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(2*RS*,4′*RS*)-3′-(3-Chloro-4-methoxyphenyl)-4′-phenyl-4′*H*-spiro[indene-2,5′-isoxazol]-1(3*H*)-one ethanol monosolvate

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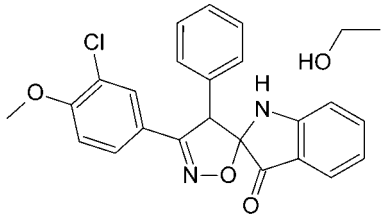
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.096; data-to-parameter ratio = 16.0.

The title compound, $C_{23}H_{17}ClN_2O_3\cdot C_2H_6O$, is the stoichiometric 1:1 ethanol solvate of a racemic reaction product, which forms a conglomerate. The refined Flack parameter of 0.36 (3) indicates racemic twinning. In the structure, molecules are linked into zigzag chains by a series of intermolecular N—H···O and O—H···O hydrogen bonds.

Related literature

For general background to dipolar 1,3-cycloaddition reactions, see: Al Houari *et al.* (2010); Toth *et al.* (1999); El yazidi *et al.* (1994).



Experimental

Crystal data

$C_{23}H_{17}ClN_2O_3\cdot C_2H_6O$
M_r = 450.90
Orthorhombic, $P2_12_12_1$
a = 8.7112 (2) Å
b = 11.3051 (2) Å
c = 22.5913 (5) Å
V = 2224.81 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 296 K
0.24 × 0.17 × 0.16 mm

Data collection

Bruker APEXII CCD diffractometer
13160 measured reflections
4757 independent reflections
3815 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.096
S = 1.06
4757 reflections
297 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983); 1986 Friedel pairs
Flack parameter: 0.36 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4	0.88 (3)	2.12 (3)	2.906 (2)	149 (2)
O4—H4A···O2^{i}	0.82	2.02	2.813 (2)	164

Symmetry code: (i) $x+1, y, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FY2017).

References

Al Houari, G., Bennani, A. K., Bennani, B., Daoudi, M., Benlarbi, N., El Yazidi, M., Garrigues, B. & Kerbal, A. (2010). *J. Maroc. Chim. Heterocycl.* **9**, 36–43.
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
El yazidi, M., Daou, B., Bougrin, K. & Soufiaoui, M. (1994). *J. Soc. Maroc. Chim.* **3**, 54–51.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Toth, G., Balazs, B., Levai, A., Fisera, L. & Jedlovska, E. (1999). *J. Mol. Struct.* **508**, 29–36.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

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(2*RS*,4′*RS*)-3′-(3-Chloro-4-methoxyphenyl)-4′-phenyl-4′*H*-spiro[indene-2,5′-isoxazol]-1(3*H*)-one ethanol monosolvate

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S1. Comment

In general, the 1,3-dipolar cycloaddition of arylnitrile oxides with ethylenic dipolarophiles leads to the regioselective formation of isoxazolines so that the electron withdrawing substituent of the dipolarophile is connected to position 5 of the isoxazoline ring (Al Houari *et al.*, 2010; Toth *et al.*, 1999; El yazidi *et al.*, 1994).

The crystal structure shows that the carbonyl group is bonded to position 5 of the isoxazoline ring, and that the hydrogen atom in position 4 is situated on the same side of the ring as the carbonyl group. The structural study by X-rays is in perfect agreement with the results of IR, ^{1}H and ^{13}C NMR spectroscopic analysis.

The 1,3-dipolar cycloaddition gave the title compound as a racemic product. However, the crystallization process from ethanol resulted in the formation of a conglomerate in space group $P2_12_12_1$.

In the crystal molecules are linked into zigzag chains by a series of intermolecular N—H···O and O—H···O hydrogen-bonding interactions, where both the main and the solvent molecules take part (Table 1).

S2. Experimental

4 mmol of (2*Z*)-2-benzylidene-1,2-dihydro-3*H*-indol-3-one and 4 mmol of 3-chloro-*N*-hydroxy-4-methoxybenzene-carboximidoyl chloride were dissolved in 30 ml of THF in a 100 ml flask equipped with a condenser. The reaction mixture was refluxed until the complete dissolution of the reagents, and then 1 ml of *N*,*N*-diethylethanamine was added to the reaction. Monitoring the reaction by thin film chromatography revealed the formation of a single cycloaddition product. After filtration, the organic solution was evaporated under reduced pressure. The residue obtained was recrystallized from ethanol.

