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Crystal structures of 3-methoxy-4-{[5-(4-methoxyphenyl)-1,3,4-oxadiazol-2-yl]methoxy}benzonitrile and *N*-(4-{[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]methoxy}phenyl)acetamide

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Keywords: crystal structure; oxadiazole derivatives; superposition; intramolecular C—H···O interactions; intermolecular C—H···N and N—H···N hydrogen bonds.

CCDC references: 1881075; 1881074

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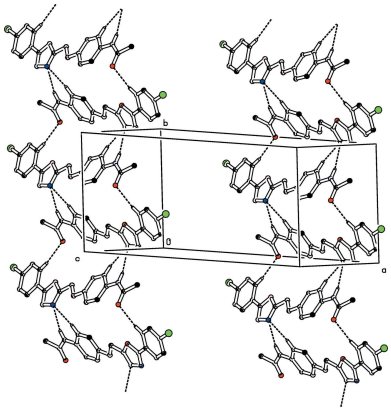
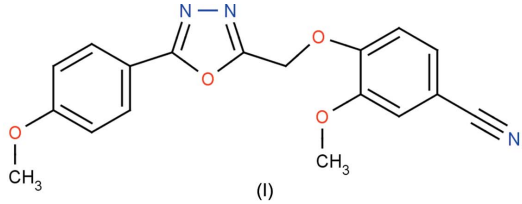
The title compounds, $C_{18}H_{15}N_3O_4$ and $C_{17}H_{14}ClN_3O_3$, are heterocyclic 1,3,4-oxadiazole derivatives which differ from each other in the groups attached to the carbon atoms: a methoxyphenyl ring and a benzonitrile group in (I) and a chlorophenyl ring and an acetamide group in (II). Short intramolecular C—H···O hydrogen bonds occur in both molecules. The crystal structure of (I) features C—H···N hydrogen bonds, while in the crystal structure of (II), N—H···N, C—H···N and C—H···O hydrogen bonds are observed.

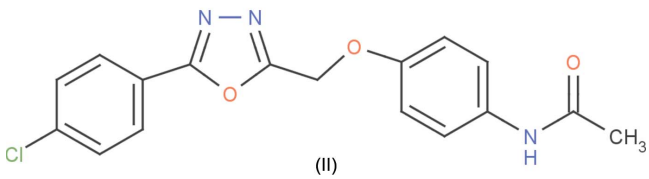
1. Chemical context

Oxadiazole is a versatile heterocyclic nucleus, which has attracted a wide attention of the medicinal chemists for the development of new drugs. Compounds containing a heterocyclic ring system are of great importance both medicinally and industrially (Pace & Pierro, 2009). This stable and neutral hetero aromatic nucleus is associated with potent pharmacological activity that can be attributed to the presence of the toxophoric —N=C—O— linkage (Rigo & Couturier, 1985). Furthermore, 1,3,4-oxadiazole heterocycles are very good bioisosteres of amides and esters, which can contribute substantially in increasing pharmacological activity by participating in hydrogen-bonding interactions with the receptors (Guimaraes *et al.*, 2005). In view of the above importance of the title compounds, we have undertaken single-crystal X-ray diffraction studies for the both compounds and the results are presented here.





(I)



(II)

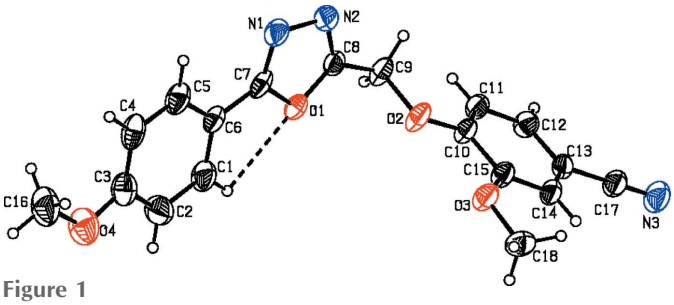


Figure 1
A view of the molecular structure of compound (I), showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The dashed line represent the intramolecular C—H···O interaction (Table 1).

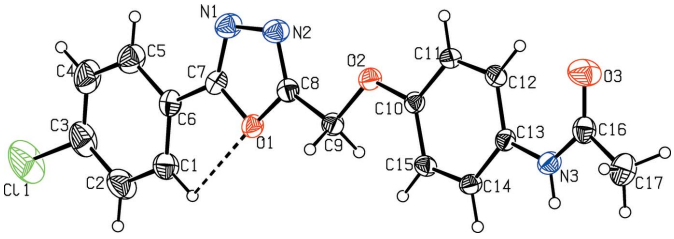


Figure 2
A view of the molecular structure of compound (II), showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The dashed line represents the intramolecular C—H···O interaction (Table 2).

2. Structural commentary

The molecular structures of (I) and (II) are illustrated in Figs. 1 and 2, respectively. In (I), the 4-methoxyphenyl and oxadiazole (r.m.s. deviation 0.007 Å) rings are almost coplanar with a dihedral angle of 1.4 (1)°. The methoxy atoms O4 and C16 are also coplanar with the rings, deviating by 0.080 (1) and 0.020 (1) Å from the mean plane of the phenyl ring, respectively. In (II), the chlorophenyl ring is almost coplanar with the oxadiazole ring, the angle between their mean planes being 4.0 (1)°. The whole molecule is almost planar: the r.m.s. deviation is 0.098 Å and the largest deviation from the mean plane of 0.230 (2) Å is observed for atom C17. Such planarity is not observed in (I) since the methoxyphenyl ring and the benzonitrile moiety are oriented at a dihedral angle of 66.8 (1)°. This difference can be seen in Fig. 3, which shows a superposition of the two molecular structures through the oxadiazole ring (C7/N1/N2/C8/O1) obtained using *Qmol* (Gans & Shalloway, 2001).

