791 (3)	0.17682 (17)	0.0492 (8)
C43	0.27125 (14)	0.6785 (3)	0.19846 (15)	0.0461 (8)
C44	0.23184 (19)	0.7498 (3)	0.1694 (2)	0.0476 (11)
C45	0.21333 (18)	0.7428 (3)	0.1096 (2)	0.0669 (12)
H45A	0.172705	0.750332	0.107690	0.100*
H45B	0.224720	0.663201	0.093658	0.100*
H45C	0.230514	0.810161	0.088332	0.100*
C46	0.16706 (13)	0.9221 (3)	0.20848 (16)	0.0469 (8)
C47	0.15412 (16)	0.9841 (3)	0.1592 (2)	0.0620 (10)
H47	0.174095	0.965779	0.126070	0.074*
C48	0.11147 (17)	1.0742 (3)	0.1582 (2)	0.0674 (10)
H48	0.101794	1.113553	0.124210	0.081*
C49	0.08361 (16)	1.1052 (4)	0.2073 (2)	0.0673 (11)
H49	0.055413	1.166738	0.206908	0.081*
C50	0.09739 (16)	1.0451 (3)	0.2572 (2)	0.0670 (10)

H50	0.078657	1.066711	0.290717	0.080*
C51	0.13889 (15)	0.9528 (3)	0.25809 (19)	0.0583 (9)
H51	0.147784	0.911680	0.291905	0.070*
C52	0.65410 (13)	0.4155 (3)	−0.05930 (16)	0.0466 (8)
C53	0.66535 (15)	0.4163 (3)	−0.11737 (17)	0.0555 (9)
H53	0.648762	0.355997	−0.140871	0.067*
C54	0.70110 (19)	0.5064 (3)	−0.1403 (3)	0.0603 (13)
H54	0.708771	0.506226	−0.179130	0.072*
C55	0.72531 (14)	0.5962 (3)	−0.10589 (19)	0.0597 (9)
H55	0.748379	0.658362	−0.121620	0.072*
C56	0.71551 (15)	0.5944 (3)	−0.04802 (18)	0.0592 (10)
H56	0.733170	0.653368	−0.024629	0.071*
C57	0.67922 (19)	0.5045 (3)	−0.0245 (3)	0.0511 (12)
H57	0.671961	0.504467	0.014406	0.061*
C58	0.61569 (13)	0.3242 (3)	−0.03402 (16)	0.0468 (8)
C59	0.55618 (14)	0.1736 (3)	−0.03043 (16)	0.0469 (8)
C60	0.51907 (14)	0.0751 (3)	−0.05139 (15)	0.0478 (8)
C61	0.48725 (19)	−0.0095 (3)	−0.0205 (2)	0.0455 (11)
C62	0.48588 (18)	−0.0312 (4)	0.04252 (19)	0.0633 (10)
H62A	0.453125	0.009666	0.058463	0.095*
H62B	0.519692	0.002959	0.059443	0.095*
H62C	0.483955	−0.120202	0.050036	0.095*
C63	0.41686 (13)	−0.1732 (3)	−0.05550 (15)	0.0467 (8)
C64	0.41034 (15)	−0.2563 (3)	−0.1005 (2)	0.0572 (10)
H64	0.432833	−0.248868	−0.132885	0.069*
C65	0.37000 (17)	−0.3502 (4)	−0.0965 (2)	0.0755 (12)
H65	0.364905	−0.405810	−0.126750	0.091*
C66	0.33719 (17)	−0.3627 (4)	−0.0484 (2)	0.0742 (12)
H66	0.310304	−0.426860	−0.045961	0.089*
C67	0.34430 (16)	−0.2802 (4)	−0.0041 (2)	0.0695 (11)
H67	0.322549	−0.289554	0.028741	0.083*
C68	0.38317 (14)	−0.1841 (3)	−0.00753 (18)	0.0586 (9)
H68	0.386835	−0.126574	0.022166	0.070*
