IUCrData

ISSN 2414-3146

(*E*)-5-(4-Methoxyphenyl)-*N*′-(2-oxoindolin-3-ylidene)-1-phenyl-1*H*-pyrazole-3-carbohydrazide

Bakr F. Abdel-Wahab,[a] Abdelbasset A. Farahat,[b,c] Mohamed S. Bekheit,[d] Emad Yousif,[e] Benson M. Kariuki[f] and Gamal A. El-Hiti[g]*

[a]Applied Organic Chemistry Department, Chemical Industries Research Institute, National Research Centre, Dokki, Giza 12622, Egypt, [b]Master of Pharmaceutical Sciences Program, California Northstate University, Elk Grove, CA 95757, USA, [c]Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt, [d]Department of Pesticide Chemistry, National Research Centre, Dokki, Giza 12622, Egypt, [e]Department of Chemistry, College of Science, Al-Nahrain University, Baghdad 64021, Iraq, [f]School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, United Kingdom, and [g]Department of Optometry, College of Applied Medical Sciences, King Saud University, Riyadh 11433, Saudi Arabia. *Correspondence e-mail: gelhiti@ksu.edu.sa

Received 20 April 2023
Accepted 23 May 2023

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

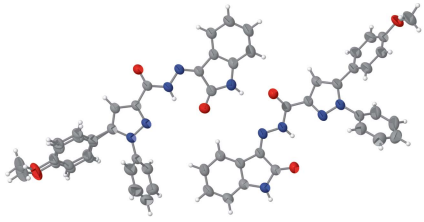
Keywords: crystal structure; pyrazoles; carbohydrazides; isatin; heterocycles; synthesis.

CCDC reference: 2235858

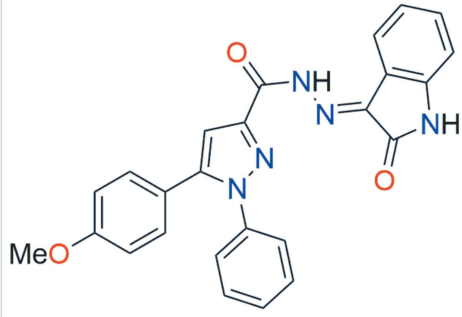
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{25}H_{19}N_5O_3$, is composed of two independent molecules with slightly different conformations. The extended structure features N—H···O hydrogen bonds as well as π–π interactions.

3D view



Chemical scheme



Structure description

The synthesis of hydrazides and hydrazones is of interest because of their involvement in various synthetic transformations. In addition, they have potential pharmacological applications (see, for example, Afsah *et al.*, 2016). Isatin-containing heterocycles also exhibit biological activities, such as anticonvulsant, antimicrobial and antioxidant properties (see, for example, Kaur *et al.*, 2016). The most common synthetic methods for isatins involve the oxidation of indoles (Zi *et al.*, 2014), oxindoles (Wei *et al.*, 2017; Ying *et al.*, 2018) and aminoacetophenones (Qian *et al.*, 2017). Pyrazoles have several medicinal uses and can act as analgesics and antipyretics (see, for example, Rios & Portilla, 2022). Many synthetic procedures have been reported for the synthesis of pyrazoles (see, for example, Zora *et al.*, 2011; Karrouchi *et al.*, 2018; Li *et al.*, 2021). Recently, we have been investigating the synthesis and structure elucidation of various heterocycles. The current work describes the synthesis and the crystal structure of a hydrazone containing both isatin and pyrazole moieties using a simple procedure.

The crystal structure of the title compound, $C_{25}H_{19}N_5O_3$, contains two independent molecules, M_1 and M_2 (Fig. 1). Each molecule comprises indole-2-one (M_1A: C1–C8, N1,

OPEN ACCESS
Published under a CC BY 4.0 licence

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O5^{i}	0.86	2.13	2.8594 (16)	142
N3—H3···O1	0.86	2.07	2.7419 (17)	135
N6—H6A···O2	0.86	2.13	2.8512 (17)	142
N8—H8A···O4	0.86	2.07	2.7396 (16)	134
C5—H5···O5^{i}	0.93	2.49	3.172 (2)	130
C30—H30···O2	0.93	2.52	3.187 (2)	129
C36—H36···O3^{ii}	0.93	2.44	3.330 (2)	159

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

O1 and M_2A: C26–C33, N6, O4), formohydrazide (M_1B: C9, N2, N3, O2 and M_2B: C34, N7, N8, O5), pyrazole (M_1C: C10–C12, N4, N5 and M_2C: C35–C37, N9, N10), methoxybenzene (M_1D: C13–C19, O3 and M_2D: C38–C44, O6) and phenyl (M_1E: C20–C25 and M_2E: C45–C50) moieties.

In both molecules, the indole-2-one, formohydrazide and pyrazole groups are close to coplanar: the twist angles M_1A/M_1B and M_1B/M_1C are 5.0 (1) and 10.7 (1)°, respectively, for molecule M_1 and the corresponding angles M_2A/M_2B and M_2B/M_2C for molecule M_2 are 4.1 (2) and 9.7 (2)°, respectively. The near coplanarity of the indole-2-one and formohydrazide groups is similar to that observed for the related 1-(4-methoxyphenyl)-5-methyl-N'-(2-oxoindolin-3-ylidene)-1H-1,2,3-triazole-4-carbohydrazide, **3** (Kariuki *et al.*, 2022) and 1-(4-fluorophenyl)-N'-(2-oxoindolin-3-ylidene)-5-phenyl-1H-1,2,3-triazole-4-carbohydrazide, **4** (Mohamed *et al.*, 2023).

The methoxybenzene and phenyl groups deviate from the plane of the indole-2-one and formohydrazide groups. The twist angles M_1C/M_1D and M_1C/M_1E are 51.9 (2) and 55.8 (1)°, respectively, for molecule M_1 while M_2C/M_2D and M_2C/M_2E are 51.7 (2) and 57.7 (1)°, respectively, for molecule M_2. The twists of the two aromatic rings from the plane of the pyrazole group is of the same order as observed in **3** (Mohamed *et al.*, 2023) as well as in 4-{3-[2-(4-methoxybenzylidene)hydrazine-1-carbonyl]-5-(4-methoxyphenyl)-1H-pyrazol-1-yl}benzenesulfonamide and 4-{5-(4-bromophenyl)-3-[2-(4-methylbenzylidene)hydrazine-1-carbonyl]-1H-pyrazol-1-yl}benzenesulfonamide, **5** (Lu *et al.*, 2016). Intramolecular N—H···O hydrogen bonds (Table 1) contribute to the observed molecular planarity. Similar intramolecular N—H···O hydrogen bonds also occur in **3** and **4**.

