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1-[2-(3,4-Dichlorophenyl)-5-(3,4,5-trimethoxyphenyl)-2,3-dihydro-1,3,4-oxadiazol-3-yl]ethanone

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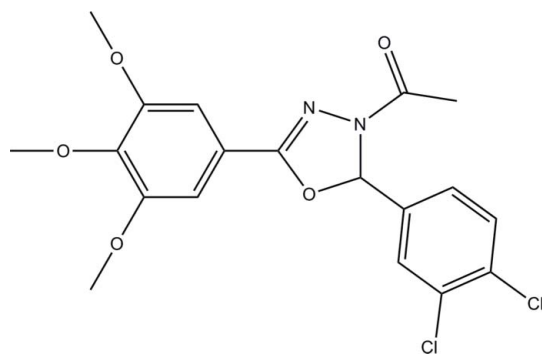
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 Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.041; wR factor = 0.126; data-to-parameter ratio = 16.2.

The title compound, $\text{C}_{19}\text{H}_{18}\text{Cl}_2\text{N}_2\text{O}_5$, was synthesized by the reaction of N' -(3,4-dichlorobenzylidene)-3,4,5-trimethoxybenzohydrazide and acetic anhydride. The oxadiazole ring makes dihedral angles of 82.82 (7) and 9.92 (7)° with the 3,4-dichlorobenzene and the 3,4,5-trimethoxybenzene ring planes, respectively. The crystal structure is stabilized by intermolecular $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds. Intramolecular $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds are also present.

Related literature

For related literature, see: Abdel *et al.* (2003); Abdel-Rahman & Farghaly (2004); Chai *et al.* (2002); Jin *et al.* (2006); Mohd *et al.* (2004).



Experimental

Crystal data

 $\text{C}_{19}\text{H}_{18}\text{Cl}_2\text{N}_2\text{O}_5$
 $M_r = 425.25$

 Monoclinic, $P2_1/c$
 $a = 7.6743$ (4) Å
 $b = 15.9516$ (8) Å
 $c = 15.7483$ (8) Å
 $\beta = 90.8940$ (10)°
 $V = 1927.63$ (17) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.37$ mm⁻¹
 $T = 173$ (2) K
 $0.47 \times 0.39 \times 0.32$ mm

Data collection

 Bruker SMART 1000 CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{\min} = 0.845$, $T_{\max} = 0.890$

 10032 measured reflections
 4159 independent reflections
 3238 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.125$
 $S = 1.04$
 4159 reflections

 257 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.34$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.31$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C6}-\text{H6}\cdots\text{O4}$	0.95	2.43	2.772 (2)	101
$\text{C8}-\text{H8}\cdots\text{O2}^{\text{i}}$	1.00	2.56	3.184 (3)	121
$\text{C10}-\text{H10}\cdots\text{O1}^{\text{ii}}$	0.95	2.43	3.302 (3)	153
$\text{C13}-\text{H13}\cdots\text{O5}^{\text{iii}}$	0.95	2.53	3.426 (3)	156
$\text{C16}-\text{H16B}\cdots\text{N1}$	0.98	2.42	2.839 (3)	105
$\text{C18}-\text{H18A}\cdots\text{N1}^{\text{ii}}$	0.98	2.53	3.468 (3)	160
$\text{C18}-\text{H18C}\cdots\text{O3}$	0.98	2.36	2.916 (3)	116
$\text{C19}-\text{H19A}\cdots\text{O5}^{\text{iv}}$	0.98	2.58	3.233 (3)	124

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2003); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2269).

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supporting information

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1-[2-(3,4-Dichlorophenyl)-5-(3,4,5-trimethoxyphenyl)-2,3-dihydro-1,3,4-oxadiazol-3-yl]ethanone

Dao-Hang He and Yong-Chuang Zhu

S1. Comment

1,3,4-Oxadiazole derivatives are well known to possess a diverse range of bioactivities in the pharmaceutical and agrochemical fields; these include insecticidal, antibacterial, anticancer, and anti-inflammatory activities (Abdel *et al.*, 2003; Abdel-Rahman & Farghaly, 2004; Chai *et al.*, 2002; Mohd *et al.*, 2004). Here we report the synthesis and crystal structure of a 1,3,4-oxadiazole derivative containing the 3,4,5-trimethoxyphenyl unit (Fig. 1).