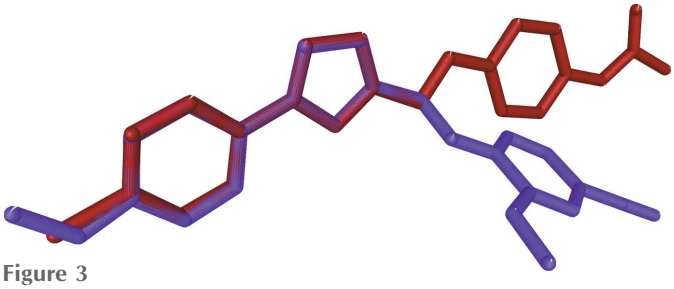


Figure 3
Superposition of oxadiazole ring system of compound (I) (blue) and compound (II)(red).

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1	0.93	2.50	2.835 (6)	101
C9—H9A···N1^{i}	0.97	2.57	3.540 (6)	178
C18—H18A···N2^{ii}	0.96	2.60	3.470 (6)	151
C16—H16B···O3^{iii}	0.96	2.59	3.094 (7)	113

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

The molecular structures of both (1) and (II) are influenced by intramolecular C—H···O interactions (Tables 1 and 2), which form $S(5)$ ring motifs (Figs. 1 and 2).

3. Supramolecular features

In the crystal of compound (I), molecules are associated via C—H···O interactions into inversion dimers (C16—H16B···O3^{iii}, Table 1), generating an $R_2^2(30)$ motif (Fig. 4). Further C—H···N hydrogen bonds (C9—H9A···N1^{i}, Table 1) link the molecules, forming $C(5)$ chains propagating along [010] (Fig. 5). There is also a weak C—H···N interaction (C18—H18A···N2^{ii}, Table 1) that links the molecules, forming $C(9)$ chains propagating in an anti-parallel manner along [110]. These C—H···N hydrogen bonds along with the C—

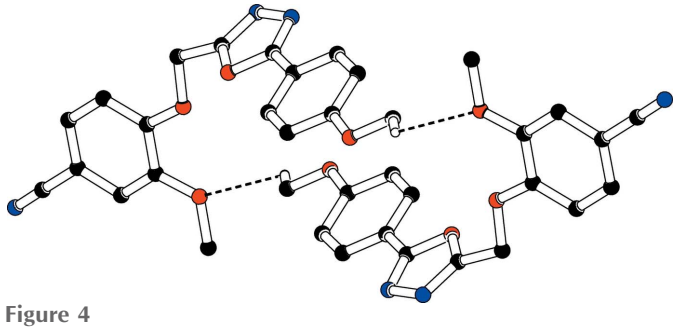


Figure 4
The inversion dimer formed in compound (I) via C—H···O interactions (dashed lines). For clarity H atoms not involved in these hydrogen bonds have been omitted.

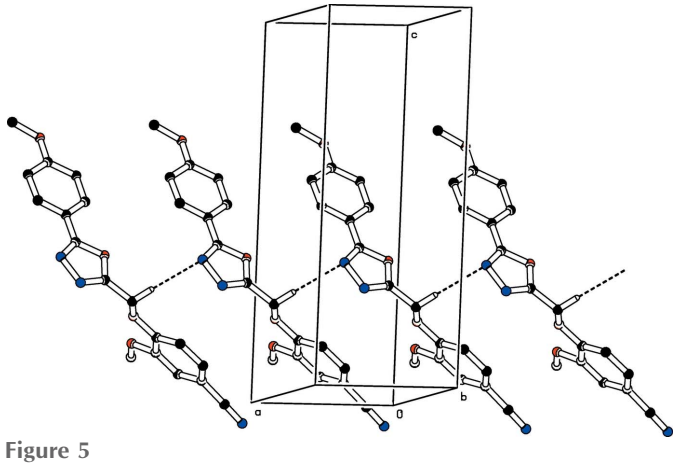


Figure 5
The crystal packing of compound (I) viewed down the *b* axis. The C—H···N hydrogen bonds (see Table 1) are shown as dashed lines. For clarity H atoms not involved in these hydrogen bonds have been omitted.

Table 2
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1	0.93	2.54	2.853 (3)	100
N3—H3···N2^{i}	0.86	2.55	3.377 (3)	161
C1—H1···O3^{i}	0.93	2.46	3.359 (3)	163
C14—H14···N2^{i}	0.93	2.59	3.443 (3)	152
C17—H17*C*···O3^{ii}	0.96	2.56	3.357 (4)	140

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

H···O dimers form a closed cavity shape arrangement consisting of 26 atoms in the unit cell (Fig. 6). In addition, offset π–π interactions are observed between the centroids of inversion-related oxadiazole and 4-methoxyphenyl rings with a centroid–centroid distance of 3.700 (3) Å and a slippage of 1.037 Å.

In the crystal of compound (II), molecules are connected by N—H···N hydrogen bonds forming $C(10)$ chains, C—H···N hydrogen bonds forming $C(8)$ chains and C—H···O interactions forming $C(15)$ chains (Fig. 7). All these chains propagate along [010] in a helical manner. In addition, C—H···O interactions involving atoms H17*C* and O3 are also observed (Table 2). No π–π interactions are observed in compound (II) because of the coplanarity between the oxadiazole and chlorophenyl rings.

