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Crystal structure of dimethomorph

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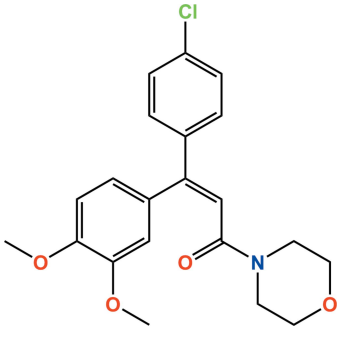
In the title compound, $C_{21}H_{22}ClNO_4$ [systematic name: (*E*)-3-(4-chlorophenyl)-3-(3,4-dimethoxyphenyl)-1-(morpholin-4-yl)-prop-2-en-1-one], which is the morpholine fungicide dimethomorph, the dihedral angles between the mean planes of the central chlorophenyl and the terminal benzene and morpholine (r.m.s. deviation = 0.2233 Å) rings are 71.74 (6) and 63.65 (7)°, respectively. In the crystal, molecules are linked *via* C—H···O hydrogen bonds and weak Cl···π interactions [3.8539 (11) Å], forming a three-dimensional structure.

Keywords: crystal structure; dimethomorph; prop-2-en-1-one; fungicide.

CCDC reference: 1417163

1. Related literature

For information on the fungicidal properties of the title compound, see: Xu *et al.* (2015). For related crystal structures, see: Chai & Liu (2011); Lu & Shi (2011).



2. Experimental

2.1. Crystal data

$C_{21}H_{22}ClNO_4$
M_r = 387.84
Monoclinic, $P2_1/c$
a = 6.6238 (2) Å
b = 13.2232 (4) Å
c = 21.4810 (7) Å
β = 97.1674 (19)°
V = 1866.77 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 173 K
0.38 × 0.06 × 0.03 mm

2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.917, T_{max} = 0.993
18090 measured reflections
4276 independent reflections
3119 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.133
S = 1.04
4276 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···O2^{i}	0.99	2.53	3.167 (2)	122
C13—H13···O2^{ii}	0.95	2.38	3.166 (2)	140
C20—H20B···O1^{iii}	0.98	2.64	3.010 (2)	103

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

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5456).

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supporting information

Acta Cryst. (2015). E**71**, o654 [https://doi.org/10.1107/S2056989015014735]

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S1. Comment

Dimethomorph [systematic name: (*E*)-3-(4-chlorophenyl)-3-(3,4-dimethoxyphenyl)-1-(morpholin-4-yl)prop-2-en-1-one] is a morpholine fungicide that has been mainly applied on grapevines, apples, ginsengs, tomatoes, potatoes, cucumbers, Chinese cabbage and other crops. (Xu *et al.*, 2015). The dihedral angles between the planes of the central chlorophenyl and the terminal benzene and mean plane [r.m.s. deviation = 0.2233] of morpholine rings are 71.74 (6) and 63.65 (7)°, respectively. All bond lengths and bond angles are normal and comparable to those observed in similar crystal structures (Chai & Liu, 2011; Lu & Shi, 2011).

In the crystal structure (Fig. 2), C—H···O hydrogen bonds (Table 1) and weak intermolecular C11—Cl1···*Cg*1^{iv} (*Cg*1 is the centroid of the C8—C13 ring) interaction with a chlorophenyl ring are present, resulting in a three-dimensional network [for symmetry code: (iv), -*x*, -*y* + 1, -*z* + 1].

S2. Experimental

The title compound was purchased from the Dr. Ehrenstorfer GmbH Company. Slow evaporation of a solution in CH_3OH gave single crystals suitable for X-ray analysis.

S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.98 Å, U_{iso} = 1.5U_{eq}(C) for methyl group, d(C—H) = 0.99 Å, U_{iso} = 1.2U_{eq}(C) for CH_2 group, d(C—H) = 0.95 Å, U_{iso} = 1.2U_{eq}(C) for Csp^2—H and aromatic C—H.