In the extended structure of the title compound, the molecules form layers oriented parallel to (102) (Fig. 2*a*). Intermolecular N—H···O hydrogen bonds (Table 1) occur within the layers. In the layers, aromatic ring edge-to-face interactions occur with ring centroid-to-centroid distances in the range 5.4–5.7 Å (Fig. 2*b*). Interactions of the type π–π between rings are also observed with centroid–centroid distances of about 4.17 Å.

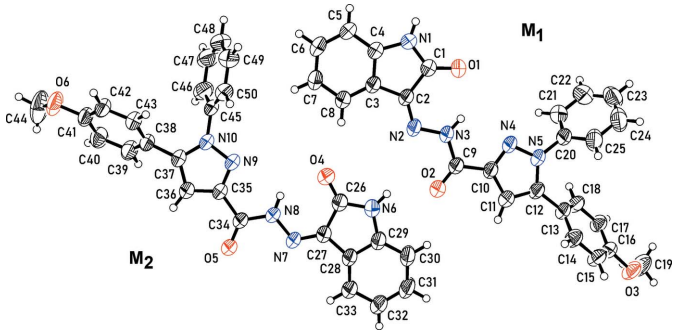


Figure 1
An *ORTEP* representation of the asymmetric unit of the title compound showing 50% probability atomic displacement parameters. Only the major disorder component of the disordered methoxybenzene group of molecule M_2 is shown.

Synthesis and crystallization

A mixture of 5-(4-methoxyphenyl)-1-phenyl-1H-pyrazole-3-carbohydrazide **1** (0.62 g, 2.0 mmol) and isatin **2** (0.30 g, 2.0 mmol) in dry EtOH (15 ml) containing a catalytic quantity of concentrated HCl (0.1 ml) was refluxed for 2 h. The mixture was left to cool to 20°C and the orange solid produced was collected by filtration. The product was washed with EtOH, dried, and recrystallized from DMF to give the title compound in 90% yield, m.p. 280–281°C. ^{1}H NMR (p.p.m.): 3.72 (*s*, 3H, OMe), 6.89 (*d*, 9.1 Hz, 2H, Ar), 6.92 (*d*, 1H, 7.7 Hz, Ar), 7.08 (*t*, 7.7 Hz, 1H, Ar), 7.15 (*s*, 1H, pyrazolyl), 7.18 (*d*, 9.1 Hz, 2H, Ar), 7.33–7.36 (*m*, 3H, Ar), 7.44–7.48 (*m*, 3H, Ar), 7.58 (*d*, 7.7 Hz, 1H, Ar), 11.17 (*s*, exch., 1H, NH), 14.08 (*s*, exch., 1H, NH). ^{13}C NMR (p.p.m.): 55.7, 108.4, 111.6, 114.7, 120.5, 121.6, 123.1, 126.2, 129.2, 129.3, 129.8, 130.6, 132.2, 138.3, 139.8, 143.1, 145.5, 145.7, 158.4, 160.2, 163.1. Analysis calculated for $C_{25}H_{19}N_5O_3$ (437.46): C, 68.64; H, 4.38; N, 16.01. Found: C, 68.77; H, 4.47; N, 16.13%.

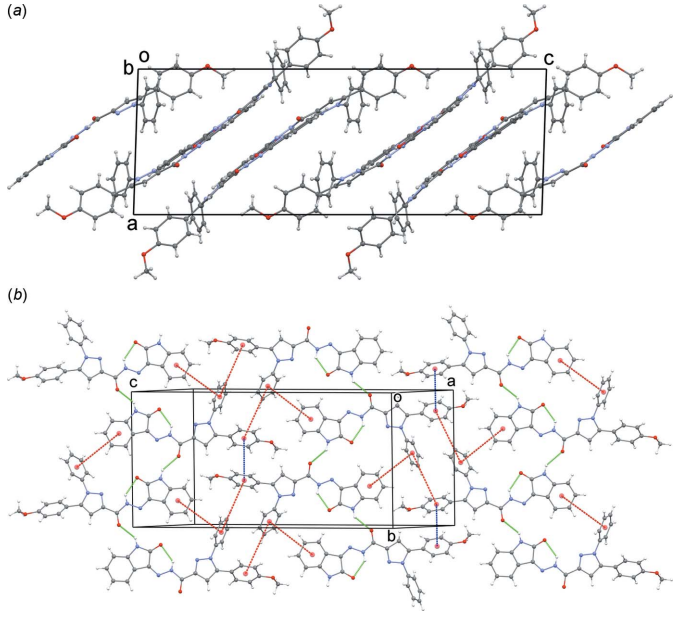


Figure 2
(*a*) Crystal packing for the title compound and (*b*) a layer showing the edge-to-face interactions (red dotted lines), π–π interactions (blue) and N—H···O hydrogen bonds (green).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The methoxybenzene group of one molecule is disordered and was modelled with two components of 0.66 (2) and 0.34 (2) occupancy.

Acknowledgements

We thank Cardiff University and the National Research Centre for technical support.

Funding information

Funding for this research was provided by: Researchers Supporting Project, King Saud University, Riyadh, Saudi Arabia. (award No. RSP2023R404).

References

Afsah, E. M., Elmorsy, S. S., Abdelmageed, S. M. & Zaki, Z. E. (2016). *Z. Naturforsch. B*, **71**, 1147–1157.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Kariuki, B. M., Abdel-Wahab, B. F., Farahat, A. A. & El-Hiti, G. A. (2022). *Molbank*, **2022**, M1374.

Karrouchi, K., Radi, S., Ramli, Y., Taoufik, J., Mabkhot, Y. N., Al-aizari, F. A. & Ansar, M. (2018). *Molecules*, **23**, 134131.

Kaur, M., Singh, M., Chadha, N. & Silakari, O. (2016). *Eur. J. Med. Chem.* **123**, 858–894.

Li, X., Yu, Y. & Tu, Z. (2021). *Molecules*, **26**, 1202.