The bond lengths and angles in the title compound are in good agreement with expected values. Though the C8 carbon of the oxadiazole ring is sp^3 hybridized, the oxadiazole ring is essentially planar. The oxadiazole ring makes dihedral angles of $82.82(7)^\circ$ and $9.92(7)^\circ$ with the 3,4-dichlorobenzene and the 3,4,5-trimethoxybenzene ring planes, respectively. These angles are somewhat different from those in a similar crystal structure (Jin *et al.*, 2006). The crystal structure exhibits intermolecular C—H \cdots O and C—H \cdots N hydrogen bonds which stabilize the molecule. Intramolecular C—H \cdots O and C—H \cdots N hydrogen bonds are also present.

S2. Experimental

N'-(3,4-Dichlorobenzylidene)-3,4,5-trimethoxybenzohydrazide (0.38 g, 1 mmol) in acetic anhydride (8 ml) was refluxed for 2 h until the starting material disappeared, as evidenced by TLC. The resulting cool mixture was then poured into cold water, after filtration. The residue was recrystallized by slow evaporation of a methanol solution.

S3. Refinement

All H atoms were included in the refinement at idealized positions and refined as riding, with C—H = 0.95 (aromatic), 0.98 (methyl), 1.00 Å (methine) and $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{carrier atom})$, where $x = 1.5$ for methyl, 1.2 for all other H atoms.

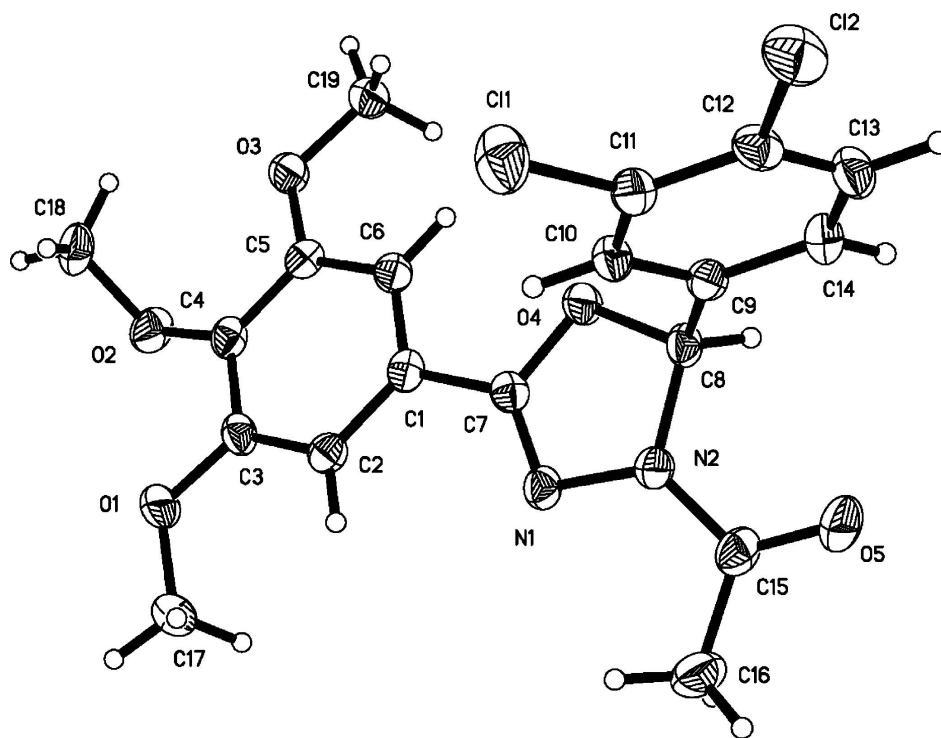


Figure 1

A view of the molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms are represented by spheres of arbitrary radius.