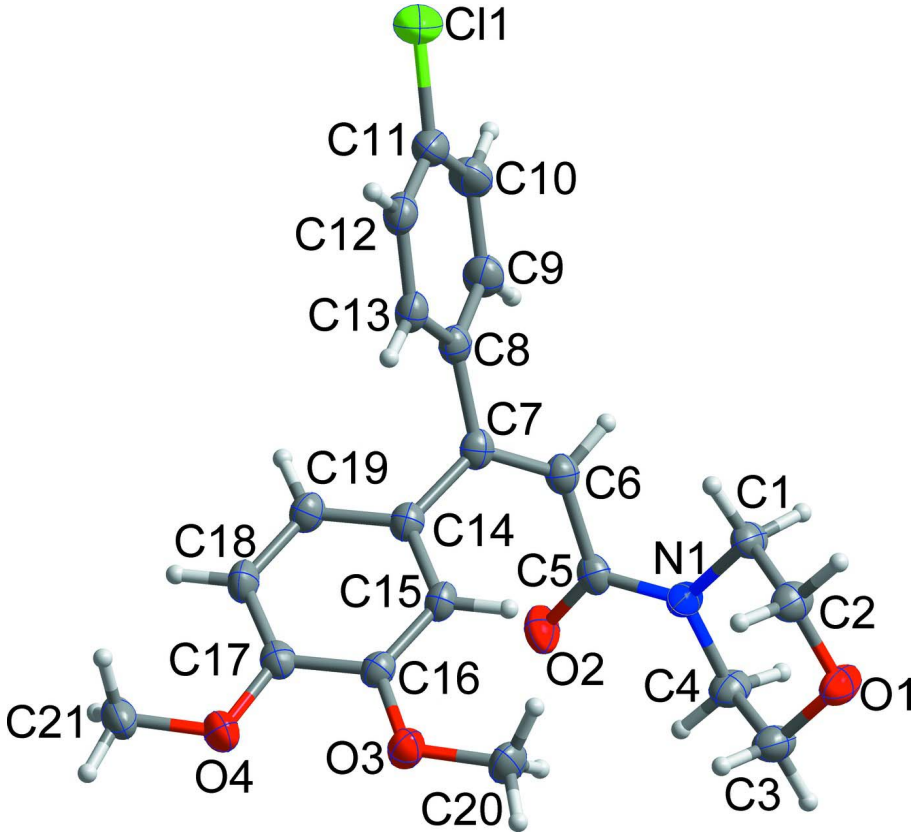

Figure 1

The asymmetric unit of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

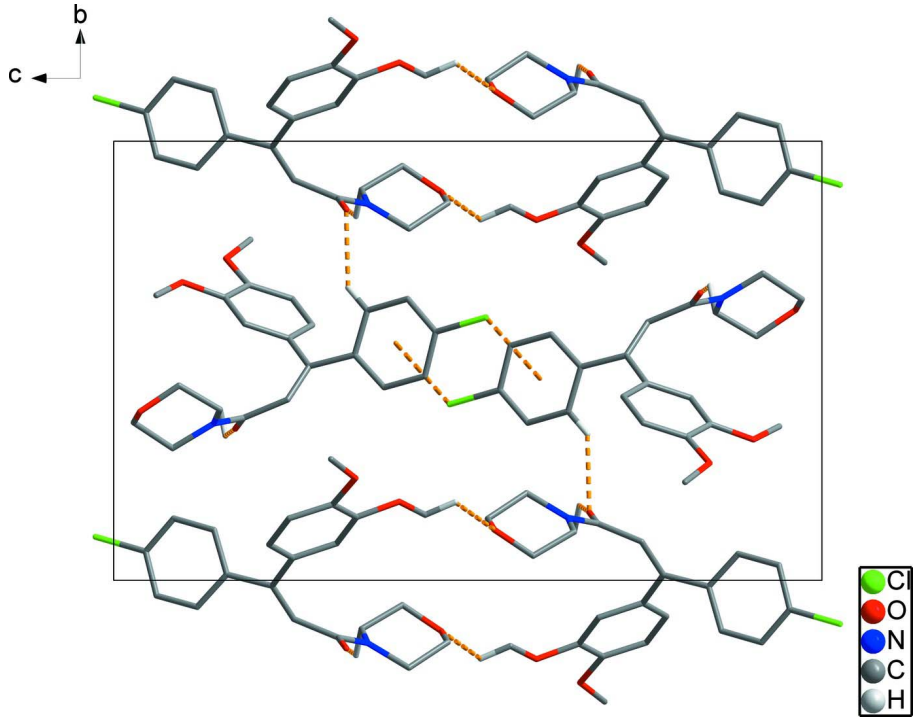

Figure 2

Crystal packing viewed along the *a* axis. The intermolecular interactions are shown as dashed lines.