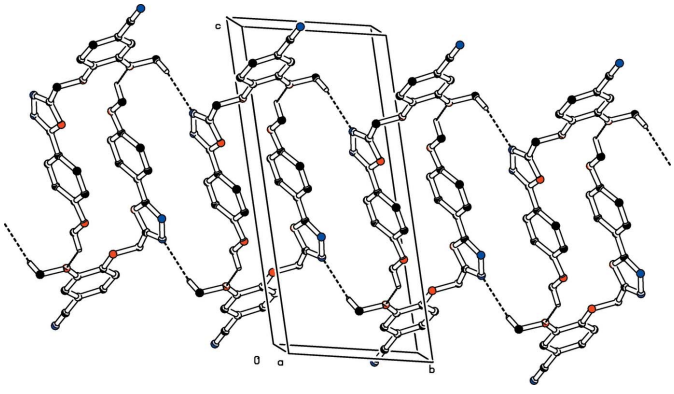


Figure 6
The crystal packing of the title compound (I) viewed along the *a* axis. The C—H···N hydrogen bonds and C—H···O interactions (see Table 1) are shown as dashed lines. For clarity H atoms not involved in these hydrogen bonds have been omitted.

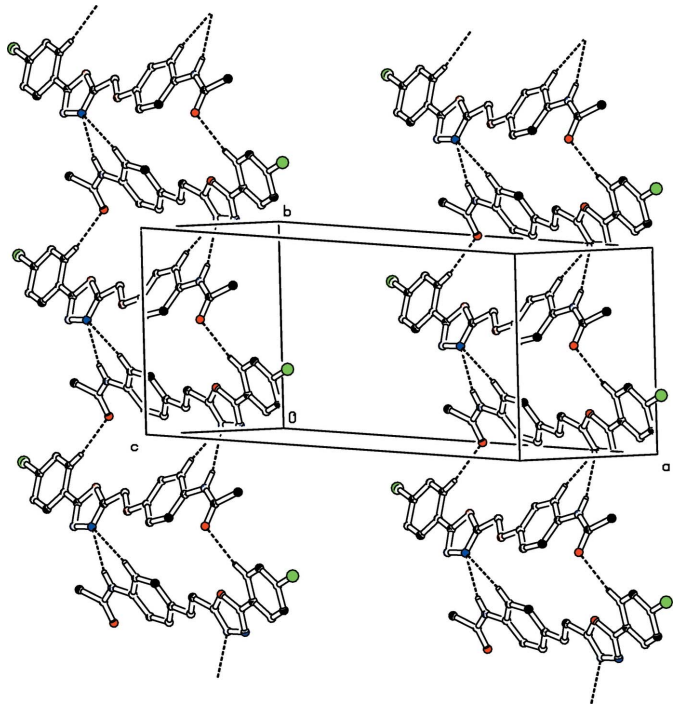


Figure 7
The crystal packing of (II) viewed along the *c* axis. The N—H···N, C—H···N and C—H···O interactions (see Table 2) are shown as dashed lines. For clarity H atoms not involved in these hydrogen bonds have been omitted.

4. Synthesis and crystallization

Compound (I) was synthesized from a solution of 4-hydroxy-3-methoxybenzonitrile (1mmol), K_2CO_3 (3 mmol) in DMF (4 mL), 2-(chloromethyl)-5-(4-methoxyphenyl)-1,3,4-oxadiazole and KI (0.5 mmol). The reaction mixture was stirred at room temperature for about 2 h until the starting material had been consumed (TLC monitoring), and then washed with cold water. The solid product was collected by filtration and dried under vacuum. The pure compound was further recrystallized from ethyl acetate/petroleum ether solution (*v*:*v* = 1:1).

Compound (II) was synthesized from a solution of *N*-(4-hydroxyphenyl)acetamide (1mmol), K_2CO_3 (3 mmol) in ACN (5mL), 2-(chloromethyl)-5-(4-chlorophenyl)-1,3,4-oxadiazole and KI (0.5 mmol). The reaction mixture was stirred under reflux condition for about 16 h, until completion of the reaction (TLC monitoring), then it was diluted with ethyl acetate (30 mL) and washed with saturated $NaHCO_3$ and cold water. The organic layer was separated, dried over anhydrous Na_2SO_4 and concentrated under vacuum. The pure compound was further recrystallized from an ethyl acetate/petroleum ether solution (*v*:*v* = 1:1), giving colourless block-like crystals suitable for X-ray diffraction analysis.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. In both crystal structures, H atoms were placed in idealized positions and allowed to ride on their parent atoms: C—H = 0.93–0.97 Å with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C) for other H atoms.

Funding information

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Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{18}H_{15}N_3O_4$	$C_{17}H_{14}ClN_3O_3$
M_r	337.33	343.76
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $C2/c$
Temperature (K)	298	298
a, b, c (Å)	6.0847 (14), 8.5048 (19), 17.286 (4)	42.24 (1), 10.233 (3), 7.496 (2)
α, β, γ (°)	102.668 (7), 90.646 (6), 109.813 (8)	90, 91.016 (11), 90
V (Å^3)	817.5 (3)	3239.6 (15)
Z	2	8
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.10	0.26
Crystal size (mm)	0.24 × 0.21 × 0.19	0.22 × 0.20 × 0.18
Data collection		
Diffractometer	Bruker SMART APEX CCD area-detector	Bruker SMART APEX CCD area-detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4701, 3593, 1137	8758, 3650, 2733
R_{int}	0.087	0.117
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650	0.649
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.086, 0.282, 0.95	0.063, 0.182, 1.05
No. of reflections	3593	3650
No. of parameters	228	218
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.33	0.25, −0.36

Computer programs: *SMART* and *SAINT* (Bruker, 2002), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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supporting information

Acta Cryst. (2018). E**74**, 1919-1922 [https://doi.org/10.1107/S2056989018016754]

Crystal structures of 3-methoxy-4-{[5-(4-methoxyphenyl)-1,3,4-oxadiazol-2-yl]methoxy}benzonitrile and *N*-(4-{[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]methoxy}phenyl)acetamide