Lu, X.-Y., Wang, Z.-C., Wei, T., Yan, X.-Q., Wang, P.-F. & Zhu, H.-L. (2016). *RSC Adv.* **6**, 22917–22935.

Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.

Mohamed, H. A., Bekheit, M. S., Ewies, E. F., Awad, H. M., Betz, R., Hosten, E. C. & Abdel-Wahab, B. F. (2023). *J. Mol. Struct.* **1274**, 134415.

Qian, P., Su, J.-H., Wang, Y., Bi, M., Zha, Z. & Wang, Z. (2017). *J. Org. Chem.* **82**, 6434–6440.

Rigaku OD. (2022). *CrysAlis PRO*. Rigaku Oxford Diffraction, Oxford, England.

Ríos, M.-C. & Portilla, J. (2022). *Chemistry*, **4**, 940–968.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{19}N_5O_3$
M_r	437.45
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	10.8353 (2), 13.3587 (2), 30.3697 (4)
β (°)	91.838 (1)
V (Å^3)	4393.62 (12)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.74
Crystal size (mm)	0.28 × 0.24 × 0.13
Data collection	
Diffractometer	SuperNova, Dual, Cu at home/near, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.663, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33362, 8632, 6902
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.620
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.122, 1.02
No. of reflections	8632
No. of parameters	671
No. of restraints	389
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.15

Computer programs: *CrysAlis PRO* 1.171.42.54a (Rigaku OD, 2022), *SHELXT (Sheldrick, 2015a), SHELXL* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012).

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Wei, W.-T., Ying, W.-W., Zhu, W.-M., Wu, Y., Huang, Y.-L., Cao, Y.-Q., Wang, Y.-N. & Liang, H. (2017). *Synlett*, **28**, 2307–2310.

Ying, W.-W., Zhu, W.-M., Liang, H. & Wei, W.-T. (2018). *Synlett*, **29**, 215–218.

Zi, Y., Cai, Z.-J., Wang, S.-Y. & Ji, S.-J. (2014). *Org. Lett.* **16**, 3094–3097.

Zora, M., Kivrak, A. & Yazici, C. (2011). *J. Org. Chem.* **76**, 6726–6742.

full crystallographic data

IUCrData (2023). **8**, x230455 [https://doi.org/10.1107/S2414314623004558]

(*E*)-5-(4-Methoxyphenyl)-*N*′-(2-oxoindolin-3-ylidene)-1-phenyl-1*H*-pyrazole-3-carbohydrazide

Bakr F. Abdel-Wahab, Abdelbasset A. Farahat, Mohamed S. Bekheit, Emad Yousif, Benson M. Kariuki and Gamal A. El-Hiti

(*E*)-5-(4-Methoxyphenyl)-*N*′-(2-oxoindolin-3-ylidene)-1-phenyl-1*H*-pyrazole-3-carbohydrazide

Crystal data

$C_{25}H_{19}N_5O_3$
M_r = 437.45
Monoclinic, $P2_1/c$
a = 10.8353 (2) Å
b = 13.3587 (2) Å
c = 30.3697 (4) Å
β = 91.838 (1)°
V = 4393.62 (12) Å^3
Z = 8
$F(000)$ = 1824
D_x = 1.323 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 14981 reflections
θ = 4.4–72.8°
μ = 0.74 mm^{-1}
T = 293 K
Needle, yellow
0.28 × 0.24 × 0.13 mm

Data collection

SuperNova, Dual, Cu at home/near, Atlas diffractometer
ω scans
Absorption correction: gaussian (Crysalispro; Rigaku OD, 2022)
T_{min} = 0.663, T_{max} = 1.000
33362 measured reflections
8632 independent reflections
6902 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 72.8°, θ_{min} = 3.6°
h = −11→13
k = −16→16
l = −37→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.122
S = 1.02
8632 reflections
671 parameters
389 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0662P)^2 + 0.4435P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.52252 (15)	0.83217 (11)	0.32663 (5)	0.0592 (3)	
C2	0.52711 (14)	0.72003 (11)	0.32210 (4)	0.0537 (3)	
C3	0.60695 (14)	0.69953 (11)	0.28547 (5)	0.0555 (3)	
C4	0.64382 (14)	0.79218 (11)	0.26934 (5)	0.0572 (3)	
C5	0.72114 (16)	0.79927 (13)	0.23416 (6)	0.0677 (4)	
H5	0.744764	0.861007	0.223064	0.081*	
C6	0.76180 (18)	0.71073 (14)	0.21621 (6)	0.0742 (5)	
H6	0.815196	0.713327	0.192862	0.089*	
C7	0.72579 (18)	0.61836 (14)	0.23178 (6)	0.0764 (5)	
H7	0.754893	0.560287	0.218787	0.092*	
C8	0.64635 (17)	0.61160 (12)	0.26675 (5)	0.0669 (4)	
H8	0.620651	0.549789	0.277148	0.080*	
C9	0.34347 (14)	0.62106 (11)	0.40400 (5)	0.0550 (3)	
C10	0.28695 (13)	0.66435 (11)	0.44319 (4)	0.0540 (3)	
C11	0.22281 (14)	0.61278 (12)	0.47516 (5)	0.0579 (3)	
H11	0.201499	0.545339	0.475096	0.070*	
C12	0.19783 (14)	0.68269 (11)	0.50672 (5)	0.0568 (3)	
C13	0.14081 (14)	0.66994 (11)	0.54983 (4)	0.0557 (3)	
C14	0.02927 (15)	0.61940 (12)	0.55308 (5)	0.0627 (4)	
H14	−0.011180	0.596060	0.527635	0.075*	
C15	−0.02234 (15)	0.60332 (13)	0.59332 (5)	0.0642 (4)	
H15	−0.097426	0.569987	0.594876	0.077*	
C16	0.03778 (14)	0.63689 (11)	0.63153 (5)	0.0565 (3)	
C17	0.14915 (14)	0.68614 (12)	0.62901 (5)	0.0603 (4)	
H17	0.190144	0.708292	0.654564	0.072*	
C18	0.19988 (14)	0.70257 (12)	0.58833 (5)	0.0609 (4)	
H18	0.274864	0.736086	0.586850	0.073*	
C19	0.0467 (2)	0.63903 (18)	0.71002 (5)	0.0877 (6)	
H19A	0.126011	0.606946	0.709974	0.132*	
H19B	0.001109	0.614749	0.734410	0.132*	
H19C	0.057706	0.710098	0.712737	0.132*	
O3	−0.01949 (11)	0.61720 (10)	0.66988 (3)	0.0730 (3)	
C20	0.24421 (16)	0.86755 (11)	0.51263 (5)	0.0606 (4)	
C21	0.35404 (19)	0.91566 (14)	0.52136 (7)	0.0795 (5)	
H21	0.428034	0.886374	0.513509	0.095*	
C22	0.3541 (2)	1.00840 (16)	0.54202 (8)	0.0942 (6)	
H22	0.428447	1.040920	0.548336	0.113*	
C23	0.2460 (2)	1.05185 (15)	0.55304 (7)	0.0898 (6)	
H23	0.246316	1.114663	0.566242	0.108*	
C24	0.1367 (2)	1.00314 (16)	0.54470 (7)	0.0913 (6)	
H24	0.063160	1.032631	0.552936	0.110*	
C25	0.13386 (19)	0.91034 (15)	0.52413 (6)	0.0787 (5)	
H25	0.059320	0.877735	0.518236	0.094*	
C26	0.54022 (15)	0.33380 (11)	0.32501 (5)	0.0601 (3)	
C27	0.53916 (14)	0.22196 (11)	0.33016 (5)	0.0550 (3)	