N1	−0.10785 (14)	0.7962 (3)	0.51957 (13)	0.0561 (7)
N2	−0.06963 (14)	0.6961 (3)	0.52138 (14)	0.0570 (8)
N3	−0.02346 (13)	0.5340 (3)	0.39151 (13)	0.0540 (7)
N4	0.01326 (13)	0.4438 (3)	0.38410 (13)	0.0547 (7)
N5	0.03861 (11)	0.4211 (2)	0.43539 (12)	0.0463 (6)
N6	0.35325 (15)	−0.0603 (3)	0.12444 (14)	0.0583 (8)
N7	0.31322 (15)	0.0395 (3)	0.12258 (13)	0.0576 (8)
N8	0.25813 (14)	0.1867 (3)	0.25203 (14)	0.0567 (8)
N9	0.22086 (13)	0.2761 (3)	0.25810 (14)	0.0562 (8)
N10	0.20740 (11)	0.3194 (2)	0.20498 (12)	0.0444 (6)
N11	0.35356 (15)	0.4434 (3)	0.12637 (14)	0.0583 (8)
N12	0.31466 (14)	0.5453 (3)	0.12471 (14)	0.0579 (8)
N13	0.27303 (13)	0.7150 (3)	0.25429 (14)	0.0579 (7)
N14	0.23577 (14)	0.8041 (3)	0.26178 (14)	0.0592 (8)
N15	0.21067 (11)	0.8276 (2)	0.21034 (12)	0.0473 (6)

N16	0.60203 (15)	0.3104 (3)	0.01853 (14)	0.0614 (8)
N17	0.56280 (16)	0.2118 (3)	0.02124 (15)	0.0636 (8)
N18	0.50895 (13)	0.0576 (3)	−0.10765 (13)	0.0564 (8)
N19	0.47243 (14)	−0.0334 (3)	−0.11341 (14)	0.0590 (8)
N20	0.45830 (11)	−0.0750 (2)	−0.06031 (12)	0.0458 (6)
O1	−0.08810 (12)	0.7411 (2)	0.43137 (16)	0.0479 (8)
O2	0.33694 (12)	0.00500 (18)	0.21168 (15)	0.0438 (7)
O3	0.33675 (12)	0.5077 (2)	0.21364 (16)	0.0488 (8)
O4	0.58785 (12)	0.2398 (2)	−0.06883 (17)	0.0508 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0471 (16)	0.0483 (16)	0.040 (2)	−0.0061 (15)	0.0015 (14)	−0.0016 (14)
C2	0.070 (2)	0.0546 (18)	0.039 (2)	0.0100 (18)	0.0023 (18)	−0.0047 (16)
C3	0.070 (3)	0.065 (2)	0.045 (3)	0.007 (2)	−0.005 (2)	0.0009 (18)
C4	0.063 (2)	0.0518 (18)	0.058 (3)	0.0016 (17)	−0.0029 (19)	−0.0005 (18)
C5	0.065 (2)	0.060 (2)	0.055 (3)	0.0040 (18)	0.0038 (19)	−0.0146 (18)
C6	0.057 (3)	0.058 (2)	0.041 (3)	0.0008 (16)	−0.004 (2)	−0.0060 (15)
C7	0.0493 (17)	0.0539 (17)	0.0350 (19)	−0.0049 (15)	0.0008 (15)	−0.0036 (15)
C8	0.0474 (17)	0.0533 (17)	0.0347 (19)	−0.0020 (15)	−0.0019 (14)	0.0044 (15)
C9	0.0470 (17)	0.0567 (18)	0.0355 (19)	−0.0043 (16)	0.0000 (14)	0.0052 (15)
C10	0.047 (2)	0.049 (2)	0.034 (3)	−0.0049 (14)	0.001 (2)	0.0023 (14)
C11	0.072 (3)	0.078 (2)	0.039 (2)	0.0130 (19)	−0.011 (2)	−0.0045 (18)
C12	0.0450 (16)	0.0460 (16)	0.049 (2)	−0.0049 (14)	−0.0018 (15)	0.0008 (16)
C13	0.068 (2)	0.065 (2)	0.048 (2)	0.002 (2)	−0.0012 (19)	−0.0030 (19)