S3. Refinement

The H atoms bound to C were treated as riding with their parent atoms [C—H distances are 0.93 Å for CH groups with U_{iso}(H) = 1.2 U_{eq}(C), and 0.97 Å for CH_3 groups with U_{iso}(H) = 1.5 U_{eq}(C). The nitrogen- and oxygen-bound H atoms were located in a difference Fourier map. The nitrogen-bound H atom was refined freely, while the H atom of the hydroxyl group was refined as an idealised rotating group and with U_{iso}(H) = 1.5 U_{eq}(O).

Refinment with TWIN and BASF instructions in *SHELXL* indicated racemic twinning.

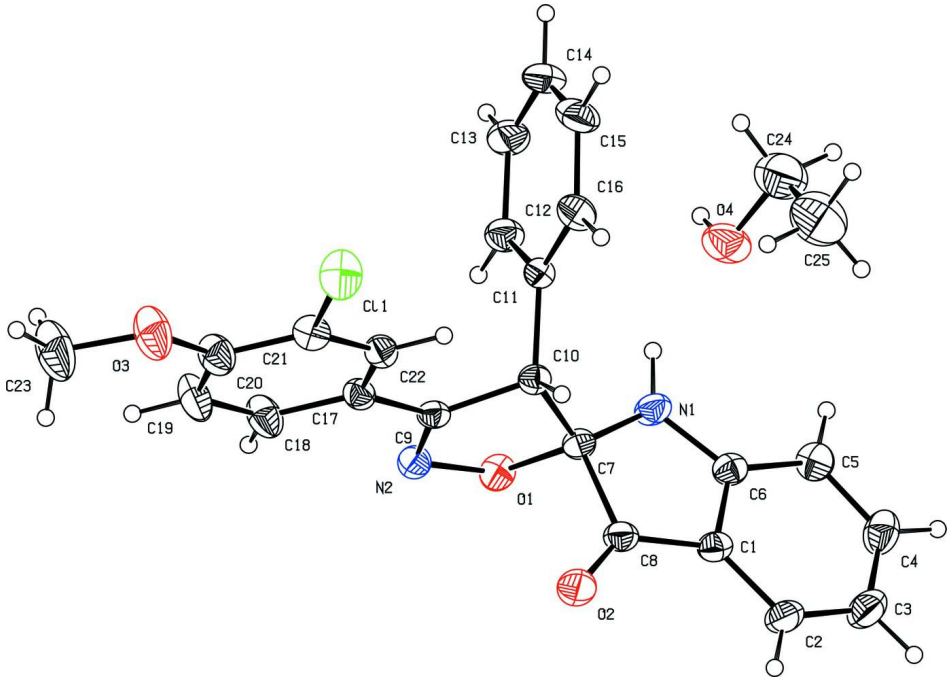

Figure 1

Molecular view of the title compound showing the atom labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