1-[2-(3,4-Dichlorophenyl)-5-(3,4,5-trimethoxyphenyl)-2,3-dihydro-1,3,4-oxadiazol-3-yl]ethanone

Crystal data

$C_{19}H_{18}Cl_2N_2O_5$

$M_r = 425.25$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 7.6743\ (4)\ \text{\AA}$

$b = 15.9516\ (8)\ \text{\AA}$

$c = 15.7483\ (8)\ \text{\AA}$

$\beta = 90.894\ (1)^\circ$

$V = 1927.63\ (17)\ \text{\AA}^3$

$Z = 4$

$F(000) = 880$

$D_x = 1.465\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5138 reflections

$\theta = 2.6\text{--}27.1^\circ$

$\mu = 0.37\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Block, colorless

$0.47 \times 0.39 \times 0.32\ \text{mm}$

Data collection

Bruker SMART 1000 CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 2003)

$T_{\min} = 0.845$, $T_{\max} = 0.891$

10032 measured reflections

4159 independent reflections

3238 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 27.2^\circ$, $\theta_{\min} = 1.8^\circ$

$h = -8 \rightarrow 9$

$k = -20 \rightarrow 18$

$l = -13 \rightarrow 20$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.125$
 $S = 1.04$
 4159 reflections
 257 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
 $w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 1.3473P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.29475 (7)	0.36125 (4)	0.89108 (4)	0.04132 (18)
C12	0.44596 (8)	0.54237 (4)	0.85758 (4)	0.03835 (17)
C1	0.7817 (3)	0.05267 (12)	0.99579 (13)	0.0233 (4)
C2	0.7051 (3)	-0.00409 (13)	1.05104 (13)	0.0243 (4)
H2	0.6667	0.0136	1.1053	0.029*
C3	0.6857 (3)	-0.08687 (12)	1.02552 (13)	0.0254 (4)
C4	0.7416 (3)	-0.11303 (12)	0.94532 (13)	0.0250 (4)
C5	0.8160 (3)	-0.05492 (13)	0.89080 (12)	0.0239 (4)
C6	0.8351 (3)	0.02847 (12)	0.91572 (13)	0.0245 (4)
H6	0.8842	0.0683	0.8782	0.029*
C7	0.8153 (3)	0.13859 (12)	1.02448 (13)	0.0229 (4)
C8	0.9032 (3)	0.27301 (12)	1.00923 (13)	0.0240 (4)
H8	1.0284	0.2903	1.0080	0.029*
C9	0.7883 (3)	0.33955 (12)	0.97007 (12)	0.0231 (4)
C10	0.6145 (3)	0.32243 (12)	0.95089 (13)	0.0248 (4)
H10	0.5676	0.2685	0.9619	0.030*
C11	0.5100 (3)	0.38450 (13)	0.91558 (13)	0.0262 (4)
C12	0.5775 (3)	0.46408 (12)	0.90009 (13)	0.0263 (4)
C13	0.7498 (3)	0.48130 (13)	0.91895 (14)	0.0297 (5)
H13	0.7963	0.5354	0.9081	0.036*
C14	0.8548 (3)	0.41901 (13)	0.95392 (13)	0.0268 (4)
H14	0.9735	0.4308	0.9670	0.032*
C15	0.9181 (3)	0.29242 (13)	1.16484 (14)	0.0297 (5)
C16	0.8863 (4)	0.25497 (16)	1.25067 (15)	0.0428 (6)
H16A	0.9930	0.2277	1.2717	0.064*

