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4-Chloro-5-(morpholin-4-yl)-2-[(5-phenyl-1,3,4-oxadiazol-2-yl)methyl]pyridazin-3(2*H*)-one

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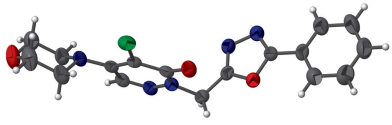
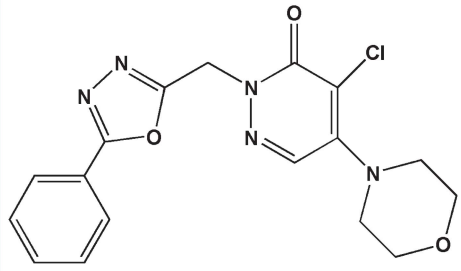
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{17}H_{16}ClN_5O_3$, the phenyl and the oxadiazole rings are almost coplanar, subtending a dihedral angle of 4.34 (19)°. These rings lie almost normal to the pyridazine ring, making dihedral angles of 87.35 (16) and 89.06 (15)°, respectively. The morpholine ring has the usual chair conformation and its mean plane is inclined to the pyridazine ring by 39.45 (17)°. There is a short intramolecular C—H···Cl contact present. In the crystal, molecules are linked by bifurcated C—(H,H)···O hydrogen bonds and a C—H···N hydrogen bond, forming layers parallel to the *ab* plane.

3D view



Chemical scheme



Structure description

1,3,4-Oxadiazole derivatives are a promising field of study because they possess good bioactivity (Liu *et al.*, 2014). This substructural unit has been used as a scaffold to design and synthesize chemical compounds with biological, medicinal and agricultural activities (Gan *et al.*, 2016; Shaikh & Meshram, 2016; Luqman *et al.*, 2015; Fershtat *et al.* 2016; Pattison *et al.*, 2009). A series of oxadiazoles containing a pyridazinone ring have been designed and synthesized, and we report herein on the crystal structure of one such compound.

The molecular structure of the title compound is shown in Fig. 1. The phenyl (C1–C6) and the oxadiazole (O1/N1/N2/C7/C8) rings are almost coplanar, subtending a dihedral angle of 4.34 (19)°. These rings lie almost normal to the pyridazine (N3/N4/C10–C13) ring, making dihedral angles of 87.35 (16) and 89.06 (15)°, respectively. The morpholine (O3/N5/C14–C17) ring has a chair conformation and its mean plane is inclined to the pyridazine ring by 39.45 (17)°. There is a short intramolecular C—H···Cl contact present (Table 1, Fig. 1).

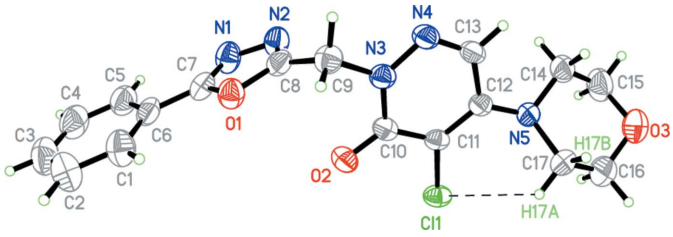


Figure 1
The molecular structure of the title compound, with the atom labelling and displacement ellipsoids drawn at the 50% probability level.

In the crystal, molecules are linked by bifurcated C—(H,H)···O hydrogen bonds and C—H···N hydrogen bond bonds, forming layers parallel to the *ab* plane (Table 1 and Fig. 2).