K. Lakshmithendral, K. Archana, K. Saravanan, S. Kabilan and S. Selvanayagam

Computing details

For both structures, data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT* (Bruker, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2018* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

3-Methoxy-4-{[5-(4-methoxyphenyl)-1,3,4-oxadiazol-2-yl]methoxy}benzonitrile (I)

Crystal data

$C_{18}H_{15}N_3O_4$
$M_r = 337.33$
Triclinic, $P\overline{1}$
$a = 6.0847$ (14) Å
$b = 8.5048$ (19) Å
$c = 17.286$ (4) Å
$\alpha = 102.668$ (7)°
$\beta = 90.646$ (6)°
$\gamma = 109.813$ (8)°
$V = 817.5$ (3) Å^3
$Z = 2$
$F(000) = 352$
$D_x = 1.370$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3118 reflections
$\theta = 3.2$–27.4°
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, colourless
0.24 × 0.21 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω and φ scans
4701 measured reflections
3593 independent reflections
1137 reflections with $I > 2\sigma(I)$
$R_{int} = 0.087$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -7\rightarrow7$
$k = -9\rightarrow10$
$l = -22\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.086$
$wR(F^2) = 0.282$
$S = 0.95$
3593 reflections
228 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0956P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ 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}
O1	0.1843 (5)	0.2454 (3)	0.36727 (18)	0.0573 (8)
O2	−0.1120 (5)	0.0785 (3)	0.21803 (19)	0.0672 (10)
O3	−0.2533 (6)	−0.2488 (4)	0.16208 (19)	0.0661 (10)
O4	0.6234 (7)	0.1389 (5)	0.6784 (2)	0.0999 (13)
N1	0.5537 (7)	0.3888 (5)	0.3540 (2)	0.0666 (11)
N2	0.4067 (7)	0.3864 (5)	0.2876 (2)	0.0679 (12)
N3	−1.0776 (8)	−0.3032 (5)	−0.0393 (3)	0.0818 (14)
C1	0.3016 (9)	0.1713 (6)	0.5111 (3)	0.0746 (15)
H1	0.145930	0.131974	0.490115	0.089*
C2	0.3548 (10)	0.1334 (7)	0.5810 (3)	0.0810 (17)
H2	0.235535	0.069914	0.606852	0.097*
C3	0.5834 (10)	0.1892 (7)	0.6124 (3)	0.0737 (15)
C4	0.7621 (9)	0.2890 (7)	0.5738 (3)	0.0744 (15)
H4	0.917781	0.329479	0.594902	0.089*
C5	0.7024 (9)	0.3258 (6)	0.5045 (3)	0.0734 (14)
H5	0.820509	0.392725	0.479518	0.088*
C6	0.4759 (7)	0.2674 (5)	0.4710 (3)	0.0534 (11)
C7	0.4163 (7)	0.3047 (5)	0.3975 (3)	0.0563 (12)
C8	0.1976 (8)	0.3015 (5)	0.2998 (3)	0.0510 (11)
C9	−0.0194 (8)	0.2584 (5)	0.2476 (3)	0.0617 (13)
H9A	−0.132615	0.297492	0.277473	0.074*
H9B	0.015621	0.314695	0.203787	0.074*
C10	−0.3104 (7)	0.0114 (5)	0.1662 (3)	0.0524 (11)
C11	−0.4371 (8)	0.1049 (5)	0.1460 (3)	0.0559 (12)
H11	−0.387569	0.222949	0.167178	0.067*
C12	−0.6385 (8)	0.0239 (6)	0.0940 (3)	0.0572 (12)
H12	−0.723785	0.087491	0.080049	0.069*
C13	−0.7123 (8)	−0.1506 (6)	0.0632 (2)	0.0531 (11)
C14	−0.5881 (7)	−0.2481 (5)	0.0840 (2)	0.0545 (12)
H14	−0.640032	−0.366455	0.063238	0.065*
C15	−0.3888 (8)	−0.1680 (5)	0.1354 (3)	0.0545 (12)
C16	0.8476 (11)	0.1995 (8)	0.7151 (4)	0.110 (2)
H16A	0.939257	0.139919	0.684979	0.165*
H16B	0.842598	0.180561	0.767860	0.165*
H16C	0.917417	0.320492	0.718006	0.165*
C17	−0.9170 (9)	−0.2349 (6)	0.0064 (3)	0.0621 (13)
C18	−0.3336 (9)	−0.4316 (5)	0.1354 (3)	0.0741 (15)
H18A	−0.454760	−0.482003	0.166887	0.111*
H18B	−0.205201	−0.471141	0.140725	0.111*