H16B	0.7925	0.2134	1.2461	0.064*
H16C	0.8525	0.2993	1.2902	0.064*
C17	0.5778 (3)	-0.12792 (16)	1.16051 (15)	0.0383 (6)
H17A	0.6858	-0.1100	1.1892	0.058*
H17B	0.5312	-0.1774	1.1893	0.058*
H17C	0.4923	-0.0824	1.1623	0.058*
C18	0.6289 (3)	-0.22110 (15)	0.85465 (16)	0.0368 (5)
H18A	0.5145	-0.1941	0.8580	0.055*
H18B	0.6143	-0.2821	0.8544	0.055*
H18C	0.6861	-0.2036	0.8024	0.055*
C19	0.9654 (3)	-0.03053 (15)	0.76156 (14)	0.0351 (5)
H19A	0.8912	0.0169	0.7450	0.053*
H19B	1.0019	-0.0607	0.7106	0.053*
H19C	1.0685	-0.0098	0.7925	0.053*
N1	0.7969 (2)	0.16636 (10)	1.09988 (11)	0.0248 (4)
N2	0.8524 (2)	0.25043 (10)	1.09633 (10)	0.0251 (4)
O1	0.6131 (2)	-0.14829 (9)	1.07411 (10)	0.0345 (4)
O2	0.7344 (2)	-0.19688 (9)	0.92680 (10)	0.0354 (4)
O3	0.8701 (2)	-0.08591 (9)	0.81492 (9)	0.0304 (3)
O4	0.87792 (19)	0.19385 (8)	0.96599 (9)	0.0265 (3)
O5	0.9955 (2)	0.35859 (10)	1.15404 (11)	0.0401 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0272 (3)	0.0402 (3)	0.0563 (4)	-0.0036 (2)	-0.0087 (2)	0.0089 (3)
C12	0.0433 (3)	0.0298 (3)	0.0419 (3)	0.0081 (2)	-0.0035 (2)	0.0093 (2)
C1	0.0220 (9)	0.0187 (9)	0.0290 (10)	0.0012 (8)	-0.0052 (8)	0.0011 (8)
C2	0.0229 (10)	0.0251 (10)	0.0249 (10)	0.0007 (8)	-0.0009 (8)	-0.0016 (8)
C3	0.0252 (10)	0.0206 (10)	0.0303 (11)	-0.0032 (8)	-0.0026 (8)	0.0056 (8)
C4	0.0283 (10)	0.0160 (9)	0.0307 (11)	0.0004 (8)	-0.0043 (8)	0.0000 (8)
C5	0.0243 (10)	0.0225 (10)	0.0247 (10)	0.0030 (8)	-0.0026 (8)	-0.0024 (7)
C6	0.0255 (10)	0.0217 (10)	0.0261 (10)	0.0000 (8)	-0.0034 (8)	0.0027 (8)
C7	0.0217 (9)	0.0210 (10)	0.0260 (10)	0.0009 (8)	-0.0011 (7)	0.0024 (7)
C8	0.0276 (10)	0.0172 (9)	0.0273 (10)	-0.0030 (8)	0.0015 (8)	-0.0023 (7)
C9	0.0280 (10)	0.0194 (9)	0.0219 (9)	0.0003 (8)	0.0017 (8)	-0.0018 (7)
C10	0.0277 (10)	0.0201 (10)	0.0266 (10)	-0.0032 (8)	0.0012 (8)	0.0004 (8)
C11	0.0243 (10)	0.0283 (11)	0.0261 (10)	-0.0029 (8)	0.0004 (8)	0.0007 (8)
C12	0.0328 (11)	0.0211 (10)	0.0250 (10)	0.0042 (8)	0.0020 (8)	0.0035 (8)
C13	0.0363 (12)	0.0201 (10)	0.0328 (11)	-0.0040 (9)	0.0030 (9)	0.0025 (8)
C14	0.0257 (10)	0.0216 (10)	0.0332 (11)	-0.0039 (8)	0.0016 (8)	-0.0016 (8)
C15	0.0363 (12)	0.0215 (10)	0.0312 (11)	0.0032 (9)	-0.0006 (9)	-0.0070 (8)
C16	0.0668 (17)	0.0339 (13)	0.0277 (12)	-0.0001 (12)	-0.0001 (11)	-0.0065 (10)
C17	0.0478 (14)	0.0373 (13)	0.0300 (12)	-0.0120 (11)	0.0034 (10)	0.0064 (10)
C18	0.0350 (12)	0.0305 (12)	0.0448 (13)	-0.0101 (10)	-0.0005 (10)	-0.0107 (10)
C19	0.0431 (13)	0.0345 (12)	0.0279 (11)	-0.0098 (10)	0.0052 (9)	-0.0017 (9)
N1	0.0291 (9)	0.0177 (8)	0.0277 (9)	-0.0016 (7)	-0.0018 (7)	-0.0001 (7)
N2	0.0309 (9)	0.0199 (8)	0.0245 (9)	-0.0015 (7)	0.0001 (7)	-0.0013 (7)

O1	0.0480 (10)	0.0232 (8)	0.0325 (8)	-0.0107 (7)	0.0041 (7)	0.0023 (6)
O2	0.0520 (10)	0.0185 (7)	0.0355 (9)	-0.0018 (7)	-0.0072 (7)	-0.0029 (6)
O3	0.0388 (9)	0.0246 (8)	0.0278 (8)	-0.0043 (6)	0.0048 (6)	-0.0035 (6)
O4	0.0367 (8)	0.0168 (7)	0.0262 (7)	-0.0013 (6)	0.0029 (6)	-0.0010 (5)
O5	0.0531 (10)	0.0255 (8)	0.0416 (10)	-0.0062 (7)	-0.0027 (8)	-0.0096 (7)

Geometric parameters (Å, °)