C28	0.46467 (15)	0.20092 (11)	0.36808 (5)	0.0586 (3)	
C29	0.42502 (16)	0.29316 (12)	0.38402 (5)	0.0629 (4)	
C30	0.35281 (19)	0.29935 (14)	0.42042 (6)	0.0774 (5)	
H30	0.326915	0.360849	0.431113	0.093*	
C31	0.3203 (2)	0.21097 (15)	0.44043 (6)	0.0851 (6)	
H31	0.271896	0.213253	0.465138	0.102*	
C32	0.3577 (2)	0.11927 (15)	0.42481 (6)	0.0822 (5)	
H32	0.333820	0.061035	0.438997	0.099*	
C33	0.43062 (18)	0.11295 (13)	0.38810 (6)	0.0711 (4)	
H33	0.455702	0.051259	0.377367	0.085*	
C34	0.71499 (14)	0.12317 (11)	0.24600 (5)	0.0549 (3)	
C35	0.79638 (14)	0.16684 (11)	0.21296 (4)	0.0543 (3)	
C36	0.87553 (15)	0.11368 (12)	0.18615 (5)	0.0598 (4)	
H36	0.884597	0.044595	0.184313	0.072*	
C37	0.93705 (14)	0.18535 (11)	0.16310 (5)	0.0565 (3)	
C38	1.0266 (9)	0.1775 (9)	0.1271 (3)	0.0520 (12)	0.66 (2)
C39	1.1282 (9)	0.1166 (8)	0.1344 (3)	0.0658 (14)	0.66 (2)
H39	1.140769	0.086717	0.161813	0.079*	0.66 (2)
C40	1.2120 (8)	0.0992 (7)	0.1015 (3)	0.0681 (13)	0.66 (2)
H40	1.279234	0.057051	0.106735	0.082*	0.66 (2)
C41	1.1947 (6)	0.1448 (5)	0.0612 (2)	0.0566 (11)	0.66 (2)
C42	1.0961 (7)	0.2093 (7)	0.0542 (2)	0.0561 (11)	0.66 (2)
H42	1.086000	0.242043	0.027293	0.067*	0.66 (2)
C43	1.0129 (8)	0.2254 (8)	0.0868 (3)	0.0535 (11)	0.66 (2)
H43	0.946860	0.268871	0.081729	0.064*	0.66 (2)
C44	1.3854 (6)	0.0877 (11)	0.0336 (3)	0.099 (2)	0.66 (2)
H44A	1.432010	0.129168	0.053915	0.148*	0.66 (2)
H44B	1.427862	0.082929	0.006447	0.148*	0.66 (2)
H44C	1.376545	0.022038	0.046014	0.148*	0.66 (2)
O6	1.2671 (7)	0.1303 (5)	0.0256 (2)	0.0755 (11)	0.66 (2)
C38B	1.0365 (18)	0.1668 (18)	0.1326 (6)	0.053 (2)	0.34 (2)
C39B	1.1343 (16)	0.1024 (14)	0.1406 (5)	0.0577 (18)	0.34 (2)
H39B	1.141568	0.070045	0.167671	0.069*	0.34 (2)
C40B	1.2218 (13)	0.0848 (12)	0.1093 (5)	0.0607 (18)	0.34 (2)
H40B	1.289063	0.043364	0.115625	0.073*	0.34 (2)
C41B	1.2078 (11)	0.1296 (9)	0.0685 (4)	0.0589 (18)	0.34 (2)
C42B	1.1093 (14)	0.1924 (12)	0.0595 (5)	0.060 (2)	0.34 (2)
H42B	1.099795	0.221976	0.031910	0.073*	0.34 (2)
C43B	1.0247 (16)	0.2114 (15)	0.0916 (6)	0.058 (2)	0.34 (2)
H43B	0.959046	0.254638	0.085587	0.069*	0.34 (2)
C44B	1.3891 (12)	0.0531 (12)	0.0426 (7)	0.089 (3)	0.34 (2)
H44D	1.436829	0.077974	0.067431	0.134*	0.34 (2)
H44E	1.439382	0.051794	0.017149	0.134*	0.34 (2)
H44F	1.360994	−0.013464	0.048798	0.134*	0.34 (2)
O6B	1.2863 (12)	0.1161 (11)	0.0344 (4)	0.076 (2)	0.34 (2)
C45	0.93673 (15)	0.37295 (11)	0.16561 (5)	0.0583 (4)	
C46	1.06071 (18)	0.39405 (15)	0.17271 (6)	0.0735 (4)	
H46	1.114035	0.345599	0.184366	0.088*	