H18C	−0.394768	−0.464801	0.080479	0.111*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0402 (18)	0.0536 (18)	0.059 (2)	−0.0017 (14)	−0.0116 (15)	0.0045 (15)
O2	0.062 (2)	0.0410 (16)	0.081 (2)	0.0082 (15)	−0.0299 (18)	−0.0021 (16)
O3	0.065 (2)	0.0469 (18)	0.075 (2)	0.0105 (15)	−0.0204 (18)	0.0094 (16)
O4	0.087 (3)	0.126 (3)	0.086 (3)	0.039 (3)	−0.016 (2)	0.023 (3)
N1	0.044 (2)	0.072 (3)	0.061 (3)	−0.002 (2)	0.002 (2)	0.003 (2)
N2	0.059 (3)	0.069 (3)	0.055 (3)	0.000 (2)	0.004 (2)	0.010 (2)
N3	0.078 (3)	0.074 (3)	0.078 (3)	0.013 (3)	−0.027 (3)	0.010 (2)
C1	0.063 (3)	0.078 (3)	0.068 (3)	0.014 (3)	−0.021 (3)	0.009 (3)
C2	0.066 (4)	0.098 (4)	0.073 (4)	0.015 (3)	−0.003 (3)	0.029 (3)
C3	0.074 (4)	0.083 (4)	0.065 (3)	0.037 (3)	−0.007 (3)	0.005 (3)
C4	0.049 (3)	0.089 (4)	0.070 (4)	0.025 (3)	−0.021 (3)	−0.010 (3)
C5	0.047 (3)	0.078 (3)	0.073 (4)	0.009 (3)	−0.011 (3)	−0.004 (3)
C6	0.042 (3)	0.049 (2)	0.054 (3)	0.007 (2)	−0.005 (2)	−0.005 (2)
C7	0.035 (2)	0.047 (2)	0.064 (3)	0.002 (2)	−0.006 (2)	−0.013 (2)
C8	0.054 (3)	0.041 (2)	0.048 (3)	0.012 (2)	0.002 (2)	−0.002 (2)
C9	0.063 (3)	0.041 (2)	0.069 (3)	0.013 (2)	−0.020 (3)	−0.004 (2)
C10	0.048 (3)	0.039 (2)	0.059 (3)	0.009 (2)	−0.013 (2)	0.002 (2)
C11	0.062 (3)	0.043 (2)	0.057 (3)	0.014 (2)	−0.008 (2)	0.008 (2)
C12	0.051 (3)	0.058 (3)	0.062 (3)	0.018 (2)	−0.005 (2)	0.014 (2)
C13	0.049 (3)	0.058 (3)	0.041 (2)	0.007 (2)	−0.002 (2)	0.007 (2)
C14	0.055 (3)	0.048 (2)	0.050 (3)	0.009 (2)	−0.011 (2)	0.004 (2)
C15	0.051 (3)	0.045 (2)	0.060 (3)	0.013 (2)	−0.013 (2)	0.006 (2)
C16	0.093 (5)	0.145 (6)	0.077 (4)	0.033 (4)	−0.019 (4)	0.015 (4)
C17	0.063 (3)	0.053 (3)	0.061 (3)	0.013 (2)	−0.011 (3)	0.008 (2)
C18	0.087 (4)	0.049 (3)	0.087 (4)	0.020 (3)	0.006 (3)	0.022 (3)

Geometric parameters (Å, º)

O1—C8	1.347 (5)	C5—H5	0.9300
O1—C7	1.381 (5)	C6—C7	1.446 (6)
O2—C10	1.368 (5)	C8—C9	1.480 (6)
O2—C9	1.409 (5)	C9—H9A	0.9700
O3—C15	1.371 (5)	C9—H9B	0.9700
O3—C18	1.426 (5)	C10—C11	1.371 (5)
O4—C3	1.350 (6)	C10—C15	1.409 (5)
O4—C16	1.375 (6)	C11—C12	1.383 (6)
N1—C7	1.274 (5)	C11—H11	0.9300
N1—N2	1.439 (5)	C12—C13	1.373 (6)
N2—C8	1.278 (5)	C12—H12	0.9300
N3—C17	1.146 (5)	C13—C14	1.392 (5)
C1—C2	1.380 (6)	C13—C17	1.445 (6)
C1—C6	1.396 (6)	C14—C15	1.369 (5)
C1—H1	0.9300	C14—H14	0.9300

C2—C3	1.370 (7)	C16—H16A	0.9600
C2—H2	0.9300	C16—H16B	0.9600
C3—C4	1.409 (7)	C16—H16C	0.9600
C4—C5	1.377 (6)	C18—H18A	0.9600
C4—H4	0.9300	C18—H18B	0.9600
C5—C6	1.369 (6)	C18—H18C	0.9600

C8—O1—C7	102.6 (3)	C8—C9—H9B	110.0
C10—O2—C9	117.8 (3)	H9A—C9—H9B	108.4
C15—O3—C18	116.4 (3)	C11—C10—O2	124.7 (4)
C3—O4—C16	119.1 (5)	C11—C10—C15	119.8 (4)
C7—N1—N2	106.0 (4)	O2—C10—C15	115.4 (3)
C8—N2—N1	105.4 (4)	C10—C11—C12	120.2 (4)
C2—C1—C6	121.6 (5)	C10—C11—H11	119.9
C2—C1—H1	119.2	C12—C11—H11	119.9
C6—C1—H1	119.2	C13—C12—C11	119.8 (4)
C1—C2—C3	120.0 (5)	C13—C12—H12	120.1
C1—C2—H2	120.0	C11—C12—H12	120.1
C3—C2—H2	120.0	C12—C13—C14	120.9 (4)
O4—C3—C2	116.6 (5)	C12—C13—C17	120.1 (4)
O4—C3—C4	123.8 (5)	C14—C13—C17	119.0 (4)
C2—C3—C4	119.5 (5)	C15—C14—C13	119.3 (4)
C5—C4—C3	118.9 (5)	C15—C14—H14	120.4
C5—C4—H4	120.5	C13—C14—H14	120.4
C3—C4—H4	120.5	O3—C15—C14	125.3 (4)
C6—C5—C4	122.5 (5)	O3—C15—C10	114.7 (4)
C6—C5—H5	118.8	C14—C15—C10	120.0 (4)
C4—C5—H5	118.8	O4—C16—H16A	109.5
C5—C6—C1	117.5 (5)	O4—C16—H16B	109.5
C5—C6—C7	121.9 (5)	H16A—C16—H16B	109.5
C1—C6—C7	120.7 (4)	O4—C16—H16C	109.5
N1—C7—O1	112.4 (4)	H16A—C16—H16C	109.5
N1—C7—C6	128.2 (4)	H16B—C16—H16C	109.5
O1—C7—C6	119.4 (4)	N3—C17—C13	179.0 (6)
N2—C8—O1	113.6 (4)	O3—C18—H18A	109.5
N2—C8—C9	127.0 (4)	O3—C18—H18B	109.5
O1—C8—C9	119.4 (4)	H18A—C18—H18B	109.5
O2—C9—C8	108.3 (3)	O3—C18—H18C	109.5
O2—C9—H9A	110.0	H18A—C18—H18C	109.5
C8—C9—H9A	110.0	H18B—C18—H18C	109.5
O2—C9—H9B	110.0		