Synthesis and crystallization

To a three-necked flask, 4,5-dichloro-2-((5- phenyl-1,3,4-oxadiazol-2-yl)methyl)-pyridazin-3-(2*H*)-one (3.0 g, 9.3 mmol; Li *et al.*, 2005) and morpholine (14.0 mmol, 1.22 g) were added and reacted at 333 K for 8 h in the presence of potassium carbonate (2 g) and 20 ml dry DMF. The reaction was monitored by TLC. On completion of the reaction, the mixture was poured into ice–water. The precipitate formed was collected by filtration, dried to give the pure title compound (yield 2.23 g, 64.2%). It was recrystallized from chloroform, ethyl acetate and petroleum (2:2:5) to give pale-yellow prismatic crystals (m.p. 461–463 K).

^{1}H NMR ($CDCl_3$): 3.47 (*t*, 4H), 3.86 (*t*, 4H), 5.64 (*s*, 2H), 7.53 (*m*, 3H), 7.68 (*s*, 1H), 8.06 (*m*, 2H). IR (KBr, cm^{-1}) ν 2957, 2857, 1641, 1593, 1549, 1487, 1446, 1423, 1257, 1117, 780.

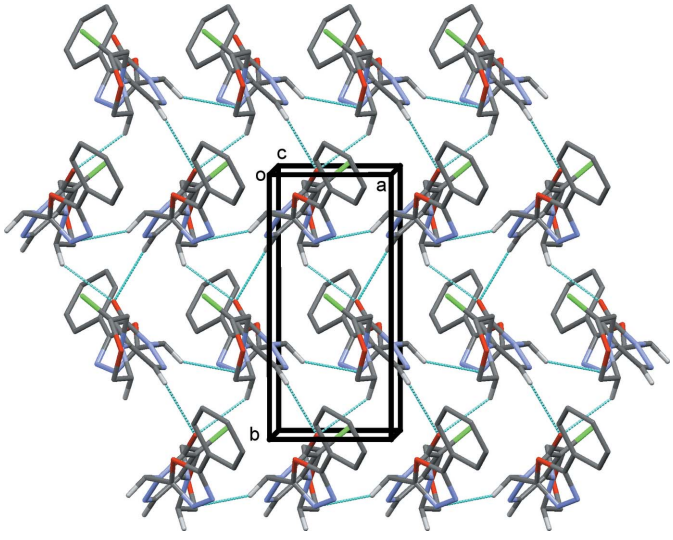


Figure 2
A view along the *c* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17*A*···Cl1	0.97	2.57	3.252 (3)	127
C14—H14*B*···O2^{i}	0.97	2.57	3.373 (4)	141
C13—H13···O2^{ii}	0.93	2.60	3.507 (3)	165
C9—H9*A*···N2^{iii}	0.97	2.50	3.310 (4)	141

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{16}ClN_5O_3$
M_r	373.80
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	293
a, *b*, *c* (Å)	4.7931 (7), 10.4177 (15), 33.685 (5)
V (Å^3)	1682.0 (4)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.26
Crystal size (mm)	0.20 × 0.16 × 0.11
Data collection	
Diffractometer	Bruker SMART CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.658, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10022, 3282, 2995
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.041, 0.096, 1.07
No. of reflections	3282
No. of parameters	235
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.17
Absolute structure	Flack *x* determined using 1105 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.05 (3)

Computer programs: *SMART* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

Refinement

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

Funding information

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full crystallographic data

IUCrData (2017). **2**, x170370 [https://doi.org/10.1107/S2414314617003704]

4-Chloro-5-(morpholin-4-yl)-2-[(5-phenyl-1,3,4-oxadiazol-2-yl)methyl]-pyridazin-3(2*H*)-one

Yanwen Sun, Haolei Wu, Changheng Wei, Mei Gao, Zeyi Shen and Hongsen Li

4-Chloro-5-(morpholin-4-yl)-2-[(5-phenyl-1,3,4-oxadiazol-2-yl)methyl]pyridazin-3(2*H*)-one