C14	0.070 (2)	0.068 (2)	0.070 (3)	0.005 (2)	0.010 (2)	−0.009 (2)
C15	0.060 (2)	0.058 (2)	0.088 (4)	0.0032 (18)	−0.001 (2)	0.001 (2)
C16	0.074 (3)	0.073 (2)	0.070 (3)	0.012 (2)	−0.009 (2)	0.013 (2)
C17	0.075 (2)	0.071 (2)	0.048 (2)	0.012 (2)	0.005 (2)	0.0105 (19)
C18	0.0455 (16)	0.0434 (16)	0.041 (2)	−0.0040 (14)	0.0033 (14)	0.0009 (14)
C19	0.055 (3)	0.057 (2)	0.042 (3)	−0.0018 (17)	0.003 (2)	−0.0043 (16)
C20	0.0559 (19)	0.0516 (18)	0.055 (3)	0.0036 (17)	0.0036 (17)	−0.0083 (16)
C21	0.0559 (19)	0.0527 (18)	0.055 (3)	0.0019 (16)	−0.0085 (17)	0.0029 (17)
C22	0.076 (3)	0.057 (2)	0.040 (3)	0.0055 (19)	−0.005 (2)	0.0024 (16)
C23	0.064 (2)	0.0546 (18)	0.040 (2)	0.0058 (17)	−0.0012 (18)	−0.0019 (16)
C24	0.0492 (17)	0.0488 (16)	0.037 (2)	−0.0044 (15)	0.0043 (15)	−0.0007 (15)
C25	0.0464 (17)	0.0495 (16)	0.039 (2)	−0.0022 (15)	−0.0029 (15)	0.0092 (15)
C26	0.0456 (17)	0.0485 (16)	0.0362 (19)	−0.0023 (15)	−0.0001 (13)	0.0043 (14)
C27	0.041 (2)	0.050 (2)	0.037 (3)	−0.0025 (13)	−0.0020 (19)	0.0041 (13)
C28	0.066 (2)	0.073 (2)	0.037 (2)	0.009 (2)	−0.0042 (19)	0.0055 (19)
C29	0.0436 (17)	0.0474 (17)	0.045 (2)	−0.0040 (15)	0.0007 (14)	0.0060 (15)
C30	0.058 (2)	0.064 (2)	0.056 (2)	0.0050 (18)	−0.0021 (19)	0.0057 (18)
C31	0.053 (2)	0.087 (3)	0.073 (3)	0.009 (2)	−0.008 (2)	0.023 (2)
C32	0.060 (2)	0.066 (2)	0.094 (4)	0.015 (2)	0.005 (2)	0.010 (2)
C33	0.075 (3)	0.066 (2)	0.078 (3)	0.008 (2)	0.009 (2)	−0.006 (2)
C34	0.063 (2)	0.061 (2)	0.057 (3)	0.0027 (18)	−0.005 (2)	−0.0031 (18)
C35	0.0471 (17)	0.0541 (18)	0.043 (2)	−0.0056 (16)	0.0034 (15)	0.0005 (15)

C36	0.065 (3)	0.068 (3)	0.046 (3)	−0.0060 (19)	0.006 (3)	−0.0043 (18)
C37	0.066 (2)	0.057 (2)	0.062 (3)	0.0025 (19)	0.008 (2)	−0.0117 (18)
C38	0.059 (2)	0.064 (2)	0.060 (3)	0.0057 (18)	−0.0015 (19)	0.000 (2)
C39	0.071 (3)	0.073 (3)	0.042 (3)	0.006 (2)	−0.002 (2)	0.0026 (18)
C40	0.064 (2)	0.069 (2)	0.044 (2)	0.0074 (19)	0.0025 (19)	−0.0036 (18)
C41	0.0469 (17)	0.0578 (18)	0.041 (2)	−0.0078 (16)	0.0089 (16)	−0.0008 (16)
C42	0.0464 (17)	0.0577 (18)	0.043 (2)	−0.0097 (16)	−0.0011 (16)	0.0114 (16)
C43	0.0475 (17)	0.0549 (17)	0.0359 (19)	−0.0087 (16)	−0.0033 (14)	0.0042 (14)
C44	0.047 (2)	0.056 (2)	0.041 (3)	−0.0081 (14)	−0.005 (2)	0.0049 (14)