(*E*)-3-(4-Chlorophenyl)-3-(3,4-dimethoxyphenyl)-1-(morpholin-4-yl)prop-2-en-1-one

Crystal data

$C_{21}H_{22}ClNO_4$
$M_r = 387.84$
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$b = 13.2232$ (4) Å
$c = 21.4810$ (7) Å
$\beta = 97.1674$ (19)°
$V = 1866.77$ (10) Å^3
$Z = 4$
$F(000) = 816$
$D_x = 1.380$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3670 reflections
$\theta = 2.5$–24.0°
$\mu = 0.23$ mm^{-1}
$T = 173$ K
Needle, colourless
0.38 × 0.06 × 0.03 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
$T_{min} = 0.917$, $T_{max} = 0.993$
18090 measured reflections
4276 independent reflections
3119 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -8 \rightarrow 8$
$k = -14 \rightarrow 17$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.133$
$S = 1.04$
4276 reflections
246 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.6606P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.31366 (10)	0.59912 (5)	0.47448 (3)	0.0574 (2)
O1	0.5956 (2)	0.38430 (11)	0.96279 (6)	0.0370 (4)
O2	−0.0418 (2)	0.34526 (10)	0.82830 (7)	0.0370 (4)
O3	−0.1413 (2)	0.67931 (10)	0.90317 (6)	0.0337 (3)
O4	−0.4849 (2)	0.73290 (10)	0.84142 (6)	0.0368 (4)
N1	0.2962 (2)	0.35718 (12)	0.85873 (7)	0.0281 (4)
C1	0.5023 (3)	0.38939 (15)	0.84994 (9)	0.0305 (4)
H1A	0.4969	0.4347	0.8131	0.037*
H1B	0.5855	0.3296	0.8421	0.037*
C2	0.5976 (3)	0.44402 (16)	0.90772 (9)	0.0347 (5)
H2A	0.7399	0.4617	0.9027	0.042*
H2B	0.5226	0.5078	0.9125	0.042*
C3	0.3918 (3)	0.35949 (17)	0.97178 (9)	0.0364 (5)
H3A	0.3150	0.4224	0.9772	0.044*
H3B	0.3928	0.3187	1.0104	0.044*
C4	0.2872 (3)	0.30099 (16)	0.91686 (9)	0.0335 (5)
H4A	0.3542	0.2345	0.9142	0.040*
H4B	0.1434	0.2890	0.9229	0.040*
C5	0.1286 (3)	0.37008 (13)	0.81674 (9)	0.0267 (4)
C6	0.1627 (3)	0.41177 (14)	0.75448 (9)	0.0277 (4)
H6	0.2683	0.3819	0.7346	0.033*
C7	0.0584 (3)	0.48755 (13)	0.72382 (9)	0.0263 (4)
C8	0.1046 (3)	0.51370 (14)	0.65975 (9)	0.0274 (4)
C9	0.1513 (3)	0.43952 (16)	0.61797 (9)	0.0354 (5)
H9	0.1412	0.3702	0.6289	0.043*
C10	0.2124 (3)	0.46527 (17)	0.56054 (10)	0.0411 (5)
H10	0.2424	0.4140	0.5321	0.049*
C11	0.2291 (3)	0.56604 (18)	0.54519 (10)	0.0378 (5)
C12	0.1811 (3)	0.64122 (16)	0.58492 (10)	0.0350 (5)
H12	0.1923	0.7103	0.5737	0.042*
C13	0.1159 (3)	0.61476 (15)	0.64179 (9)	0.0303 (4)
H13	0.0785	0.6664	0.6689	0.036*
C14	−0.0896 (3)	0.55131 (13)	0.75275 (9)	0.0261 (4)
C15	−0.0445 (3)	0.58425 (13)	0.81488 (8)	0.0254 (4)