Crystal data

$C_{17}H_{16}ClN_5O_3$
M_r = 373.80
Orthorhombic, $P2_12_12_1$
a = 4.7931 (7) Å
b = 10.4177 (15) Å
c = 33.685 (5) Å
V = 1682.0 (4) Å^3
Z = 4
$F(000)$ = 776
D_x = 1.476 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3057 reflections
θ = 4.6–50.4°
μ = 0.26 mm^{-1}
T = 293 K
Prismatic, pale-yellow
0.20 × 0.16 × 0.11 mm

Data collection

Bruker SMART CCD area detector diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.658, T_{max} = 0.746
10022 measured reflections
3282 independent reflections
2995 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 26.0°, θ_{min} = 2.1°
h = −5→5
k = −12→12
l = −40→41

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.096
S = 1.07
3282 reflections
235 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack x determined using 1105 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.05 (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	0.59088 (15)	−0.01685 (6)	0.76733 (2)	0.0433 (2)
N1	0.4856 (6)	0.2459 (3)	0.59442 (7)	0.0529 (7)
N2	0.3286 (6)	0.2745 (3)	0.62853 (7)	0.0486 (7)
N3	0.0445 (5)	0.1687 (2)	0.70294 (7)	0.0368 (5)
N4	−0.0777 (6)	0.2543 (2)	0.72725 (7)	0.0396 (5)
N5	0.2681 (5)	0.1739 (2)	0.82072 (7)	0.0405 (6)
O1	0.1658 (5)	0.09679 (19)	0.60219 (6)	0.0451 (5)
O2	0.3400 (4)	0.00730 (18)	0.68817 (6)	0.0452 (5)
O3	0.2610 (7)	0.1845 (3)	0.90460 (7)	0.0765 (9)
C1	0.3377 (8)	−0.0400 (4)	0.53314 (10)	0.0608 (10)
H1	0.2004	−0.0757	0.5492	0.073*
C2	0.4134 (11)	−0.1013 (4)	0.49869 (11)	0.0736 (11)
H2	0.3278	−0.1779	0.4914	0.088*
C3	0.6176 (10)	−0.0483 (4)	0.47491 (11)	0.0722 (11)
H3	0.6687	−0.0890	0.4514	0.087*
C4	0.7437 (9)	0.0626 (4)	0.48555 (10)	0.0690 (11)
H4	0.8819	0.0972	0.4694	0.083*
C5	0.6695 (8)	0.1252 (4)	0.52024 (10)	0.0581 (9)
H5	0.7578	0.2012	0.5274	0.070*
C6	0.4629 (7)	0.0738 (3)	0.54413 (8)	0.0462 (8)
C7	0.3820 (7)	0.1421 (3)	0.57997 (8)	0.0430 (7)
C8	0.1487 (7)	0.1844 (3)	0.63175 (8)	0.0400 (7)
C9	−0.0686 (7)	0.1662 (3)	0.66278 (8)	0.0421 (7)
H9A	−0.2075	0.2334	0.6602	0.050*
H9B	−0.1610	0.0845	0.6584	0.050*
C10	0.2450 (6)	0.0805 (3)	0.71332 (8)	0.0342 (6)
C11	0.3255 (5)	0.0852 (2)	0.75441 (8)	0.0316 (6)
C12	0.2033 (6)	0.1676 (2)	0.78069 (8)	0.0334 (6)
C13	−0.0014 (6)	0.2522 (2)	0.76394 (8)	0.0378 (7)
H13	−0.0863	0.3106	0.7810	0.045*
C14	0.1841 (9)	0.2897 (3)	0.84206 (9)	0.0505 (9)
H14A	−0.0167	0.2901	0.8456	0.061*
H14B	0.2352	0.3650	0.8268	0.061*
C15	0.3242 (10)	0.2938 (4)	0.88161 (10)	0.0663 (11)
H15A	0.5245	0.2991	0.8778	0.080*
H15B	0.2650	0.3702	0.8958	0.080*
C16	0.3517 (11)	0.0713 (4)	0.88451 (10)	0.0739 (12)
H16A	0.3067	−0.0032	0.9005	0.089*
H16B	0.5528	0.0742	0.8814	0.089*