C45	0.076 (3)	0.084 (3)	0.041 (3)	0.011 (2)	−0.014 (2)	−0.0049 (18)
C46	0.0467 (17)	0.0492 (17)	0.045 (2)	−0.0080 (15)	−0.0003 (15)	0.0032 (16)
C47	0.067 (2)	0.071 (2)	0.048 (2)	0.004 (2)	0.0023 (19)	0.0092 (19)
C48	0.074 (2)	0.067 (2)	0.061 (3)	0.006 (2)	−0.004 (2)	0.014 (2)
C49	0.063 (2)	0.063 (2)	0.076 (3)	0.0016 (19)	0.000 (2)	0.002 (2)
C50	0.069 (2)	0.071 (2)	0.061 (3)	−0.003 (2)	0.011 (2)	−0.004 (2)
C51	0.065 (2)	0.062 (2)	0.048 (2)	−0.0070 (19)	−0.0007 (19)	0.0044 (19)
C52	0.0448 (16)	0.0499 (16)	0.045 (2)	0.0055 (15)	−0.0059 (15)	−0.0028 (15)
C53	0.061 (2)	0.0590 (19)	0.046 (2)	−0.0052 (18)	−0.0055 (18)	−0.0062 (17)
C54	0.057 (3)	0.075 (3)	0.049 (3)	−0.0029 (19)	0.004 (2)	−0.0025 (18)
C55	0.0567 (19)	0.0580 (19)	0.065 (3)	−0.0056 (17)	−0.0029 (19)	−0.0012 (19)
C56	0.062 (2)	0.059 (2)	0.056 (3)	0.0018 (18)	−0.0084 (19)	−0.0121 (18)
C57	0.055 (3)	0.053 (2)	0.045 (3)	0.0045 (15)	−0.002 (3)	−0.0065 (15)
C58	0.0488 (17)	0.0506 (17)	0.041 (2)	0.0022 (15)	−0.0045 (16)	−0.0031 (15)
C59	0.0511 (17)	0.0526 (17)	0.037 (2)	0.0032 (15)	−0.0009 (15)	0.0018 (15)
C60	0.0512 (18)	0.0527 (18)	0.039 (2)	0.0043 (16)	0.0006 (15)	0.0028 (15)
C61	0.051 (2)	0.049 (2)	0.036 (3)	0.0059 (14)	0.001 (2)	−0.0017 (14)
C62	0.069 (2)	0.082 (2)	0.039 (2)	−0.009 (2)	0.001 (2)	0.005 (2)
C63	0.0464 (17)	0.0486 (16)	0.045 (2)	0.0052 (15)	0.0022 (15)	0.0029 (15)
C64	0.061 (2)	0.062 (2)	0.048 (3)	−0.0018 (17)	0.0001 (19)	−0.0036 (17)
C65	0.080 (3)	0.070 (2)	0.076 (3)	−0.011 (2)	−0.010 (2)	−0.012 (2)
C66	0.065 (2)	0.072 (2)	0.086 (4)	−0.013 (2)	−0.002 (2)	0.011 (2)
C67	0.061 (2)	0.079 (2)	0.069 (3)	−0.002 (2)	0.015 (2)	0.015 (2)
C68	0.060 (2)	0.063 (2)	0.053 (2)	0.0006 (18)	0.0072 (18)	0.0007 (18)
N1	0.0617 (18)	0.0669 (18)	0.0396 (19)	0.0076 (16)	0.0013 (15)	−0.0039 (15)
N2	0.0631 (18)	0.069 (2)	0.039 (2)	0.0070 (17)	−0.0022 (15)	0.0054 (16)
N3	0.0639 (18)	0.0613 (15)	0.0368 (17)	0.0045 (15)	−0.0075 (15)	−0.0008 (15)
N4	0.0659 (18)	0.0618 (17)	0.0364 (17)	0.0039 (15)	−0.0109 (15)	−0.0025 (14)
N5	0.0514 (14)	0.0530 (14)	0.0345 (16)	−0.0020 (13)	−0.0066 (12)	0.0011 (12)
N6	0.0688 (19)	0.0645 (18)	0.0416 (19)	0.0125 (16)	0.0006 (16)	0.0010 (15)
N7	0.070 (2)	0.0676 (17)	0.0351 (19)	0.0126 (17)	0.0023 (16)	0.0016 (15)