H15	0.0808	0.5648	0.8382	0.030*
C16	−0.1772 (3)	0.64407 (13)	0.84292 (8)	0.0255 (4)
C17	−0.3626 (3)	0.67311 (13)	0.80926 (9)	0.0278 (4)
C18	−0.4093 (3)	0.64144 (14)	0.74781 (9)	0.0304 (4)
H18	−0.5351	0.6606	0.7247	0.037*
C19	−0.2734 (3)	0.58161 (14)	0.71962 (9)	0.0293 (4)
H19	−0.3067	0.5612	0.6772	0.035*
C20	0.0428 (3)	0.64921 (17)	0.93982 (9)	0.0369 (5)
H20A	0.0476	0.5753	0.9428	0.055*
H20B	0.0485	0.6782	0.9820	0.055*
H20C	0.1591	0.6734	0.9199	0.055*
C21	−0.6601 (3)	0.77604 (16)	0.80687 (10)	0.0388 (5)
H21A	−0.6192	0.8187	0.7733	0.058*
H21B	−0.7324	0.8172	0.8349	0.058*
H21C	−0.7499	0.7220	0.7885	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0525 (4)	0.0813 (5)	0.0412 (3)	0.0133 (3)	0.0173 (3)	0.0147 (3)
O1	0.0326 (8)	0.0484 (8)	0.0281 (7)	−0.0095 (7)	−0.0041 (6)	0.0043 (6)
O2	0.0226 (7)	0.0352 (7)	0.0529 (9)	−0.0019 (6)	0.0031 (6)	0.0124 (7)
O3	0.0356 (8)	0.0358 (7)	0.0283 (7)	0.0058 (6)	−0.0015 (6)	−0.0037 (6)
O4	0.0333 (8)	0.0410 (8)	0.0362 (8)	0.0113 (6)	0.0048 (6)	0.0003 (6)
N1	0.0243 (8)	0.0340 (9)	0.0255 (8)	−0.0049 (7)	0.0017 (7)	0.0040 (7)
C1	0.0235 (10)	0.0395 (11)	0.0283 (10)	−0.0039 (8)	0.0028 (8)	0.0010 (9)
C2	0.0310 (11)	0.0399 (11)	0.0325 (11)	−0.0102 (9)	0.0011 (9)	0.0024 (9)
C3	0.0363 (12)	0.0462 (12)	0.0270 (10)	−0.0058 (10)	0.0045 (9)	0.0025 (9)
C4	0.0324 (11)	0.0373 (11)	0.0309 (11)	−0.0074 (9)	0.0045 (9)	0.0065 (9)
C5	0.0241 (9)	0.0211 (9)	0.0346 (10)	0.0003 (7)	0.0028 (8)	−0.0010 (8)
C6	0.0238 (9)	0.0271 (9)	0.0313 (10)	−0.0006 (8)	−0.0001 (8)	−0.0017 (8)
C7	0.0236 (9)	0.0252 (9)	0.0285 (10)	−0.0032 (8)	−0.0027 (8)	−0.0029 (8)
C8	0.0228 (9)	0.0302 (10)	0.0279 (10)	0.0004 (8)	−0.0020 (8)	−0.0016 (8)
C9	0.0378 (12)	0.0332 (10)	0.0347 (11)	0.0031 (9)	0.0020 (9)	−0.0045 (9)
C10	0.0394 (12)	0.0484 (13)	0.0361 (12)	0.0060 (10)	0.0077 (10)	−0.0077 (10)
C11	0.0301 (11)	0.0539 (13)	0.0298 (11)	0.0056 (10)	0.0046 (9)	0.0057 (10)
C12	0.0290 (11)	0.0387 (11)	0.0360 (11)	0.0038 (9)	−0.0013 (9)	0.0073 (9)
C13	0.0279 (10)	0.0313 (10)	0.0299 (10)	0.0036 (8)	−0.0031 (8)	0.0015 (8)
C14	0.0251 (9)	0.0232 (9)	0.0291 (10)	−0.0019 (7)	−0.0003 (8)	0.0024 (8)
C15	0.0236 (9)	0.0229 (9)	0.0278 (10)	−0.0012 (7)	−0.0032 (8)	0.0029 (7)
C16	0.0270 (10)	0.0235 (9)	0.0253 (10)	−0.0024 (7)	0.0008 (8)	0.0025 (7)
C17	0.0250 (10)	0.0245 (9)	0.0343 (11)	−0.0001 (8)	0.0051 (8)	0.0042 (8)
C18	0.0224 (9)	0.0326 (10)	0.0345 (11)	0.0010 (8)	−0.0033 (8)	0.0043 (8)
C19	0.0281 (10)	0.0304 (10)	0.0279 (10)	−0.0015 (8)	−0.0024 (8)	−0.0010 (8)
C20	0.0337 (11)	0.0473 (12)	0.0275 (11)	0.0019 (10)	−0.0055 (9)	−0.0033 (9)
C21	0.0278 (10)	0.0437 (12)	0.0458 (13)	0.0082 (9)	0.0084 (9)	0.0084 (10)