C17	0.2186 (9)	0.0577 (3)	0.84467 (9)	0.0538 (9)
H17A	0.2956	−0.0165	0.8311	0.065*
H17B	0.0196	0.0444	0.8478	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0348 (4)	0.0369 (4)	0.0584 (4)	0.0064 (3)	0.0008 (3)	0.0035 (3)
N1	0.0579 (19)	0.0594 (17)	0.0416 (14)	−0.0151 (15)	0.0007 (13)	0.0019 (12)
N2	0.0553 (17)	0.0510 (14)	0.0395 (14)	−0.0093 (14)	−0.0015 (12)	0.0000 (11)
N3	0.0351 (13)	0.0353 (12)	0.0399 (12)	0.0023 (11)	0.0019 (10)	0.0019 (10)
N4	0.0379 (13)	0.0357 (12)	0.0451 (14)	0.0058 (11)	0.0071 (12)	0.0019 (10)
N5	0.0495 (15)	0.0341 (13)	0.0379 (13)	−0.0002 (12)	0.0075 (11)	0.0012 (10)
O1	0.0496 (13)	0.0460 (11)	0.0396 (11)	−0.0079 (11)	0.0004 (9)	−0.0011 (9)
O2	0.0496 (13)	0.0407 (11)	0.0455 (11)	0.0067 (11)	0.0072 (9)	−0.0061 (9)
O3	0.108 (2)	0.0816 (18)	0.0397 (13)	0.0122 (19)	0.0130 (14)	0.0015 (12)
C1	0.062 (2)	0.072 (2)	0.0486 (19)	−0.007 (2)	0.0062 (17)	−0.0053 (17)
C2	0.081 (3)	0.078 (3)	0.062 (2)	−0.004 (3)	0.000 (2)	−0.019 (2)
C3	0.077 (3)	0.094 (3)	0.046 (2)	0.007 (3)	0.005 (2)	−0.0082 (19)
C4	0.074 (3)	0.085 (3)	0.048 (2)	0.004 (2)	0.0156 (19)	0.0109 (19)
C5	0.067 (2)	0.062 (2)	0.0454 (19)	−0.0025 (19)	0.0026 (17)	0.0083 (15)
C6	0.0483 (19)	0.0574 (18)	0.0329 (15)	0.0057 (16)	−0.0071 (13)	0.0068 (13)
C7	0.0435 (17)	0.0503 (17)	0.0352 (14)	−0.0045 (15)	−0.0040 (13)	0.0107 (13)
C8	0.0439 (18)	0.0416 (15)	0.0345 (14)	0.0000 (14)	−0.0076 (13)	0.0044 (12)
C9	0.0376 (16)	0.0464 (16)	0.0422 (16)	0.0002 (15)	−0.0043 (14)	0.0006 (12)
C10	0.0294 (14)	0.0295 (13)	0.0438 (15)	−0.0030 (12)	0.0085 (12)	−0.0009 (12)
C11	0.0269 (13)	0.0256 (13)	0.0423 (15)	−0.0021 (11)	0.0031 (11)	0.0022 (11)
C12	0.0333 (14)	0.0265 (13)	0.0405 (14)	−0.0049 (12)	0.0063 (12)	0.0014 (11)
C13	0.0398 (16)	0.0288 (13)	0.0448 (16)	0.0040 (12)	0.0096 (13)	−0.0009 (12)
C14	0.066 (2)	0.0415 (16)	0.0437 (17)	−0.0024 (16)	0.0098 (16)	−0.0045 (13)
C15	0.080 (3)	0.068 (2)	0.0501 (19)	−0.006 (2)	0.0091 (19)	−0.0116 (17)
C16	0.100 (4)	0.075 (2)	0.0470 (19)	0.025 (3)	0.008 (2)	0.0126 (17)
C17	0.073 (2)	0.0413 (16)	0.0475 (18)	0.0036 (17)	0.0125 (17)	0.0095 (14)