N8	0.0671 (18)	0.0622 (17)	0.0407 (19)	0.0112 (16)	0.0004 (15)	0.0070 (15)
N9	0.0655 (19)	0.0654 (16)	0.0376 (18)	0.0096 (16)	0.0000 (15)	0.0083 (15)
N10	0.0487 (14)	0.0488 (14)	0.0358 (16)	0.0018 (12)	−0.0028 (12)	0.0047 (11)
N11	0.0624 (18)	0.0703 (19)	0.0421 (19)	−0.0001 (16)	0.0025 (16)	0.0059 (16)
N12	0.0637 (19)	0.0715 (19)	0.039 (2)	0.0013 (17)	0.0024 (15)	0.0058 (16)
N13	0.0640 (19)	0.0661 (16)	0.0437 (19)	0.0027 (16)	−0.0076 (16)	0.0054 (16)
N14	0.0690 (19)	0.0721 (19)	0.0365 (18)	0.0070 (16)	−0.0085 (16)	0.0020 (16)
N15	0.0527 (15)	0.0557 (14)	0.0336 (16)	−0.0058 (13)	−0.0057 (12)	0.0056 (13)

N16	0.070 (2)	0.071 (2)	0.043 (2)	−0.0083 (17)	−0.0021 (16)	−0.0052 (16)
N17	0.076 (2)	0.0679 (18)	0.047 (2)	−0.0125 (19)	0.0030 (18)	0.0011 (17)
N18	0.0692 (18)	0.0623 (17)	0.0378 (18)	−0.0144 (16)	0.0024 (15)	0.0036 (15)
N19	0.078 (2)	0.0635 (16)	0.0353 (18)	−0.0113 (17)	0.0039 (16)	0.0051 (16)
N20	0.0520 (15)	0.0517 (14)	0.0336 (16)	0.0013 (13)	0.0032 (12)	0.0031 (12)
O1	0.0485 (17)	0.0560 (15)	0.039 (2)	0.0030 (10)	−0.0006 (15)	0.0016 (11)
O2	0.0532 (18)	0.0482 (15)	0.0301 (17)	0.0039 (10)	0.0031 (14)	0.0023 (10)
O3	0.0542 (18)	0.0588 (16)	0.0335 (18)	0.0014 (11)	0.0026 (15)	0.0049 (11)
O4	0.0514 (18)	0.0556 (15)	0.045 (2)	−0.0032 (11)	0.0007 (15)	−0.0012 (11)

Geometric parameters (Å, º)

C1—C6	1.373 (5)	C37—H37	0.9300
C1—C2	1.390 (5)	C38—C39	1.377 (6)
C1—C7	1.445 (4)	C38—H38	0.9300
C2—C3	1.382 (5)	C39—C40	1.371 (6)
C2—H2	0.9300	C39—H39	0.9300
C3—C4	1.367 (6)	C40—H40	0.9300
C3—H3	0.9300	C41—N11	1.286 (5)
C4—C5	1.377 (5)	C41—O3	1.358 (4)
C4—H4	0.9300	C42—N12	1.288 (5)
C5—C6	1.385 (5)	C42—O3	1.347 (5)
C5—H5	0.9300	C42—C43	1.438 (5)
C6—H6	0.9300	C43—N13	1.368 (5)
C7—N1	1.284 (4)	C43—C44	1.377 (5)
C7—O1	1.377 (4)	C44—N15	1.360 (6)
C8—N2	1.292 (4)	C44—C45	1.474 (8)
C8—O1	1.364 (5)	C45—H45A	0.9600
C8—C9	1.446 (5)	C45—H45B	0.9600
C9—N3	1.354 (4)	C45—H45C	0.9600
C9—C10	1.372 (5)	C46—C47	1.365 (5)
C10—N5	1.349 (5)	C46—C51	1.379 (5)
C10—C11	1.494 (7)	C46—N15	1.434 (4)
C11—H11A	0.9600	C47—C48	1.385 (5)
C11—H11B	0.9600	C47—H47	0.9300
C11—H11C	0.9600	C48—C49	1.366 (6)
C12—C17	1.376 (5)	C48—H48	0.9300
C12—C13	1.387 (5)	C49—C50	1.373 (6)
C12—N5	1.435 (4)	C49—H49	0.9300