Geometric parameters (Å, º)

Cl1—C11	1.739 (2)	C8—C9	1.390 (3)
O1—C2	1.424 (2)	C8—C13	1.395 (3)
O1—C3	1.426 (2)	C9—C10	1.388 (3)
O2—C5	1.230 (2)	C9—H9	0.9500
O3—C16	1.368 (2)	C10—C11	1.380 (3)
O3—C20	1.423 (2)	C10—H10	0.9500
O4—C17	1.378 (2)	C11—C12	1.373 (3)
O4—C21	1.417 (2)	C12—C13	1.390 (3)
N1—C5	1.351 (2)	C12—H12	0.9500
N1—C4	1.461 (2)	C13—H13	0.9500
N1—C1	1.464 (2)	C14—C19	1.390 (3)
C1—C2	1.505 (3)	C14—C15	1.400 (3)
C1—H1A	0.9900	C15—C16	1.376 (3)
C1—H1B	0.9900	C15—H15	0.9500
C2—H2A	0.9900	C16—C17	1.398 (3)
C2—H2B	0.9900	C17—C18	1.383 (3)
C3—C4	1.505 (3)	C18—C19	1.392 (3)
C3—H3A	0.9900	C18—H18	0.9500
C3—H3B	0.9900	C19—H19	0.9500
C4—H4A	0.9900	C20—H20A	0.9800
C4—H4B	0.9900	C20—H20B	0.9800
C5—C6	1.490 (3)	C20—H20C	0.9800
C6—C7	1.342 (3)	C21—H21A	0.9800
C6—H6	0.9500	C21—H21B	0.9800
C7—C14	1.487 (3)	C21—H21C	0.9800
C7—C8	1.487 (3)		
C2—O1—C3	110.32 (15)	C8—C9—H9	119.5
C16—O3—C20	117.63 (15)	C11—C10—C9	119.3 (2)
C17—O4—C21	117.58 (15)	C11—C10—H10	120.3
C5—N1—C4	121.14 (16)	C9—C10—H10	120.3
C5—N1—C1	125.36 (16)	C12—C11—C10	121.2 (2)
C4—N1—C1	113.35 (15)	C12—C11—Cl1	119.04 (17)
N1—C1—C2	109.58 (15)	C10—C11—Cl1	119.71 (17)
N1—C1—H1A	109.8	C11—C12—C13	119.03 (19)
C2—C1—H1A	109.8	C11—C12—H12	120.5
N1—C1—H1B	109.8	C13—C12—H12	120.5
C2—C1—H1B	109.8	C12—C13—C8	121.15 (19)
H1A—C1—H1B	108.2	C12—C13—H13	119.4
O1—C2—C1	111.87 (16)	C8—C13—H13	119.4
O1—C2—H2A	109.2	C19—C14—C15	117.86 (17)
C1—C2—H2A	109.2	C19—C14—C7	122.03 (17)
O1—C2—H2B	109.2	C15—C14—C7	120.10 (17)
C1—C2—H2B	109.2	C16—C15—C14	121.60 (17)
H2A—C2—H2B	107.9	C16—C15—H15	119.2
O1—C3—C4	111.29 (16)	C14—C15—H15	119.2