Geometric parameters (Å, º)

Cl1—C11	1.714 (3)	C4—C5	1.385 (5)
N1—C7	1.285 (4)	C4—H4	0.9300
N1—N2	1.405 (4)	C5—C6	1.384 (5)
N2—C8	1.278 (4)	C5—H5	0.9300
N3—N4	1.345 (3)	C6—C7	1.454 (4)
N3—C10	1.375 (4)	C8—C9	1.488 (4)
N3—C9	1.457 (4)	C9—H9A	0.9700
N4—C13	1.289 (4)	C9—H9B	0.9700
N5—C12	1.385 (4)	C10—C11	1.438 (4)
N5—C14	1.461 (4)	C11—C12	1.365 (4)
N5—C17	1.474 (4)	C12—C13	1.435 (4)
O1—C8	1.354 (3)	C13—H13	0.9300

O1—C7	1.363 (4)	C14—C15	1.493 (5)
O2—C10	1.228 (3)	C14—H14A	0.9700
O3—C15	1.411 (4)	C14—H14B	0.9700
O3—C16	1.427 (4)	C15—H15A	0.9700
C1—C2	1.373 (5)	C15—H15B	0.9700
C1—C6	1.380 (5)	C16—C17	1.493 (5)
C1—H1	0.9300	C16—H16A	0.9700
C2—C3	1.380 (6)	C16—H16B	0.9700
C2—H2	0.9300	C17—H17A	0.9700
C3—C4	1.351 (6)	C17—H17B	0.9700
C3—H3	0.9300		

C7—N1—N2	106.3 (3)	C8—C9—H9B	109.0
C8—N2—N1	106.0 (2)	H9A—C9—H9B	107.8
N4—N3—C10	126.3 (2)	O2—C10—N3	119.9 (3)
N4—N3—C9	114.5 (2)	O2—C10—C11	125.9 (3)
C10—N3—C9	119.0 (2)	N3—C10—C11	114.2 (2)
C13—N4—N3	116.7 (2)	C12—C11—C10	122.0 (3)
C12—N5—C14	117.1 (2)	C12—C11—Cl1	122.9 (2)
C12—N5—C17	117.2 (2)	C10—C11—Cl1	115.0 (2)
C14—N5—C17	111.4 (2)	C11—C12—N5	124.4 (3)
C8—O1—C7	102.5 (2)	C11—C12—C13	115.1 (2)
C15—O3—C16	110.0 (3)	N5—C12—C13	120.5 (2)
C2—C1—C6	120.8 (4)	N4—C13—C12	125.5 (2)
C2—C1—H1	119.6	N4—C13—H13	117.2
C6—C1—H1	119.6	C12—C13—H13	117.2
C1—C2—C3	119.5 (4)	N5—C14—C15	109.8 (3)
C1—C2—H2	120.3	N5—C14—H14A	109.7
C3—C2—H2	120.3	C15—C14—H14A	109.7
C4—C3—C2	120.4 (4)	N5—C14—H14B	109.7
C4—C3—H3	119.8	C15—C14—H14B	109.7
C2—C3—H3	119.8	H14A—C14—H14B	108.2
C3—C4—C5	120.8 (4)	O3—C15—C14	111.7 (3)
C3—C4—H4	119.6	O3—C15—H15A	109.3
C5—C4—H4	119.6	C14—C15—H15A	109.3
C6—C5—C4	119.5 (4)	O3—C15—H15B	109.3
C6—C5—H5	120.3	C14—C15—H15B	109.3
C4—C5—H5	120.3	H15A—C15—H15B	107.9
C1—C6—C5	119.2 (3)	O3—C16—C17	112.0 (3)
C1—C6—C7	121.8 (3)	O3—C16—H16A	109.2
C5—C6—C7	119.0 (3)	C17—C16—H16A	109.2
N1—C7—O1	112.2 (3)	O3—C16—H16B	109.2
N1—C7—C6	128.5 (3)	C17—C16—H16B	109.2
O1—C7—C6	119.3 (3)	H16A—C16—H16B	107.9
N2—C8—O1	113.1 (3)	N5—C17—C16	110.2 (3)
N2—C8—C9	128.7 (3)	N5—C17—H17A	109.6
O1—C8—C9	118.2 (3)	C16—C17—H17A	109.6
N3—C9—C8	112.9 (3)	N5—C17—H17B	109.6