C7—N1—N2—C8	0.3 (5)	C7—O1—C8—N2	−0.5 (5)
C6—C1—C2—C3	−0.5 (8)	C7—O1—C8—C9	178.1 (3)
C16—O4—C3—C2	−176.1 (5)	C10—O2—C9—C8	−178.1 (4)
C16—O4—C3—C4	5.9 (8)	N2—C8—C9—O2	114.2 (5)
C1—C2—C3—O4	−176.3 (5)	O1—C8—C9—O2	−64.2 (5)
C1—C2—C3—C4	1.7 (8)	C9—O2—C10—C11	−5.7 (7)

O4—C3—C4—C5	176.8 (5)	C9—O2—C10—C15	176.9 (4)
C2—C3—C4—C5	−1.1 (8)	O2—C10—C11—C12	−178.7 (4)
C3—C4—C5—C6	−0.7 (8)	C15—C10—C11—C12	−1.4 (7)
C4—C5—C6—C1	1.8 (7)	C10—C11—C12—C13	0.4 (7)
C4—C5—C6—C7	−179.0 (4)	C11—C12—C13—C14	0.6 (7)
C2—C1—C6—C5	−1.2 (7)	C11—C12—C13—C17	−177.4 (4)
C2—C1—C6—C7	179.6 (4)	C12—C13—C14—C15	−0.6 (7)
N2—N1—C7—O1	−0.7 (5)	C17—C13—C14—C15	177.5 (4)
N2—N1—C7—C6	179.2 (4)	C18—O3—C15—C14	−2.0 (7)
C8—O1—C7—N1	0.8 (5)	C18—O3—C15—C10	176.9 (4)
C8—O1—C7—C6	−179.2 (4)	C13—C14—C15—O3	178.5 (4)
C5—C6—C7—N1	1.4 (7)	C13—C14—C15—C10	−0.4 (7)
C1—C6—C7—N1	−179.5 (4)	C11—C10—C15—O3	−177.6 (4)
C5—C6—C7—O1	−178.7 (4)	O2—C10—C15—O3	−0.1 (6)
C1—C6—C7—O1	0.5 (6)	C11—C10—C15—C14	1.4 (7)
N1—N2—C8—O1	0.1 (5)	O2—C10—C15—C14	178.9 (4)
N1—N2—C8—C9	−178.3 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1	0.93	2.50	2.835 (6)	101
C9—H9*A*···N1^{i}	0.97	2.57	3.540 (6)	178
C18—H18*A*···N2^{ii}	0.96	2.60	3.470 (6)	151
C16—H16*B*···O3^{iii}	0.96	2.59	3.094 (7)	113

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

N-(4-{[5-(4-Chlorophenyl)-1,3,4-oxadiazol-2-yl]methoxy}phenyl)acetamide (II)

Crystal data

$C_{17}H_{14}ClN_3O_3$	*F*(000) = 1424
M_r = 343.76	D_x = 1.410 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *Kα* radiation, *λ* = 0.71073 Å
a = 42.24 (1) Å	Cell parameters from 5528 reflections
b = 10.233 (3) Å	*θ* = 3.3–27.2°
c = 7.496 (2) Å	*μ* = 0.26 mm^{-1}
β = 91.016 (11)°	*T* = 298 K
V = 3239.6 (15) Å^3	Block, colourless
Z = 8	0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2733 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.117
ω and *φ* scans	θ_{max} = 27.5°, θ_{min} = 3.1°
8758 measured reflections	*h* = −52→54
3650 independent reflections	*k* = −13→12
	l = −6→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.182$
$S = 1.05$
3650 reflections
218 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2 + 1.9656P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ 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}
Cl1	1.01226 (2)	0.28663 (15)	−0.00562 (17)	0.1223 (5)
O1	0.85574 (3)	0.18095 (14)	0.0915 (2)	0.0407 (4)
O2	0.77454 (3)	0.07687 (14)	0.0967 (2)	0.0425 (4)
O3	0.62394 (4)	0.0180 (2)	0.2485 (3)	0.0729 (6)
N1	0.86735 (5)	−0.00435 (19)	−0.0435 (3)	0.0519 (5)
N2	0.83462 (4)	−0.00355 (19)	−0.0042 (3)	0.0487 (5)
N3	0.65271 (4)	0.19545 (18)	0.3324 (3)	0.0446 (4)
H3	0.651157	0.270429	0.383345	0.053*
C1	0.91898 (6)	0.2770 (3)	0.0713 (4)	0.0552 (6)
H1	0.903405	0.332106	0.114707	0.066*
C2	0.95026 (7)	0.3187 (3)	0.0652 (4)	0.0723 (8)
H2	0.955862	0.401652	0.105345	0.087*
C3	0.97283 (6)	0.2357 (4)	−0.0008 (4)	0.0742 (9)
C4	0.96543 (6)	0.1127 (4)	−0.0627 (4)	0.0737 (8)
H4	0.981049	0.058641	−0.108061	0.088*
C5	0.93441 (6)	0.0710 (3)	−0.0564 (4)	0.0623 (7)
H5	0.929027	−0.011804	−0.097927	0.075*
C6	0.91116 (5)	0.1521 (2)	0.0118 (3)	0.0462 (5)
C7	0.87852 (5)	0.1050 (2)	0.0164 (3)	0.0417 (5)
C8	0.82940 (5)	0.1064 (2)	0.0735 (3)	0.0392 (5)
C9	0.79968 (5)	0.1607 (2)	0.1473 (3)	0.0395 (5)
H9A	0.801380	0.166062	0.276309	0.047*
H9B	0.795908	0.247872	0.100672	0.047*
C10	0.74482 (5)	0.11247 (18)	0.1555 (3)	0.0345 (4)
C11	0.72024 (5)	0.02966 (19)	0.1083 (3)	0.0376 (4)
H11	0.724354	−0.043669	0.039235	0.045*
C12	0.68942 (5)	0.05388 (19)	0.1623 (3)	0.0393 (5)
H12	0.673114	−0.002716	0.129254	0.047*
C13	0.68317 (5)	0.16400 (19)	0.2665 (3)	0.0356 (4)
C14	0.70774 (5)	0.24918 (19)	0.3082 (3)	0.0377 (4)