C47	1.1044 (2)	0.48796 (18)	0.16229 (7)	0.0912 (6)
H47	1.187712	0.502916	0.166652	0.109*
C48	1.0248 (2)	0.55904 (16)	0.14551 (8)	0.0948 (7)
H48	1.054419	0.622241	0.138518	0.114*
C49	0.9022 (2)	0.53768 (15)	0.13898 (8)	0.0929 (6)
H49	0.848859	0.586698	0.127869	0.111*
C50	0.85682 (18)	0.44350 (13)	0.14879 (6)	0.0742 (5)
H50	0.773622	0.428606	0.144026	0.089*
N1	0.59191 (13)	0.86917 (9)	0.29427 (4)	0.0644 (3)
H1	0.602962	0.931952	0.289518	0.077*
N2	0.47247 (12)	0.65335 (9)	0.34518 (4)	0.0556 (3)
N3	0.40306 (12)	0.68823 (9)	0.37855 (4)	0.0567 (3)
H3	0.397058	0.751439	0.383414	0.068*
N4	0.30144 (12)	0.76075 (10)	0.45310 (4)	0.0589 (3)
N5	0.24509 (12)	0.77127 (9)	0.49202 (4)	0.0581 (3)
N6	0.47120 (14)	0.37071 (10)	0.35775 (5)	0.0681 (4)
H6A	0.457401	0.433331	0.361942	0.082*
N7	0.59252 (12)	0.15611 (9)	0.30643 (4)	0.0557 (3)
N8	0.66029 (12)	0.19096 (9)	0.27276 (4)	0.0564 (3)
H8A	0.668472	0.254206	0.268439	0.068*
N9	0.80578 (12)	0.26548 (9)	0.20751 (4)	0.0564 (3)
N10	0.89251 (12)	0.27560 (9)	0.17665 (4)	0.0564 (3)
O1	0.46685 (13)	0.87878 (8)	0.35461 (4)	0.0761 (3)
O2	0.34031 (12)	0.53157 (8)	0.39661 (4)	0.0713 (3)
O4	0.59503 (12)	0.38076 (8)	0.29704 (4)	0.0736 (3)
O5	0.70216 (12)	0.03351 (8)	0.24977 (4)	0.0735 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0688 (9)	0.0552 (8)	0.0545 (8)	−0.0004 (7)	0.0176 (7)	−0.0021 (6)
C2	0.0599 (8)	0.0551 (8)	0.0468 (7)	0.0024 (6)	0.0134 (6)	0.0011 (6)
C3	0.0604 (8)	0.0578 (8)	0.0491 (7)	0.0024 (6)	0.0144 (6)	0.0021 (6)
C4	0.0612 (8)	0.0583 (8)	0.0528 (7)	−0.0007 (6)	0.0140 (6)	−0.0007 (6)
C5	0.0739 (10)	0.0675 (9)	0.0632 (9)	−0.0056 (8)	0.0256 (8)	0.0027 (7)
C6	0.0785 (11)	0.0798 (11)	0.0663 (10)	0.0018 (8)	0.0332 (8)	0.0023 (8)
C7	0.0900 (12)	0.0688 (10)	0.0724 (10)	0.0117 (9)	0.0342 (9)	−0.0025 (8)
C8	0.0804 (10)	0.0588 (9)	0.0632 (9)	0.0068 (7)	0.0265 (8)	0.0026 (7)
C9	0.0601 (8)	0.0550 (8)	0.0506 (7)	0.0054 (6)	0.0152 (6)	0.0013 (6)
C10	0.0600 (8)	0.0565 (8)	0.0465 (7)	0.0052 (6)	0.0149 (6)	0.0011 (6)
C11	0.0662 (8)	0.0589 (8)	0.0495 (7)	−0.0014 (6)	0.0149 (6)	0.0010 (6)
C12	0.0606 (8)	0.0626 (8)	0.0480 (7)	0.0008 (6)	0.0144 (6)	0.0032 (6)
C13	0.0621 (8)	0.0609 (8)	0.0450 (7)	−0.0003 (6)	0.0141 (6)	0.0021 (6)
C14	0.0693 (9)	0.0733 (10)	0.0459 (7)	−0.0107 (7)	0.0078 (6)	−0.0003 (6)
C15	0.0634 (9)	0.0755 (10)	0.0543 (8)	−0.0149 (7)	0.0112 (7)	0.0013 (7)
C16	0.0650 (8)	0.0597 (8)	0.0460 (7)	−0.0032 (6)	0.0169 (6)	0.0005 (6)
C17	0.0667 (9)	0.0688 (9)	0.0459 (7)	−0.0077 (7)	0.0083 (6)	−0.0030 (6)
C18	0.0574 (8)	0.0728 (9)	0.0532 (8)	−0.0082 (7)	0.0121 (6)	0.0008 (7)