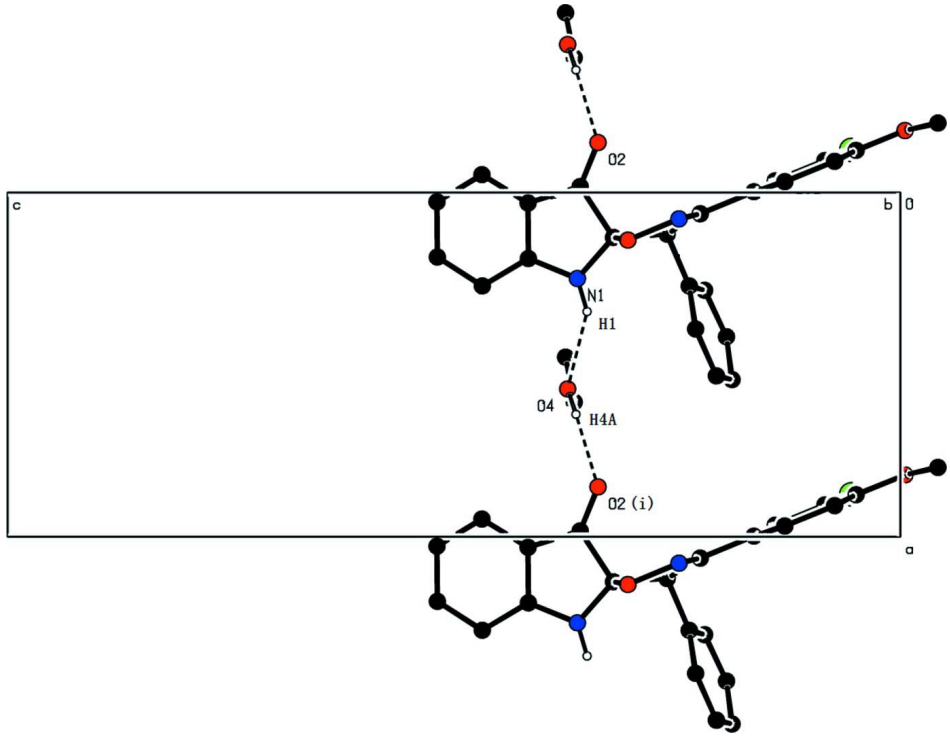

Figure 2

Partial packing view showing the chain formed by N—H···O and O—H···O hydrogen bondings. H atoms not involved in hydrogen bonds have been omitted for clarity. Symmetry codes: (i) *x*+1, *y*, *z*.

(2*RS*,4′*RS*)-3′-(3-Chloro-4-methoxyphenyl)-4′-phenyl-4′*H*- spiro[indene-2,5′-isoxazol]-1(3*H*)-one ethanol monosolvate

Crystal data

$C_{23}H_{17}ClN_2O_3 \cdot C_2H_6O$
$M_r = 450.90$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 8.7112$ (2) Å
$b = 11.3051$ (2) Å
$c = 22.5913$ (5) Å
$V = 2224.81$ (8) Å^3
$Z = 4$
$F(000) = 944$
$D_x = 1.346$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 265 reflections
$\theta = 2.6$–$26.3°$
$\mu = 0.21$ mm^{-1}
$T = 296$ K
Prism, colourless
0.24 × 0.17 × 0.16 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
13160 measured reflections
4757 independent reflections
3815 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.8°$
$h = -10 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -28 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.096$
$S = 1.06$
4757 reflections
297 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.1284P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Absolute structure: Flack (1983); 1986 Friedel pairs
Absolute structure parameter: 0.36 (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.

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0305 (2)	0.33701 (16)	0.41709 (9)	0.0378 (4)
C10	0.1211 (2)	0.35087 (15)	0.26128 (8)	0.0333 (4)
C11	0.2714 (2)	0.39793 (16)	0.23651 (8)	0.0340 (4)