O1—C3—H3A	109.4	O3—C16—C15	124.38 (17)
C4—C3—H3A	109.4	O3—C16—C17	115.68 (17)
O1—C3—H3B	109.4	C15—C16—C17	119.94 (17)
C4—C3—H3B	109.4	O4—C17—C18	125.23 (17)
H3A—C3—H3B	108.0	O4—C17—C16	115.56 (17)
N1—C4—C3	110.16 (16)	C18—C17—C16	119.21 (18)
N1—C4—H4A	109.6	C17—C18—C19	120.49 (18)
C3—C4—H4A	109.6	C17—C18—H18	119.8
N1—C4—H4B	109.6	C19—C18—H18	119.8
C3—C4—H4B	109.6	C14—C19—C18	120.89 (18)
H4A—C4—H4B	108.1	C14—C19—H19	119.6
O2—C5—N1	121.99 (18)	C18—C19—H19	119.6
O2—C5—C6	121.71 (17)	O3—C20—H20A	109.5
N1—C5—C6	116.24 (16)	O3—C20—H20B	109.5
C7—C6—C5	126.17 (17)	H20A—C20—H20B	109.5
C7—C6—H6	116.9	O3—C20—H20C	109.5
C5—C6—H6	116.9	H20A—C20—H20C	109.5
C6—C7—C14	122.97 (18)	H20B—C20—H20C	109.5
C6—C7—C8	118.35 (17)	O4—C21—H21A	109.5
C14—C7—C8	118.52 (16)	O4—C21—H21B	109.5
C9—C8—C13	118.25 (18)	H21A—C21—H21B	109.5
C9—C8—C7	121.42 (17)	O4—C21—H21C	109.5
C13—C8—C7	120.18 (17)	H21A—C21—H21C	109.5
C10—C9—C8	120.9 (2)	H21B—C21—H21C	109.5
C10—C9—H9	119.5		

C5—N1—C1—C2	132.71 (19)	Cl1—C11—C12—C13	−179.22 (15)
C4—N1—C1—C2	−51.7 (2)	C11—C12—C13—C8	1.9 (3)
C3—O1—C2—C1	−60.0 (2)	C9—C8—C13—C12	−2.9 (3)
N1—C1—C2—O1	55.2 (2)	C7—C8—C13—C12	172.68 (17)
C2—O1—C3—C4	59.7 (2)	C6—C7—C14—C19	−139.6 (2)
C5—N1—C4—C3	−132.19 (19)	C8—C7—C14—C19	45.1 (2)
C1—N1—C4—C3	52.0 (2)	C6—C7—C14—C15	41.5 (3)
O1—C3—C4—N1	−55.3 (2)	C8—C7—C14—C15	−133.79 (18)
C4—N1—C5—O2	8.1 (3)	C19—C14—C15—C16	0.5 (3)
C1—N1—C5—O2	−176.63 (17)	C7—C14—C15—C16	179.42 (16)
C4—N1—C5—C6	−169.19 (17)	C20—O3—C16—C15	−2.2 (3)
C1—N1—C5—C6	6.1 (3)	C20—O3—C16—C17	178.19 (16)
O2—C5—C6—C7	50.0 (3)	C14—C15—C16—O3	−179.46 (17)
N1—C5—C6—C7	−132.7 (2)	C14—C15—C16—C17	0.2 (3)
C5—C6—C7—C14	9.2 (3)	C21—O4—C17—C18	−8.5 (3)
C5—C6—C7—C8	−175.53 (17)	C21—O4—C17—C16	171.23 (17)
C6—C7—C8—C9	37.0 (3)	O3—C16—C17—O4	−0.4 (2)
C14—C7—C8—C9	−147.52 (18)	C15—C16—C17—O4	179.97 (16)
C6—C7—C8—C13	−138.47 (19)	O3—C16—C17—C18	179.34 (16)
C14—C7—C8—C13	37.0 (2)	C15—C16—C17—C18	−0.3 (3)
C13—C8—C9—C10	1.6 (3)	O4—C17—C18—C19	179.47 (17)
C7—C8—C9—C10	−173.99 (18)	C16—C17—C18—C19	−0.2 (3)

C8—C9—C10—C11	0.8 (3)	C15—C14—C19—C18	−1.0 (3)
C9—C10—C11—C12	−1.8 (3)	C7—C14—C19—C18	−179.93 (17)
C9—C10—C11—Cl1	177.89 (16)	C17—C18—C19—C14	0.9 (3)
C10—C11—C12—C13	0.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···O2^{i}	0.99	2.53	3.167 (2)	122
C13—H13···O2^{ii}	0.95	2.38	3.166 (2)	140
C20—H20*B*···O1^{iii}	0.98	2.64	3.010 (2)	103

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