C19	0.0961 (13)	0.1231 (16)	0.0450 (8)	−0.0197 (12)	0.0185 (8)	−0.0056 (9)
O3	0.0809 (7)	0.0924 (8)	0.0469 (5)	−0.0197 (6)	0.0211 (5)	−0.0014 (5)
C20	0.0778 (10)	0.0571 (8)	0.0480 (7)	0.0049 (7)	0.0183 (7)	0.0017 (6)
C21	0.0833 (12)	0.0680 (10)	0.0885 (12)	−0.0030 (9)	0.0238 (10)	−0.0084 (9)
C22	0.1095 (16)	0.0710 (12)	0.1028 (16)	−0.0114 (11)	0.0159 (12)	−0.0112 (11)
C23	0.1319 (19)	0.0631 (10)	0.0750 (12)	0.0113 (12)	0.0143 (12)	−0.0078 (9)
C24	0.1104 (16)	0.0816 (13)	0.0831 (13)	0.0319 (12)	0.0216 (11)	−0.0075 (10)
C25	0.0813 (11)	0.0792 (11)	0.0764 (11)	0.0142 (9)	0.0147 (9)	−0.0068 (9)
C26	0.0657 (9)	0.0563 (8)	0.0591 (8)	0.0036 (7)	0.0163 (7)	0.0006 (6)
C27	0.0606 (8)	0.0555 (8)	0.0497 (7)	0.0027 (6)	0.0153 (6)	0.0009 (6)
C28	0.0672 (9)	0.0594 (8)	0.0503 (7)	0.0046 (7)	0.0167 (6)	−0.0010 (6)
C29	0.0697 (9)	0.0633 (9)	0.0567 (8)	0.0074 (7)	0.0176 (7)	−0.0012 (7)
C30	0.0917 (12)	0.0751 (11)	0.0672 (10)	0.0139 (9)	0.0314 (9)	−0.0039 (8)
C31	0.1029 (14)	0.0889 (13)	0.0661 (10)	0.0103 (10)	0.0427 (10)	0.0021 (9)
C32	0.1050 (14)	0.0753 (11)	0.0687 (10)	0.0029 (10)	0.0392 (10)	0.0087 (8)
C33	0.0886 (11)	0.0635 (9)	0.0629 (9)	0.0047 (8)	0.0290 (8)	0.0023 (7)
C34	0.0640 (8)	0.0540 (8)	0.0476 (7)	−0.0008 (6)	0.0162 (6)	0.0017 (6)
C35	0.0627 (8)	0.0551 (8)	0.0461 (7)	−0.0029 (6)	0.0160 (6)	−0.0005 (6)
C36	0.0701 (9)	0.0557 (8)	0.0549 (8)	0.0015 (7)	0.0214 (7)	0.0000 (6)
C37	0.0616 (8)	0.0604 (8)	0.0483 (7)	−0.0016 (6)	0.0151 (6)	−0.0018 (6)
C38	0.056 (2)	0.056 (3)	0.046 (3)	−0.0001 (14)	0.0142 (19)	0.0002 (19)
C39	0.073 (2)	0.074 (3)	0.050 (2)	0.009 (2)	0.0096 (17)	0.0135 (17)
C40	0.0618 (19)	0.078 (3)	0.065 (3)	0.0170 (17)	0.0098 (18)	0.0058 (19)
C41	0.0548 (19)	0.067 (2)	0.0491 (18)	−0.0030 (16)	0.0123 (14)	−0.0025 (15)
C42	0.0629 (19)	0.061 (2)	0.0455 (19)	−0.0002 (14)	0.0121 (14)	0.0042 (15)
C43	0.057 (2)	0.057 (3)	0.0468 (19)	0.0022 (14)	0.0097 (15)	0.0048 (15)
C44	0.066 (2)	0.150 (6)	0.081 (3)	0.018 (3)	0.0134 (19)	−0.015 (4)
O6	0.062 (2)	0.107 (2)	0.059 (2)	0.0102 (14)	0.0207 (15)	−0.0021 (15)
C38B	0.058 (3)	0.057 (4)	0.045 (3)	−0.003 (3)	0.009 (3)	0.004 (3)
C39B	0.059 (3)	0.062 (4)	0.053 (4)	0.008 (2)	0.014 (3)	0.010 (3)
C40B	0.054 (3)	0.068 (4)	0.061 (3)	0.005 (3)	0.011 (3)	0.004 (3)
C41B	0.054 (3)	0.068 (3)	0.055 (3)	0.004 (2)	0.017 (3)	−0.003 (3)
C42B	0.072 (4)	0.064 (4)	0.046 (3)	0.001 (3)	0.015 (3)	0.007 (3)
C43B	0.060 (3)	0.059 (4)	0.055 (4)	0.010 (3)	0.010 (3)	0.000 (3)
C44B	0.065 (4)	0.113 (7)	0.090 (6)	0.019 (4)	0.030 (4)	−0.017 (5)
O6B	0.063 (4)	0.105 (4)	0.062 (4)	0.013 (3)	0.026 (3)	−0.005 (3)
C45	0.0724 (9)	0.0571 (8)	0.0467 (7)	−0.0090 (7)	0.0226 (6)	−0.0036 (6)
C46	0.0792 (11)	0.0818 (11)	0.0599 (9)	−0.0162 (9)	0.0080 (8)	−0.0003 (8)
C47	0.0998 (15)	0.0941 (15)	0.0808 (12)	−0.0401 (12)	0.0173 (11)	−0.0070 (11)
C48	0.1280 (19)	0.0671 (11)	0.0918 (14)	−0.0281 (12)	0.0423 (13)	−0.0041 (10)
C49	0.1182 (17)	0.0608 (10)	0.1020 (15)	0.0036 (11)	0.0387 (13)	0.0094 (10)
C50	0.0791 (11)	0.0633 (9)	0.0819 (11)	0.0010 (8)	0.0278 (9)	0.0026 (8)
N1	0.0813 (9)	0.0516 (7)	0.0619 (7)	−0.0047 (6)	0.0264 (6)	−0.0014 (5)
N2	0.0647 (7)	0.0553 (6)	0.0479 (6)	0.0042 (5)	0.0181 (5)	0.0000 (5)
N3	0.0703 (7)	0.0520 (6)	0.0490 (6)	0.0028 (5)	0.0217 (5)	0.0004 (5)
N4	0.0690 (7)	0.0611 (7)	0.0478 (6)	0.0031 (6)	0.0217 (5)	0.0010 (5)
N5	0.0697 (7)	0.0581 (7)	0.0477 (6)	0.0011 (6)	0.0205 (5)	0.0000 (5)
N6	0.0822 (9)	0.0546 (7)	0.0692 (8)	0.0079 (6)	0.0271 (7)	−0.0019 (6)

N7	0.0645 (7)	0.0559 (7)	0.0477 (6)	0.0004 (5)	0.0186 (5)	0.0017 (5)
N8	0.0676 (7)	0.0516 (6)	0.0513 (6)	−0.0004 (5)	0.0228 (5)	0.0024 (5)
N9	0.0650 (7)	0.0571 (7)	0.0484 (6)	−0.0046 (5)	0.0212 (5)	−0.0006 (5)
N10	0.0656 (7)	0.0553 (7)	0.0496 (6)	−0.0053 (5)	0.0206 (5)	−0.0016 (5)
O1	0.1001 (9)	0.0573 (6)	0.0732 (7)	0.0007 (6)	0.0383 (6)	−0.0079 (5)
O2	0.0912 (8)	0.0544 (6)	0.0703 (7)	−0.0001 (5)	0.0347 (6)	−0.0019 (5)
O4	0.0886 (8)	0.0566 (6)	0.0777 (7)	0.0020 (5)	0.0337 (6)	0.0079 (5)
O5	0.1010 (9)	0.0524 (6)	0.0696 (7)	−0.0023 (5)	0.0404 (6)	0.0010 (5)

Geometric parameters (Å, º)