C13—C14	1.381 (5)	C50—C51	1.382 (5)
C13—H13	0.9300	C50—H50	0.9300
C14—C15	1.379 (6)	C51—H51	0.9300
C14—H14	0.9300	C52—C57	1.380 (5)
C15—C16	1.362 (6)	C52—C53	1.390 (5)
C15—H15	0.9300	C52—C58	1.451 (5)
C16—C17	1.372 (5)	C53—C54	1.381 (6)
C16—H16	0.9300	C53—H53	0.9300
C17—H17	0.9300	C54—C55	1.372 (6)

C18—C23	1.384 (5)	C54—H54	0.9300
C18—C19	1.407 (5)	C55—C56	1.379 (5)
C18—C24	1.458 (4)	C55—H55	0.9300
C19—C20	1.366 (5)	C56—C57	1.393 (5)
C19—H19	0.9300	C56—H56	0.9300
C20—C21	1.378 (5)	C57—H57	0.9300
C20—H20	0.9300	C58—N16	1.284 (4)
C21—C22	1.382 (6)	C58—O4	1.377 (5)
C21—H21	0.9300	C59—N17	1.288 (5)
C22—C23	1.375 (6)	C59—O4	1.364 (5)
C22—H22	0.9300	C59—C60	1.447 (5)
C23—H23	0.9300	C60—N18	1.355 (5)
C24—N6	1.288 (4)	C60—C61	1.375 (5)
C24—O2	1.357 (4)	C61—N20	1.349 (5)
C25—N7	1.285 (4)	C61—C62	1.499 (7)
C25—O2	1.348 (4)	C62—H62A	0.9600
C25—C26	1.453 (4)	C62—H62B	0.9600
C26—N8	1.352 (4)	C62—H62C	0.9600
C26—C27	1.376 (5)	C63—C68	1.382 (5)
C27—N10	1.357 (5)	C63—C64	1.384 (5)
C27—C28	1.481 (7)	C63—N20	1.430 (4)
C28—H28A	0.9600	C64—C65	1.378 (5)
C28—H28B	0.9600	C64—H64	0.9300
C28—H28C	0.9600	C65—C66	1.375 (6)
C29—C34	1.372 (5)	C65—H65	0.9300
C29—C30	1.376 (5)	C66—C67	1.370 (6)
C29—N10	1.438 (4)	C66—H66	0.9300
C30—C31	1.386 (5)	C67—C68	1.371 (5)
C30—H30	0.9300	C67—H67	0.9300
C31—C32	1.375 (6)	C68—H68	0.9300
C31—H31	0.9300	N1—N2	1.391 (5)
C32—C33	1.362 (6)	N3—N4	1.300 (4)
C32—H32	0.9300	N4—N5	1.366 (4)
C33—C34	1.378 (5)	N6—N7	1.416 (5)
C33—H33	0.9300	N8—N9	1.299 (4)
C34—H34	0.9300	N9—N10	1.367 (4)
C35—C40	1.384 (5)	N11—N12	1.416 (5)
C35—C36	1.403 (6)	N13—N14	1.300 (4)
C35—C41	1.460 (5)	N14—N15	1.368 (4)
C36—C37	1.367 (6)	N16—N17	1.395 (5)
C36—H36	0.9300	N18—N19	1.299 (4)
C37—C38	1.370 (5)	N19—N20	1.364 (4)

C6—C1—C2	118.9 (3)	C39—C40—H40	120.0
C6—C1—C7	118.9 (4)	C35—C40—H40	120.0
C2—C1—C7	122.2 (3)	N11—C41—O3	112.3 (3)
C3—C2—C1	120.4 (4)	N11—C41—C35	128.2 (3)
C3—C2—H2	119.8	O3—C41—C35	119.5 (3)

C1—C2—H2	119.8	N12—C42—O3	112.3 (3)
C4—C3—C2	120.2 (5)	N12—C42—C43	128.5 (3)
C4—C3—H3	119.9	O3—C42—C43	119.2 (3)
C2—C3—H3	119.9	N13—C43—C44	109.9 (4)
C3—C4—C5	119.9 (4)	N13—C43—C42	121.8 (3)
C3—C4—H4	120.0	C44—C43—C42	128.2 (4)
C5—C4—H4	120.0	N15—C44—C43	103.2 (4)
C4—C5—C6	120.1 (4)	N15—C44—C45	126.6 (4)