C12	0.3965 (2)	0.32367 (18)	0.22940 (10)	0.0470 (5)
C13	0.5324 (3)	0.3680 (2)	0.20606 (11)	0.0590 (6)
C14	0.5434 (3)	0.4828 (2)	0.18859 (11)	0.0629 (7)
C15	0.4190 (3)	0.5564 (2)	0.19482 (11)	0.0585 (6)
C16	0.2839 (2)	0.51488 (18)	0.21932 (10)	0.0471 (5)
C17	−0.0022 (2)	0.26234 (16)	0.16411 (8)	0.0359 (4)
C18	−0.0316 (3)	0.16313 (18)	0.12947 (10)	0.0533 (6)
C19	−0.0905 (3)	0.17326 (19)	0.07365 (11)	0.0613 (7)
C2	−0.0518 (3)	0.36087 (19)	0.46878 (10)	0.0495 (5)
C20	−0.1223 (3)	0.28381 (19)	0.04958 (10)	0.0526 (5)
C21	−0.0928 (2)	0.38300 (17)	0.08457 (9)	0.0423 (5)
C22	−0.0338 (2)	0.37289 (17)	0.14030 (9)	0.0379 (4)
C23	−0.2016 (4)	0.2016 (3)	−0.04206 (13)	0.0908 (10)
C24	0.6087 (4)	0.5038 (3)	0.36539 (16)	0.0920 (9)
C25	0.4781 (4)	0.5779 (3)	0.37505 (16)	0.1008 (11)
C3	0.0272 (3)	0.3874 (2)	0.51910 (10)	0.0587 (6)
C4	0.1875 (3)	0.3900 (2)	0.51872 (10)	0.0569 (6)
C5	0.2713 (3)	0.36897 (19)	0.46834 (9)	0.0466 (5)
C6	0.1917 (2)	0.34114 (16)	0.41674 (9)	0.0378 (4)
C7	0.1305 (2)	0.28684 (16)	0.32140 (8)	0.0362 (4)
C8	−0.0172 (2)	0.30244 (18)	0.35872 (9)	0.0389 (5)
C9	0.0618 (2)	0.24995 (15)	0.22427 (8)	0.0330 (4)
Cl1	−0.12367 (8)	0.52300 (5)	0.05494 (3)	0.06402 (19)
H1	0.346 (3)	0.324 (2)	0.3510 (10)	0.060 (7)*
H10	0.0447	0.4144	0.2630	0.040*
H12	0.3895	0.2445	0.2402	0.056*
H13	0.6170	0.3184	0.2023	0.071*
H14	0.6345	0.5113	0.1726	0.075*
H15	0.4257	0.6348	0.1825	0.070*
H16	0.2011	0.5659	0.2243	0.056*
H18	−0.0107	0.0884	0.1446	0.064*
H19	−0.1096	0.1055	0.0515	0.074*
H2	−0.1585	0.3587	0.4688	0.059*
H22	−0.0145	0.4406	0.1625	0.045*
H23A	−0.1057	0.1606	−0.0465	0.136*
H23B	−0.2379	0.2263	−0.0802	0.136*
H23C	−0.2756	0.1497	−0.0242	0.136*
H24A	0.6892	0.5250	0.3931	0.110*
H24B	0.6475	0.5166	0.3257	0.110*
H25A	0.3977	0.5561	0.3481	0.151*
H25B	0.5062	0.6590	0.3685	0.151*
H25C	0.4427	0.5684	0.4150	0.151*
H3	−0.0258	0.4038	0.5539	0.070*
H4	0.2392	0.4066	0.5538	0.068*
H4A	0.6442	0.3400	0.3634	0.105*
H5	0.3779	0.3732	0.4687	0.056*
N1	0.2497 (2)	0.31383 (17)	0.36182 (8)	0.0444 (4)
N2	0.07647 (17)	0.14773 (13)	0.24799 (7)	0.0391 (4)