C1—O1	1.2275 (18)	C31—H31	0.9300
C1—N1	1.3500 (19)	C32—C33	1.390 (2)
C1—C2	1.505 (2)	C32—H32	0.9300
C2—N2	1.2892 (18)	C33—H33	0.9300
C2—C3	1.4568 (18)	C34—O5	1.2117 (18)
C3—C8	1.379 (2)	C34—N8	1.3650 (18)
C3—C4	1.394 (2)	C34—C35	1.4771 (18)
C4—C5	1.382 (2)	C35—N9	1.3323 (19)
C4—N1	1.4053 (19)	C35—C36	1.3955 (19)
C5—C6	1.380 (2)	C36—C37	1.371 (2)
C5—H5	0.9300	C36—H36	0.9300
C6—C7	1.382 (3)	C37—N10	1.3670 (19)
C6—H6	0.9300	C37—C38B	1.464 (14)
C7—C8	1.391 (2)	C37—C38	1.489 (7)
C7—H7	0.9300	C38—C39	1.380 (4)
C8—H8	0.9300	C38—C43	1.384 (4)
C9—O2	1.2166 (18)	C39—C40	1.391 (4)
C9—N3	1.3607 (18)	C39—H39	0.9300
C9—C10	1.4741 (18)	C40—C41	1.374 (4)
C10—N4	1.331 (2)	C40—H40	0.9300
C10—C11	1.3941 (19)	C41—O6	1.372 (4)
C11—C12	1.371 (2)	C41—C42	1.384 (4)
C11—H11	0.9300	C42—C43	1.378 (4)
C12—N5	1.3698 (19)	C42—H42	0.9300
C12—C13	1.4754 (18)	C43—H43	0.9300
C13—C18	1.385 (2)	C44—O6	1.416 (5)
C13—C14	1.391 (2)	C44—H44A	0.9600
C14—C15	1.377 (2)	C44—H44B	0.9600
C14—H14	0.9300	C44—H44C	0.9600
C15—C16	1.387 (2)	C38B—C39B	1.380 (7)
C15—H15	0.9300	C38B—C43B	1.382 (7)
C16—O3	1.3627 (16)	C39B—C40B	1.385 (6)
C16—C17	1.379 (2)	C39B—H39B	0.9300
C17—C18	1.3858 (19)	C40B—C41B	1.378 (7)
C17—H17	0.9300	C40B—H40B	0.9300
C18—H18	0.9300	C41B—O6B	1.373 (6)
C19—O3	1.425 (2)	C41B—C42B	1.378 (7)

C19—H19A	0.9600	C42B—C43B	1.384 (6)
C19—H19B	0.9600	C42B—H42B	0.9300
C19—H19C	0.9600	C43B—H43B	0.9300
C20—C21	1.371 (3)	C44B—O6B	1.412 (7)
C20—C25	1.380 (2)	C44B—H44D	0.9600
C20—N5	1.4305 (19)	C44B—H44E	0.9600
C21—C22	1.389 (3)	C44B—H44F	0.9600
C21—H21	0.9300	C45—C50	1.368 (3)
C22—C23	1.359 (3)	C45—C46	1.383 (2)
C22—H22	0.9300	C45—N10	1.4294 (18)
C23—C24	1.368 (3)	C46—C47	1.381 (3)
C23—H23	0.9300	C46—H46	0.9300
C24—C25	1.388 (3)	C47—C48	1.370 (3)
C24—H24	0.9300	C47—H47	0.9300
C25—H25	0.9300	C48—C49	1.367 (3)
C26—O4	1.2249 (18)	C48—H48	0.9300
C26—N6	1.3559 (19)	C49—C50	1.387 (3)
C26—C27	1.502 (2)	C49—H49	0.9300
C27—N7	1.2862 (18)	C50—H50	0.9300
C27—C28	1.4545 (19)	N1—H1	0.8600
C28—C33	1.379 (2)	N2—N3	1.3633 (15)
C28—C29	1.397 (2)	N3—H3	0.8600
C29—C30	1.377 (2)	N4—N5	1.3551 (15)
C29—N6	1.409 (2)	N6—H6A	0.8600
C30—C31	1.378 (3)	N7—N8	1.3600 (15)
C30—H30	0.9300	N8—H8A	0.8600
C31—C32	1.379 (3)	N9—N10	1.3552 (15)

O1—C1—N1	128.01 (14)	O5—C34—C35	121.83 (13)
O1—C1—C2	125.91 (13)	N8—C34—C35	115.00 (12)
N1—C1—C2	106.09 (12)	N9—C35—C36	112.34 (12)
N2—C2—C3	125.42 (13)	N9—C35—C34	121.64 (12)
N2—C2—C1	128.38 (12)	C36—C35—C34	125.93 (13)
C3—C2—C1	106.20 (12)	C37—C36—C35	105.10 (13)
C8—C3—C4	121.01 (13)	C37—C36—H36	127.5
C8—C3—C2	132.41 (14)	C35—C36—H36	127.5
C4—C3—C2	106.58 (12)	N10—C37—C36	106.26 (12)
C5—C4—C3	121.34 (14)	N10—C37—C38B	127.9 (10)
C5—C4—N1	129.02 (14)	C36—C37—C38B	125.7 (9)
C3—C4—N1	109.64 (12)	N10—C37—C38	121.9 (5)
C6—C5—C4	117.12 (15)	C36—C37—C38	131.6 (5)
C6—C5—H5	121.4	C39—C38—C43	118.5 (4)
C4—C5—H5	121.4	C39—C38—C37	117.3 (5)
C5—C6—C7	122.18 (15)	C43—C38—C37	124.2 (5)
C5—C6—H6	118.9	C38—C39—C40	121.3 (4)
C7—C6—H6	118.9	C38—C39—H39	119.4
C6—C7—C8	120.49 (16)	C40—C39—H39	119.4
C6—C7—H7	119.8	C41—C40—C39	119.4 (4)