C4—C5—H5	120.0	C43—C44—C45	130.1 (4)
C6—C5—H5	120.0	C44—C45—H45A	109.5
C1—C6—C5	120.5 (5)	C44—C45—H45B	109.5
C1—C6—H6	119.7	H45A—C45—H45B	109.5
C5—C6—H6	119.7	C44—C45—H45C	109.5
N1—C7—O1	111.6 (3)	H45A—C45—H45C	109.5
N1—C7—C1	129.0 (3)	H45B—C45—H45C	109.5
O1—C7—C1	119.4 (3)	C47—C46—C51	119.7 (3)
N2—C8—O1	112.6 (3)	C47—C46—N15	121.4 (3)
N2—C8—C9	128.7 (3)	C51—C46—N15	118.8 (3)
O1—C8—C9	118.6 (3)	C46—C47—C48	120.5 (4)
N3—C9—C10	109.5 (3)	C46—C47—H47	119.8
N3—C9—C8	122.1 (3)	C48—C47—H47	119.8
C10—C9—C8	128.4 (4)	C49—C48—C47	120.0 (4)
N5—C10—C9	103.9 (4)	C49—C48—H48	120.0
N5—C10—C11	127.0 (4)	C47—C48—H48	120.0
C9—C10—C11	129.0 (4)	C48—C49—C50	119.7 (4)
C10—C11—H11A	109.5	C48—C49—H49	120.1
C10—C11—H11B	109.5	C50—C49—H49	120.1
H11A—C11—H11B	109.5	C49—C50—C51	120.5 (4)
C10—C11—H11C	109.5	C49—C50—H50	119.8
H11A—C11—H11C	109.5	C51—C50—H50	119.8
H11B—C11—H11C	109.5	C46—C51—C50	119.6 (4)
C17—C12—C13	119.5 (3)	C46—C51—H51	120.2
C17—C12—N5	121.9 (3)	C50—C51—H51	120.2
C13—C12—N5	118.5 (3)	C57—C52—C53	119.7 (4)
C14—C13—C12	119.4 (4)	C57—C52—C58	118.7 (4)
C14—C13—H13	120.3	C53—C52—C58	121.6 (3)
C12—C13—H13	120.3	C54—C53—C52	120.2 (4)
C15—C14—C13	120.8 (4)	C54—C53—H53	119.9
C15—C14—H14	119.6	C52—C53—H53	119.9
C13—C14—H14	119.6	C55—C54—C53	120.1 (5)
C16—C15—C14	118.9 (4)	C55—C54—H54	119.9
C16—C15—H15	120.6	C53—C54—H54	119.9
C14—C15—H15	120.6	C54—C55—C56	120.1 (4)
C15—C16—C17	121.4 (4)	C54—C55—H55	119.9
C15—C16—H16	119.3	C56—C55—H55	119.9
C17—C16—H16	119.3	C55—C56—C57	120.2 (4)
C16—C17—C12	119.9 (4)	C55—C56—H56	119.9
C16—C17—H17	120.1	C57—C56—H56	119.9

C12—C17—H17	120.1	C52—C57—C56	119.6 (5)
C23—C18—C19	119.4 (3)	C52—C57—H57	120.2
C23—C18—C24	121.9 (3)	C56—C57—H57	120.2
C19—C18—C24	118.7 (4)	N16—C58—O4	112.2 (3)
C20—C19—C18	119.2 (5)	N16—C58—C52	128.7 (3)
C20—C19—H19	120.4	O4—C58—C52	119.1 (3)
C18—C19—H19	120.4	N17—C59—O4	113.3 (3)
C19—C20—C21	121.3 (4)	N17—C59—C60	128.3 (3)
C19—C20—H20	119.3	O4—C59—C60	118.4 (3)
C21—C20—H20	119.3	N18—C60—C61	109.3 (3)
C20—C21—C22	119.6 (4)	N18—C60—C59	122.4 (3)
C20—C21—H21	120.2	C61—C60—C59	128.2 (4)
C22—C21—H21	120.2	N20—C61—C60	104.1 (4)
C23—C22—C21	120.1 (5)	N20—C61—C62	126.5 (4)
C23—C22—H22	119.9	C60—C61—C62	129.3 (4)
C21—C22—H22	119.9	C61—C62—H62A	109.5