C11—C11	1.730 (2)	C11—C12	1.394 (3)
C12—C12	1.734 (2)	C12—C13	1.378 (3)
C1—C6	1.387 (3)	C13—C14	1.388 (3)
C1—C2	1.392 (3)	C13—H13	0.9500
C1—C7	1.465 (3)	C14—H14	0.9500
C2—C3	1.388 (3)	C15—O5	1.224 (3)
C2—H2	0.9500	C15—N2	1.360 (3)
C3—O1	1.367 (2)	C15—C16	1.501 (3)
C3—C4	1.404 (3)	C16—H16A	0.9800
C4—O2	1.370 (2)	C16—H16B	0.9800
C4—C5	1.392 (3)	C16—H16C	0.9800
C5—O3	1.364 (2)	C17—O1	1.429 (3)
C5—C6	1.394 (3)	C17—H17A	0.9800
C6—H6	0.9500	C17—H17B	0.9800
C7—N1	1.277 (3)	C17—H17C	0.9800
C7—O4	1.368 (2)	C18—O2	1.438 (3)
C8—O4	1.446 (2)	C18—H18A	0.9800
C8—N2	1.476 (3)	C18—H18B	0.9800
C8—C9	1.506 (3)	C18—H18C	0.9800
C8—H8	1.0000	C19—O3	1.429 (3)
C9—C10	1.390 (3)	C19—H19A	0.9800
C9—C14	1.391 (3)	C19—H19B	0.9800
C10—C11	1.385 (3)	C19—H19C	0.9800
C10—H10	0.9500	N1—N2	1.409 (2)
C6—C1—C2	121.40 (18)	C12—C13—H13	120.3
C6—C1—C7	119.20 (18)	C14—C13—H13	120.3
C2—C1—C7	119.32 (18)	C13—C14—C9	120.8 (2)
C3—C2—C1	118.83 (19)	C13—C14—H14	119.6
C3—C2—H2	120.6	C9—C14—H14	119.6
C1—C2—H2	120.6	O5—C15—N2	119.3 (2)
O1—C3—C2	124.24 (19)	O5—C15—C16	123.7 (2)
O1—C3—C4	115.06 (18)	N2—C15—C16	117.0 (2)
C2—C3—C4	120.70 (18)	C15—C16—H16A	109.5
O2—C4—C5	122.30 (19)	C15—C16—H16B	109.5
O2—C4—C3	118.03 (18)	H16A—C16—H16B	109.5
C5—C4—C3	119.42 (18)	C15—C16—H16C	109.5
O3—C5—C4	115.61 (18)	H16A—C16—H16C	109.5
O3—C5—C6	124.10 (19)	H16B—C16—H16C	109.5
C4—C5—C6	120.27 (19)	O1—C17—H17A	109.5