H14	0.703636	0.324139	0.374048	0.045*
C15	0.73839 (5)	0.22421 (19)	0.2532 (3)	0.0376 (4)
H15	0.754604	0.282438	0.281810	0.045*
C16	0.62573 (5)	0.1230 (2)	0.3258 (3)	0.0481 (5)
C17	0.59772 (6)	0.1809 (3)	0.4218 (4)	0.0633 (7)
H17A	0.579119	0.174637	0.346840	0.095*
H17B	0.601896	0.271026	0.448890	0.095*
H17C	0.594398	0.133676	0.530577	0.095*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0409 (4)	0.1918 (13)	0.1346 (10)	−0.0285 (6)	0.0098 (5)	−0.0347 (9)
O1	0.0337 (7)	0.0388 (7)	0.0495 (9)	0.0005 (6)	0.0009 (6)	0.0002 (6)
O2	0.0347 (7)	0.0388 (7)	0.0541 (9)	−0.0004 (6)	0.0022 (6)	−0.0049 (6)
O3	0.0530 (10)	0.0679 (12)	0.0983 (15)	−0.0194 (10)	0.0142 (10)	−0.0212 (11)
N1	0.0459 (10)	0.0484 (11)	0.0618 (12)	0.0004 (9)	0.0093 (9)	−0.0053 (9)
N2	0.0445 (10)	0.0434 (10)	0.0583 (12)	−0.0042 (8)	0.0070 (8)	−0.0058 (8)
N3	0.0391 (9)	0.0393 (9)	0.0554 (11)	0.0024 (8)	0.0032 (8)	−0.0038 (8)
C1	0.0397 (12)	0.0612 (15)	0.0648 (15)	−0.0029 (11)	0.0036 (11)	−0.0073 (12)
C2	0.0495 (15)	0.085 (2)	0.082 (2)	−0.0147 (14)	−0.0027 (14)	−0.0151 (17)
C3	0.0378 (13)	0.112 (3)	0.0733 (19)	−0.0085 (15)	0.0046 (12)	−0.0051 (18)
C4	0.0419 (13)	0.097 (2)	0.083 (2)	0.0130 (15)	0.0095 (13)	−0.0038 (17)
C5	0.0491 (13)	0.0675 (16)	0.0708 (17)	0.0051 (12)	0.0107 (12)	−0.0023 (13)
C6	0.0377 (11)	0.0514 (12)	0.0495 (12)	0.0033 (10)	0.0006 (9)	0.0048 (10)
C7	0.0389 (11)	0.0408 (11)	0.0453 (11)	0.0062 (9)	0.0024 (8)	0.0030 (9)
C8	0.0394 (10)	0.0375 (10)	0.0407 (10)	−0.0029 (8)	−0.0008 (8)	0.0062 (8)
C9	0.0372 (10)	0.0380 (10)	0.0433 (11)	−0.0016 (8)	0.0000 (8)	0.0017 (8)
C10	0.0357 (10)	0.0328 (9)	0.0349 (9)	0.0008 (8)	−0.0011 (7)	0.0032 (7)
C11	0.0414 (10)	0.0306 (9)	0.0407 (10)	0.0013 (8)	−0.0034 (8)	−0.0029 (8)
C12	0.0356 (10)	0.0363 (10)	0.0458 (11)	−0.0044 (8)	−0.0033 (8)	−0.0015 (8)
C13	0.0344 (10)	0.0338 (9)	0.0385 (10)	0.0017 (8)	−0.0009 (8)	0.0034 (8)
C14	0.0430 (11)	0.0306 (9)	0.0393 (10)	0.0014 (8)	−0.0002 (8)	−0.0023 (8)
C15	0.0376 (10)	0.0329 (9)	0.0423 (11)	−0.0061 (8)	−0.0027 (8)	−0.0011 (8)
C16	0.0398 (11)	0.0518 (13)	0.0529 (13)	−0.0011 (10)	0.0007 (9)	0.0055 (10)
C17	0.0422 (13)	0.0750 (18)	0.0729 (17)	0.0050 (12)	0.0125 (12)	0.0086 (14)

Geometric parameters (Å, º)

Cl1—C3	1.746 (3)	C5—C6	1.390 (3)
O1—C8	1.354 (2)	C5—H5	0.9300
O1—C7	1.366 (2)	C6—C7	1.461 (3)
O2—C10	1.386 (2)	C8—C9	1.488 (3)
O2—C9	1.412 (2)	C9—H9A	0.9700
O3—C16	1.222 (3)	C9—H9B	0.9700
N1—C7	1.292 (3)	C10—C11	1.381 (3)
N1—N2	1.419 (3)	C10—C15	1.387 (3)
N2—C8	1.288 (3)	C11—C12	1.392 (3)