C22—C23—C18	120.5 (4)	C61—C62—H62B	109.5
C22—C23—H23	119.8	H62A—C62—H62B	109.5
C18—C23—H23	119.8	C61—C62—H62C	109.5
N6—C24—O2	112.3 (3)	H62A—C62—H62C	109.5
N6—C24—C18	127.8 (3)	H62B—C62—H62C	109.5
O2—C24—C18	119.9 (3)	C68—C63—C64	120.4 (3)
N7—C25—O2	113.1 (3)	C68—C63—N20	121.1 (3)
N7—C25—C26	127.5 (3)	C64—C63—N20	118.5 (3)
O2—C25—C26	119.4 (3)	C65—C64—C63	118.9 (4)
N8—C26—C27	110.5 (3)	C65—C64—H64	120.5
N8—C26—C25	121.9 (3)	C63—C64—H64	120.5
C27—C26—C25	127.4 (3)	C66—C65—C64	120.8 (4)
N10—C27—C26	102.8 (4)	C66—C65—H65	119.6
N10—C27—C28	126.8 (3)	C64—C65—H65	119.6
C26—C27—C28	130.5 (4)	C67—C66—C65	119.7 (4)
C27—C28—H28A	109.5	C67—C66—H66	120.2
C27—C28—H28B	109.5	C65—C66—H66	120.2
H28A—C28—H28B	109.5	C66—C67—C68	120.7 (4)
C27—C28—H28C	109.5	C66—C67—H67	119.7
H28A—C28—H28C	109.5	C68—C67—H67	119.7
H28B—C28—H28C	109.5	C67—C68—C63	119.5 (4)
C34—C29—C30	120.7 (3)	C67—C68—H68	120.2
C34—C29—N10	118.7 (3)	C63—C68—H68	120.2
C30—C29—N10	120.6 (3)	C7—N1—N2	107.5 (3)
C29—C30—C31	119.0 (4)	C8—N2—N1	106.0 (3)
C29—C30—H30	120.5	N4—N3—C9	108.6 (3)
C31—C30—H30	120.5	N3—N4—N5	107.5 (3)
C32—C31—C30	120.5 (4)	C10—N5—N4	110.4 (3)
C32—C31—H31	119.7	C10—N5—C12	131.3 (3)
C30—C31—H31	119.7	N4—N5—C12	118.3 (3)
C33—C32—C31	119.2 (4)	C24—N6—N7	106.1 (3)
C33—C32—H32	120.4	C25—N7—N6	105.5 (3)

C31—C32—H32	120.4	N9—N8—C26	108.3 (3)
C32—C33—C34	121.3 (4)	N8—N9—N10	107.5 (3)
C32—C33—H33	119.3	C27—N10—N9	110.9 (3)
C34—C33—H33	119.3	C27—N10—C29	131.1 (3)
C29—C34—C33	119.2 (4)	N9—N10—C29	118.0 (3)
C29—C34—H34	120.4	C41—N11—N12	105.8 (3)
C33—C34—H34	120.4	C42—N12—N11	106.1 (3)
C40—C35—C36	119.4 (4)	N14—N13—C43	108.3 (3)
C40—C35—C41	121.2 (3)	N13—N14—N15	107.7 (3)
C36—C35—C41	119.4 (4)	C44—N15—N14	110.9 (3)
C37—C36—C35	119.5 (5)	C44—N15—C46	131.5 (3)
C37—C36—H36	120.2	N14—N15—C46	117.6 (3)
C35—C36—H36	120.2	C58—N16—N17	107.1 (3)
C36—C37—C38	120.7 (4)	C59—N17—N16	105.8 (3)
C36—C37—H37	119.6	N19—N18—C60	108.6 (3)
C38—C37—H37	119.6	N18—N19—N20	107.8 (3)
C37—C38—C39	119.9 (4)	C61—N20—N19	110.2 (3)
C37—C38—H38	120.0	C61—N20—C63	131.6 (3)
C39—C38—H38	120.0	N19—N20—C63	118.2 (3)
C40—C39—C38	120.5 (5)	C8—O1—C7	102.2 (4)
C40—C39—H39	119.8	C25—O2—C24	103.0 (3)
C38—C39—H39	119.8	C42—O3—C41	103.5 (4)
C39—C40—C35	119.9 (4)	C59—O4—C58	101.6 (4)