O1	0.13828 (17)	0.16082 (11)	0.30525 (6)	0.0426 (3)
O2	−0.14510 (17)	0.28485 (15)	0.33873 (7)	0.0583 (4)
O3	−0.1799 (2)	0.30291 (14)	−0.00516 (8)	0.0716 (5)
O4	0.57042 (17)	0.38095 (16)	0.37275 (9)	0.0703 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0382 (11)	0.0361 (10)	0.0391 (11)	−0.0006 (8)	0.0064 (9)	0.0047 (8)
C10	0.0287 (9)	0.0337 (9)	0.0374 (10)	0.0030 (8)	0.0024 (8)	0.0008 (7)
C11	0.0332 (11)	0.0352 (9)	0.0336 (10)	−0.0031 (8)	0.0001 (8)	−0.0006 (8)
C12	0.0396 (12)	0.0441 (11)	0.0571 (13)	−0.0002 (9)	0.0087 (10)	−0.0001 (9)
C13	0.0373 (12)	0.0655 (15)	0.0741 (17)	−0.0016 (11)	0.0164 (12)	−0.0106 (13)
C14	0.0480 (14)	0.0782 (18)	0.0625 (16)	−0.0275 (13)	0.0121 (12)	0.0003 (13)
C15	0.0599 (16)	0.0500 (13)	0.0657 (16)	−0.0216 (11)	0.0001 (13)	0.0119 (11)
C16	0.0464 (12)	0.0387 (10)	0.0561 (13)	−0.0035 (9)	−0.0030 (11)	0.0045 (10)
C17	0.0311 (10)	0.0377 (10)	0.0390 (11)	−0.0025 (8)	−0.0014 (8)	−0.0013 (8)
C18	0.0685 (15)	0.0365 (11)	0.0549 (14)	−0.0078 (10)	−0.0150 (12)	0.0033 (10)
C19	0.0843 (19)	0.0429 (12)	0.0566 (15)	−0.0146 (11)	−0.0225 (13)	−0.0047 (10)
C2	0.0509 (13)	0.0523 (13)	0.0454 (12)	−0.0015 (10)	0.0150 (11)	0.0028 (10)
C20	0.0555 (13)	0.0545 (13)	0.0476 (13)	−0.0071 (11)	−0.0158 (12)	0.0031 (10)
C21	0.0380 (12)	0.0417 (10)	0.0472 (12)	0.0030 (8)	−0.0033 (10)	0.0048 (9)
C22	0.0344 (10)	0.0375 (10)	0.0417 (11)	0.0010 (8)	−0.0001 (9)	−0.0022 (8)
C23	0.129 (3)	0.0773 (18)	0.0661 (19)	−0.0205 (18)	−0.0483 (19)	−0.0026 (15)
C24	0.078 (2)	0.090 (2)	0.108 (3)	−0.0139 (19)	0.0090 (19)	−0.0018 (18)
C25	0.106 (3)	0.074 (2)	0.122 (3)	−0.0016 (19)	−0.005 (2)	0.0111 (19)
C3	0.0709 (18)	0.0657 (15)	0.0396 (13)	0.0004 (13)	0.0141 (12)	0.0017 (11)
C4	0.0744 (18)	0.0605 (14)	0.0357 (12)	0.0038 (12)	−0.0051 (11)	0.0001 (10)
C5	0.0484 (13)	0.0502 (12)	0.0413 (12)	0.0023 (10)	−0.0078 (10)	0.0075 (9)
C6	0.0410 (11)	0.0333 (9)	0.0392 (11)	0.0020 (8)	0.0030 (9)	0.0054 (8)
C7	0.0304 (10)	0.0396 (10)	0.0387 (10)	0.0008 (8)	0.0041 (9)	−0.0017 (8)
C8	0.0334 (12)	0.0391 (10)	0.0442 (12)	−0.0022 (8)	0.0066 (9)	0.0003 (9)
C9	0.0265 (9)	0.0351 (9)	0.0374 (10)	−0.0009 (7)	0.0052 (8)	0.0013 (8)
Cl1	0.0852 (4)	0.0498 (3)	0.0571 (3)	0.0136 (3)	−0.0127 (4)	0.0081 (3)
N1	0.0296 (10)	0.0642 (11)	0.0393 (10)	−0.0021 (8)	0.0047 (8)	−0.0020 (8)
N2	0.0414 (10)	0.0371 (9)	0.0389 (9)	−0.0005 (7)	0.0019 (7)	0.0001 (7)
O1	0.0502 (8)	0.0370 (7)	0.0405 (8)	0.0051 (6)	0.0008 (7)	0.0041 (6)
O2	0.0312 (9)	0.0843 (11)	0.0595 (10)	−0.0069 (7)	0.0045 (7)	−0.0158 (8)
O3	0.0952 (14)	0.0641 (10)	0.0555 (10)	−0.0077 (9)	−0.0353 (10)	−0.0004 (8)
O4	0.0398 (9)	0.0696 (12)	0.1014 (14)	−0.0027 (8)	0.0102 (9)	−0.0073 (10)

Geometric parameters (Å, º)

C1—C2	1.397 (3)	C23—H23C	0.9600
C10—H10	0.9800	C23—H23B	0.9600
C10—C7	1.541 (3)	C23—H23A	0.9600
C10—C11	1.520 (2)	C24—H24B	0.9700
C10—C9	1.506 (2)	C24—H24A	0.9700

C11—C12	1.385 (3)	C24—C25	1.429 (5)
C11—C16	1.382 (3)	C25—H25C	0.9600
C12—H12	0.9300	C25—H25B	0.9600
C12—C13	1.389 (3)	C25—H25A	0.9600
C13—H13	0.9300	C3—H3	0.9300
C13—C14	1.361 (4)	C4—H4	0.9300
C14—H14	0.9300	C4—C3	1.396 (4)
C15—H15	0.9300	C4—C5	1.373 (3)
C15—C14	1.373 (4)	C5—H5	0.9300
C16—H16	0.9300	C6—C1	1.405 (3)
C16—C15	1.383 (3)	C6—C5	1.392 (3)
C17—C9	1.476 (3)	C8—C7	1.549 (3)
C17—C18	1.391 (3)	C8—C1	1.437 (3)
C18—H18	0.9300	N1—H1	0.88 (3)
C18—C19	1.366 (3)	N1—C7	1.416 (3)
C19—H19	0.9300	N1—C6	1.375 (3)
C2—H2	0.9300	N2—O1	1.409 (2)
C2—C3	1.362 (3)	N2—C9	1.280 (2)
C20—C19	1.391 (3)	O1—C7	1.472 (2)
C21—Cl1	1.739 (2)	O2—C8	1.218 (2)
C21—C20	1.396 (3)	O3—C23	1.429 (3)
C22—H22	0.9300	O3—C20	1.352 (3)
C22—C17	1.388 (3)	O4—H4A	0.8200
C22—C21	1.365 (3)	O4—C24	1.438 (4)