N3—C16	1.359 (3)	C11—H11	0.9300
N3—C13	1.423 (3)	C12—C13	1.399 (3)
N3—H3	0.8600	C12—H12	0.9300
C1—C2	1.390 (4)	C13—C14	1.387 (3)
C1—C6	1.391 (4)	C14—C15	1.390 (3)
C1—H1	0.9300	C14—H14	0.9300
C2—C3	1.376 (4)	C15—H15	0.9300
C2—H2	0.9300	C16—C17	1.516 (3)
C3—C4	1.375 (5)	C17—H17A	0.9600
C4—C5	1.380 (4)	C17—H17B	0.9600
C4—H4	0.9300	C17—H17C	0.9600

C8—O1—C7	102.84 (16)	O2—C9—H9A	110.1
C10—O2—C9	115.84 (15)	C8—C9—H9A	110.1
C7—N1—N2	105.90 (18)	O2—C9—H9B	110.1
C8—N2—N1	105.93 (18)	C8—C9—H9B	110.1
C16—N3—C13	128.78 (19)	H9A—C9—H9B	108.4
C16—N3—H3	115.6	C11—C10—O2	115.99 (17)
C13—N3—H3	115.6	C11—C10—C15	119.16 (19)
C2—C1—C6	119.5 (2)	O2—C10—C15	124.84 (18)
C2—C1—H1	120.3	C10—C11—C12	121.27 (18)
C6—C1—H1	120.3	C10—C11—H11	119.4
C3—C2—C1	119.2 (3)	C12—C11—H11	119.4
C3—C2—H2	120.4	C11—C12—C13	119.49 (18)
C1—C2—H2	120.4	C11—C12—H12	120.3
C4—C3—C2	122.1 (3)	C13—C12—H12	120.3
C4—C3—Cl1	118.5 (3)	C14—C13—C12	118.97 (19)
C2—C3—Cl1	119.4 (3)	C14—C13—N3	117.19 (18)
C3—C4—C5	118.8 (3)	C12—C13—N3	123.84 (18)
C3—C4—H4	120.6	C13—C14—C15	120.99 (18)
C5—C4—H4	120.6	C13—C14—H14	119.5
C4—C5—C6	120.4 (3)	C15—C14—H14	119.5
C4—C5—H5	119.8	C10—C15—C14	120.03 (18)
C6—C5—H5	119.8	C10—C15—H15	120.0
C5—C6—C1	120.0 (2)	C14—C15—H15	120.0
C5—C6—C7	119.0 (2)	O3—C16—N3	122.8 (2)
C1—C6—C7	120.9 (2)	O3—C16—C17	121.7 (2)
N1—C7—O1	112.35 (19)	N3—C16—C17	115.5 (2)
N1—C7—C6	128.0 (2)	C16—C17—H17A	109.5
O1—C7—C6	119.63 (19)	C16—C17—H17B	109.5
N2—C8—O1	112.97 (18)	H17A—C17—H17B	109.5
N2—C8—C9	130.30 (19)	C16—C17—H17C	109.5
O1—C8—C9	116.72 (17)	H17A—C17—H17C	109.5
O2—C9—C8	107.97 (17)	H17B—C17—H17C	109.5

C7—N1—N2—C8	0.6 (3)	C7—O1—C8—N2	−0.2 (2)
C6—C1—C2—C3	0.5 (5)	C7—O1—C8—C9	178.65 (17)
C1—C2—C3—C4	0.6 (5)	C10—O2—C9—C8	179.63 (16)

C1—C2—C3—Cl1	−179.1 (2)	N2—C8—C9—O2	−8.3 (3)
C2—C3—C4—C5	−0.7 (5)	O1—C8—C9—O2	173.06 (16)
Cl1—C3—C4—C5	178.9 (2)	C9—O2—C10—C11	−179.13 (17)
C3—C4—C5—C6	−0.1 (5)	C9—O2—C10—C15	2.1 (3)
C4—C5—C6—C1	1.1 (4)	O2—C10—C11—C12	178.85 (18)
C4—C5—C6—C7	179.9 (2)	C15—C10—C11—C12	−2.3 (3)
C2—C1—C6—C5	−1.3 (4)	C10—C11—C12—C13	−0.1 (3)
C2—C1—C6—C7	179.9 (2)	C11—C12—C13—C14	2.3 (3)
N2—N1—C7—O1	−0.8 (3)	C11—C12—C13—N3	−178.20 (19)
N2—N1—C7—C6	179.2 (2)	C16—N3—C13—C14	−172.9 (2)
C8—O1—C7—N1	0.6 (2)	C16—N3—C13—C12	7.6 (4)
C8—O1—C7—C6	−179.32 (18)	C12—C13—C14—C15	−2.1 (3)
C5—C6—C7—N1	−3.4 (4)	N3—C13—C14—C15	178.33 (19)
C1—C6—C7—N1	175.5 (2)	C11—C10—C15—C14	2.5 (3)
C5—C6—C7—O1	176.6 (2)	O2—C10—C15—C14	−178.79 (18)
C1—C6—C7—O1	−4.6 (3)	C13—C14—C15—C10	−0.2 (3)
N1—N2—C8—O1	−0.3 (2)	C13—N3—C16—O3	−4.4 (4)
N1—N2—C8—C9	−178.9 (2)	C13—N3—C16—C17	175.4 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1	0.93	2.54	2.853 (3)	100
N3—H3···N2^{i}	0.86	2.55	3.377 (3)	161
C1—H1···O3^{i}	0.93	2.46	3.359 (3)	163
C14—H14···N2^{i}	0.93	2.59	3.443 (3)	152
C17—H17*C*···O3^{ii}	0.96	2.56	3.357 (4)	140

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