C1—C6—C5	119.37 (19)	O1—C17—H17B	109.5
C1—C6—H6	120.3	H17A—C17—H17B	109.5
C5—C6—H6	120.3	O1—C17—H17C	109.5
N1—C7—O4	116.60 (17)	H17A—C17—H17C	109.5
N1—C7—C1	126.14 (18)	H17B—C17—H17C	109.5
O4—C7—C1	117.22 (17)	O2—C18—H18A	109.5
O4—C8—N2	100.90 (14)	O2—C18—H18B	109.5
O4—C8—C9	110.42 (16)	H18A—C18—H18B	109.5
N2—C8—C9	113.01 (16)	O2—C18—H18C	109.5
O4—C8—H8	110.7	H18A—C18—H18C	109.5
N2—C8—H8	110.7	H18B—C18—H18C	109.5
C9—C8—H8	110.7	O3—C19—H19A	109.5
C10—C9—C14	119.51 (18)	O3—C19—H19B	109.5
C10—C9—C8	120.30 (18)	H19A—C19—H19B	109.5
C14—C9—C8	120.18 (18)	O3—C19—H19C	109.5
C11—C10—C9	119.63 (19)	H19A—C19—H19C	109.5
C11—C10—H10	120.2	H19B—C19—H19C	109.5
C9—C10—H10	120.2	C7—N1—N2	104.79 (16)
C10—C11—C12	120.43 (19)	C15—N2—N1	123.09 (17)
C10—C11—Cl1	118.75 (16)	C15—N2—C8	121.12 (17)
C12—C11—Cl1	120.82 (16)	N1—N2—C8	110.70 (15)
C13—C12—C11	120.13 (19)	C3—O1—C17	117.06 (17)
C13—C12—Cl2	119.37 (16)	C4—O2—C18	116.81 (17)
C11—C12—Cl2	120.49 (17)	C5—O3—C19	117.18 (16)
C12—C13—C14	119.45 (19)	C7—O4—C8	106.95 (15)
C6—C1—C2—C3	1.4 (3)	C10—C11—C12—Cl2	-178.89 (16)
C7—C1—C2—C3	-175.26 (18)	Cl1—C11—C12—Cl2	1.2 (3)
C1—C2—C3—O1	179.76 (19)	C11—C12—C13—C14	-0.4 (3)
C1—C2—C3—C4	-0.2 (3)	Cl2—C12—C13—C14	179.24 (16)
O1—C3—C4—O2	-6.1 (3)	C12—C13—C14—C9	0.0 (3)
C2—C3—C4—O2	173.88 (18)	C10—C9—C14—C13	0.0 (3)
O1—C3—C4—C5	179.51 (18)	C8—C9—C14—C13	-179.09 (19)
C2—C3—C4—C5	-0.5 (3)	O4—C7—N1—N2	-0.3 (2)
O2—C4—C5—O3	4.6 (3)	C1—C7—N1—N2	177.36 (18)
C3—C4—C5—O3	178.68 (18)	O5—C15—N2—N1	165.36 (19)
O2—C4—C5—C6	-174.01 (18)	C16—C15—N2—N1	-16.2 (3)
C3—C4—C5—C6	0.1 (3)	O5—C15—N2—C8	12.9 (3)
C2—C1—C6—C5	-1.8 (3)	C16—C15—N2—C8	-168.66 (19)
C7—C1—C6—C5	174.89 (18)	C7—N1—N2—C15	-153.3 (2)
O3—C5—C6—C1	-177.46 (18)	C7—N1—N2—C8	1.6 (2)
C4—C5—C6—C1	1.0 (3)	O4—C8—N2—C15	153.32 (18)
C6—C1—C7—N1	-169.31 (19)	C9—C8—N2—C15	-88.8 (2)
C2—C1—C7—N1	7.4 (3)	O4—C8—N2—N1	-2.2 (2)
C6—C1—C7—O4	8.3 (3)	C9—C8—N2—N1	115.70 (18)
C2—C1—C7—O4	-174.95 (17)	C2—C3—O1—C17	-9.0 (3)
O4—C8—C9—C10	45.1 (2)	C4—C3—O1—C17	171.03 (19)
N2—C8—C9—C10	-67.1 (2)	C5—C4—O2—C18	-65.1 (3)

O4—C8—C9—C14	-135.80 (19)	C3—C4—O2—C18	120.8 (2)
N2—C8—C9—C14	112.0 (2)	C4—C5—O3—C19	-172.83 (18)
C14—C9—C10—C11	0.3 (3)	C6—C5—O3—C19	5.7 (3)
C8—C9—C10—C11	179.43 (18)	N1—C7—O4—C8	-1.2 (2)
C9—C10—C11—C12	-0.7 (3)	C1—C7—O4—C8	-179.02 (17)
C9—C10—C11—C11	179.22 (15)	N2—C8—O4—C7	1.92 (19)
C10—C11—C12—C13	0.7 (3)	C9—C8—O4—C7	-117.85 (17)
C11—C11—C12—C13	-179.17 (16)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C6—H6 \cdots O4	0.95	2.43	2.772 (2)	101
C8—H8 \cdots O2 ⁱ	1.00	2.56	3.184 (3)	121
C10—H10 \cdots O1 ⁱⁱ	0.95	2.43	3.302 (3)	153
C13—H13 \cdots O5 ⁱⁱⁱ	0.95	2.53	3.426 (3)	156
C16—H16 <i>B</i> \cdots N1	0.98	2.42	2.839 (3)	105
C18—H18 <i>A</i> \cdots N1 ⁱⁱ	0.98	2.53	3.468 (3)	160
C18—H18 <i>C</i> \cdots O3	0.98	2.36	2.916 (3)	116
C19—H19 <i>A</i> \cdots O5 ^{iv}	0.98	2.58	3.233 (3)	124

Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $-x+1, -y, -z+2$; (iii) $-x+2, -y+1, -z+2$; (iv) $x, -y+1/2, z-1/2$.