C6—C1—C8	107.05 (17)	H23A—C23—H23C	109.5
C2—C1—C8	132.17 (19)	O3—C23—H23C	109.5
C2—C1—C6	120.7 (2)	H23A—C23—H23B	109.5
C7—C10—H10	110.1	O3—C23—H23B	109.5
C11—C10—H10	110.1	O3—C23—H23A	109.5
C9—C10—H10	110.1	H24A—C24—H24B	108.0
C11—C10—C7	116.32 (16)	O4—C24—H24B	109.4
C9—C10—C7	98.72 (13)	C25—C24—H24B	109.4
C9—C10—C11	110.86 (15)	O4—C24—H24A	109.4
C12—C11—C10	120.54 (16)	C25—C24—H24A	109.4
C16—C11—C10	120.42 (17)	C25—C24—O4	111.3 (3)
C16—C11—C12	119.01 (17)	H25B—C25—H25C	109.5
C13—C12—H12	120.1	H25A—C25—H25C	109.5
C11—C12—H12	120.1	C24—C25—H25C	109.5
C11—C12—C13	119.73 (19)	H25A—C25—H25B	109.5
C12—C13—H13	119.5	C24—C25—H25B	109.5
C14—C13—H13	119.5	C24—C25—H25A	109.5
C14—C13—C12	120.9 (2)	C4—C3—H3	119.8
C15—C14—H14	120.2	C2—C3—H3	119.8
C13—C14—H14	120.2	C2—C3—C4	120.3 (2)
C13—C14—C15	119.5 (2)	C3—C4—H4	118.9
C16—C15—H15	119.8	C5—C4—H4	118.9
C14—C15—H15	119.8	C5—C4—C3	122.2 (2)

C14—C15—C16	120.4 (2)	C6—C5—H5	121.0
C15—C16—H16	119.8	C4—C5—H5	121.0
C11—C16—H16	119.8	C4—C5—C6	117.9 (2)
C11—C16—C15	120.3 (2)	C5—C6—C1	120.04 (19)
C18—C17—C9	120.73 (16)	N1—C6—C1	111.39 (18)
C22—C17—C9	121.14 (16)	N1—C6—C5	128.57 (18)
C22—C17—C18	118.13 (17)	C10—C7—C8	112.47 (16)
C17—C18—H18	119.3	O1—C7—C8	106.46 (14)
C19—C18—H18	119.3	N1—C7—C8	103.50 (15)
C19—C18—C17	121.38 (19)	O1—C7—C10	103.80 (14)
C20—C19—H19	119.6	N1—C7—C10	120.40 (16)
C18—C19—H19	119.6	N1—C7—O1	109.55 (15)
C18—C19—C20	120.74 (19)	C1—C8—C7	106.86 (16)
C1—C2—H2	120.6	O2—C8—C7	122.64 (18)
C3—C2—H2	120.6	O2—C8—C1	130.48 (19)
C3—C2—C1	118.7 (2)	C17—C9—C10	124.70 (15)
C19—C20—C21	117.63 (19)	N2—C9—C10	114.66 (16)
O3—C20—C21	117.26 (19)	N2—C9—C17	120.58 (16)
O3—C20—C19	125.11 (19)	C7—N1—H1	123.1 (15)
C20—C21—Cl1	118.99 (16)	C6—N1—H1	124.9 (15)
C22—C21—Cl1	119.30 (15)	C6—N1—C7	111.18 (17)
C22—C21—C20	121.64 (18)	C9—N2—O1	109.12 (14)
C17—C22—H22	119.8	N2—O1—C7	108.16 (12)
C21—C22—H22	119.8	C20—O3—C23	117.03 (19)
C21—C22—C17	120.49 (18)	C24—O4—H4A	109.5
H23B—C23—H23C	109.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4	0.88 (3)	2.12 (3)	2.906 (2)	149 (2)
O4—H4*A*···O2^{i}	0.82	2.02	2.813 (2)	164

Symmetry code: (i) *x*+1, *y*, *z*.