N3—C9—H9A	109.0	C16—C17—H17B	109.6
C8—C9—H9A	109.0	H17A—C17—H17B	108.1
N3—C9—H9B	109.0		

C7—N1—N2—C8	1.0 (3)	N4—N3—C10—O2	179.9 (3)
C10—N3—N4—C13	−0.9 (4)	C9—N3—C10—O2	5.1 (4)
C9—N3—N4—C13	174.2 (3)	N4—N3—C10—C11	−0.5 (4)
C6—C1—C2—C3	0.1 (6)	C9—N3—C10—C11	−175.3 (2)
C1—C2—C3—C4	0.5 (7)	O2—C10—C11—C12	−178.2 (3)
C2—C3—C4—C5	−0.4 (6)	N3—C10—C11—C12	2.3 (4)
C3—C4—C5—C6	−0.3 (6)	O2—C10—C11—Cl1	3.5 (4)
C2—C1—C6—C5	−0.8 (5)	N3—C10—C11—Cl1	−176.01 (19)
C2—C1—C6—C7	178.6 (4)	C10—C11—C12—N5	178.4 (2)
C4—C5—C6—C1	0.9 (5)	Cl1—C11—C12—N5	−3.4 (4)
C4—C5—C6—C7	−178.5 (3)	C10—C11—C12—C13	−2.5 (4)
N2—N1—C7—O1	−0.7 (3)	Cl1—C11—C12—C13	175.65 (19)
N2—N1—C7—C6	178.0 (3)	C14—N5—C12—C11	162.1 (3)
C8—O1—C7—N1	0.1 (3)	C17—N5—C12—C11	−61.4 (4)
C8—O1—C7—C6	−178.7 (3)	C14—N5—C12—C13	−16.9 (4)
C1—C6—C7—N1	177.5 (3)	C17—N5—C12—C13	119.5 (3)
C5—C6—C7—N1	−3.1 (5)	N3—N4—C13—C12	0.6 (4)
C1—C6—C7—O1	−3.9 (5)	C11—C12—C13—N4	1.0 (4)
C5—C6—C7—O1	175.5 (3)	N5—C12—C13—N4	−179.8 (3)
N1—N2—C8—O1	−1.0 (3)	C12—N5—C14—C15	−167.2 (3)
N1—N2—C8—C9	179.3 (3)	C17—N5—C14—C15	53.9 (4)
C7—O1—C8—N2	0.6 (3)	C16—O3—C15—C14	60.0 (5)
C7—O1—C8—C9	−179.7 (2)	N5—C14—C15—O3	−58.0 (4)
N4—N3—C9—C8	125.5 (3)	C15—O3—C16—C17	−58.7 (5)
C10—N3—C9—C8	−59.1 (3)	C12—N5—C17—C16	168.4 (3)
N2—C8—C9—N3	−53.4 (4)	C14—N5—C17—C16	−52.8 (4)
O1—C8—C9—N3	127.0 (3)	O3—C16—C17—N5	55.0 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17*A*···Cl1	0.97	2.57	3.252 (3)	127
C14—H14*B*···O2^{i}	0.97	2.57	3.373 (4)	141
C13—H13···O2^{ii}	0.93	2.60	3.507 (3)	165
C9—H9*A*···N2^{iii}	0.97	2.50	3.310 (4)	141

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