C8—C7—H7	119.8	C41—C40—H40	120.3
C3—C8—C7	117.84 (15)	C39—C40—H40	120.3
C3—C8—H8	121.1	O6—C41—C40	125.1 (4)
C7—C8—H8	121.1	O6—C41—C42	115.1 (4)
O2—C9—N3	123.67 (13)	C40—C41—C42	119.8 (4)
O2—C9—C10	121.62 (13)	C43—C42—C41	120.4 (4)
N3—C9—C10	114.64 (12)	C43—C42—H42	119.8
N4—C10—C11	112.24 (12)	C41—C42—H42	119.8
N4—C10—C9	120.88 (12)	C42—C43—C38	120.6 (4)
C11—C10—C9	126.71 (14)	C42—C43—H43	119.7
C12—C11—C10	105.32 (13)	C38—C43—H43	119.7
C12—C11—H11	127.3	O6—C44—H44A	109.5
C10—C11—H11	127.3	O6—C44—H44B	109.5
N5—C12—C11	106.04 (12)	H44A—C44—H44B	109.5
N5—C12—C13	124.09 (13)	O6—C44—H44C	109.5
C11—C12—C13	129.74 (14)	H44A—C44—H44C	109.5
C18—C13—C14	118.16 (13)	H44B—C44—H44C	109.5
C18—C13—C12	121.16 (13)	C41—O6—C44	117.2 (4)
C14—C13—C12	120.57 (13)	C39B—C38B—C43B	118.4 (8)
C15—C14—C13	121.15 (14)	C39B—C38B—C37	124.9 (10)
C15—C14—H14	119.4	C43B—C38B—C37	116.6 (10)
C13—C14—H14	119.4	C38B—C39B—C40B	121.6 (8)
C14—C15—C16	119.92 (14)	C38B—C39B—H39B	119.2
C14—C15—H15	120.0	C40B—C39B—H39B	119.2
C16—C15—H15	120.0	C41B—C40B—C39B	119.0 (7)
O3—C16—C17	124.25 (14)	C41B—C40B—H40B	120.5
O3—C16—C15	115.98 (13)	C39B—C40B—H40B	120.5
C17—C16—C15	119.77 (13)	O6B—C41B—C40B	124.6 (7)
C16—C17—C18	119.86 (14)	O6B—C41B—C42B	115.1 (7)
C16—C17—H17	120.1	C40B—C41B—C42B	120.3 (7)
C18—C17—H17	120.1	C41B—C42B—C43B	119.9 (7)
C13—C18—C17	121.13 (14)	C41B—C42B—H42B	120.1
C13—C18—H18	119.4	C43B—C42B—H42B	120.1
C17—C18—H18	119.4	C38B—C43B—C42B	120.7 (8)
O3—C19—H19A	109.5	C38B—C43B—H43B	119.6
O3—C19—H19B	109.5	C42B—C43B—H43B	119.6
H19A—C19—H19B	109.5	O6B—C44B—H44D	109.5
O3—C19—H19C	109.5	O6B—C44B—H44E	109.5
H19A—C19—H19C	109.5	H44D—C44B—H44E	109.5
H19B—C19—H19C	109.5	O6B—C44B—H44F	109.5
C16—O3—C19	117.47 (13)	H44D—C44B—H44F	109.5
C21—C20—C25	120.70 (16)	H44E—C44B—H44F	109.5
C21—C20—N5	119.22 (15)	C41B—O6B—C44B	116.7 (8)
C25—C20—N5	120.07 (16)	C50—C45—C46	121.20 (16)
C20—C21—C22	119.56 (19)	C50—C45—N10	120.11 (15)
C20—C21—H21	120.2	C46—C45—N10	118.69 (15)
C22—C21—H21	120.2	C47—C46—C45	119.2 (2)
C23—C22—C21	120.3 (2)	C47—C46—H46	120.4

C23—C22—H22	119.8	C45—C46—H46	120.4
C21—C22—H22	119.8	C48—C47—C46	119.9 (2)
C22—C23—C24	119.96 (19)	C48—C47—H47	120.0
C22—C23—H23	120.0	C46—C47—H47	120.0
C24—C23—H23	120.0	C49—C48—C47	120.41 (19)
C23—C24—C25	121.0 (2)	C49—C48—H48	119.8
C23—C24—H24	119.5	C47—C48—H48	119.8
C25—C24—H24	119.5	C48—C49—C50	120.5 (2)
C20—C25—C24	118.5 (2)	C48—C49—H49	119.7
C20—C25—H25	120.8	C50—C49—H49	119.7
C24—C25—H25	120.8	C45—C50—C49	118.73 (19)
O4—C26—N6	127.84 (15)	C45—C50—H50	120.6
O4—C26—C27	125.95 (13)	C49—C50—H50	120.6
N6—C26—C27	106.20 (12)	C1—N1—C4	111.48 (12)
N7—C27—C28	125.61 (13)	C1—N1—H1	124.3
N7—C27—C26	128.08 (13)	C4—N1—H1	124.3
C28—C27—C26	106.31 (12)	C2—N2—N3	116.22 (12)
C33—C28—C29	120.62 (14)	C9—N3—N2	118.68 (12)
C33—C28—C27	132.60 (14)	C9—N3—H3	120.7
C29—C28—C27	106.77 (13)	N2—N3—H3	120.7
C30—C29—C28	121.35 (15)	C10—N4—N5	104.15 (11)
C30—C29—N6	129.16 (15)	N4—N5—C12	112.22 (12)
C28—C29—N6	109.49 (13)	N4—N5—C20	118.97 (12)
C29—C30—C31	117.51 (16)	C12—N5—C20	128.78 (11)
C29—C30—H30	121.2	C26—N6—C29	111.22 (13)
C31—C30—H30	121.2	C26—N6—H6A	124.4
C30—C31—C32	121.83 (15)	C29—N6—H6A	124.4
C30—C31—H31	119.1	C27—N7—N8	116.77 (12)
C32—C31—H31	119.1	N7—N8—C34	118.41 (12)
C31—C32—C33	120.71 (17)	N7—N8—H8A	120.8
C31—C32—H32	119.6	C34—N8—H8A	120.8
C33—C32—H32	119.6	C35—N9—N10	104.00 (11)
C28—C33—C32	117.98 (16)	N9—N10—C37	112.30 (11)
C28—C33—H33	121.0	N9—N10—C45	119.87 (11)
C32—C33—H33	121.0	C37—N10—C45	127.42 (11)
O5—C34—N8	123.11 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O5^{i}	0.86	2.13	2.8594 (16)	142
N3—H3···O1	0.86	2.07	2.7419 (17)	135
N6—H6*A*···O2	0.86	2.13	2.8512 (17)	142
N8—H8*A*···O4	0.86	2.07	2.7396 (16)	134
C5—H5···O5^{i}	0.93	2.49	3.172 (2)	130

C30—H30···O2	0.93	2.52	3.187 (2)	129
C36—H36···O3^{ii}	0.93	2.44	3.330 (2)	159

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