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N-(4-Chlorophenyl)-6,7-bis(2-methoxyethoxy)quinazolin-4-amine monohydrate

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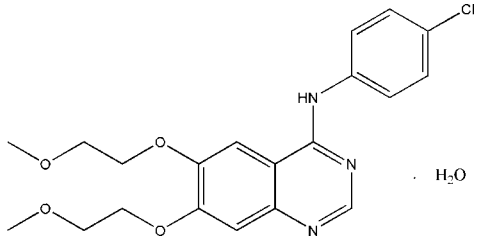
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.067; wR factor = 0.179; data-to-parameter ratio = 15.5.

In the title compound, $C_{20}H_{22}ClN_3O_4\cdot H_2O$, the quinazoline and benzene ring systems are oriented at a dihedral angle of 4.99 (3)°. Intramolecular C—H···N hydrogen bonding results in the formation of a nearly planar six-membered ring, which is nearly coplanar with the adjacent quinazoline ring system and the benzene ring, making dihedral angles of 2.39 (3) and 3.32 (3)°, respectively. In the crystal structure, intermolecular N—H···O and C—H···O hydrogen bonds link the molecules.

Related literature

For related literature, see: Dolle *et al.* (1994); Aislabie *et al.* (1990). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{22}ClN_3O_4\cdot H_2O$
M_r = 421.87
Monoclinic, $P2_1/c$
a = 5.8850 (12) Å
b = 16.231 (3) Å
c = 21.723 (4) Å
β = 93.93 (3)°
V = 2070.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 298 (2) K
0.30 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.937, T_{max} = 0.978
4474 measured reflections
4064 independent reflections
1956 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.179
S = 0.99
4064 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
OW—HWA···O3	0.85	2.38	2.794 (4)	110
C16—H16A···N2	0.93	2.21	2.825 (6)	123
N3—H3A···OW^i	0.86	2.17	2.999 (4)	163
C12—H12A···OW^i	0.93	2.38	3.299 (4)	168
C20—H20A···OW^i	0.93	2.47	3.257 (5)	143

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Siemens, 1996).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2380).

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supplementary materials

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N-(4-Chlorophenyl)-6,7-bis(2-methoxyethoxy)quinazolin-4-amine monohydrate

S.-C. Li, H. Xu and W.-L. Huang

Comment

The title compound, $C_{20}H_{24}ClN_3O_5$, is one of quinazolins which are an important class of aromatic compounds and have widespread applications from pharmaceuticals (Dolle *et al.*, 1994) to agronomy environmental microbiology (Aislabie *et al.*, 1990). As part of our studies in this area, we report herein the synthesis and crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings A (C7—C12), B (N1/N2/C10/C11/C13/C14) and C (C15—C20) are, of course, planar and the dihedral angles between them are A/B = 0.50 (3)°, A/C = 5.06 (3)° and B/C = 4.89 (2)°. So, rings A and B are also co-planar. The nearly planar quinazoline ring system is oriented with respect to ring C at a dihedral angle of 4.99 (3)°. The intramolecular C—H···N hydrogen bond (Table 1) causes to the formation of the nearly planar six-membered ring; D (N2/N3/C14—C16/H16A), in which it is also nearly co-planar with the adjacent quinazoline ring system and ring C with dihedral angles of 2.39 (3)° and 3.32 (3)°, respectively.

In the crystal structure, intermolecular N—H···O and C—H···O hydrogen bonds (Table 1) link the molecules, in which they seem to be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, a solution of 4-chloro-6,7-bis -(2-methoxyethoxy)-quinazoline (2.0 g, 6.4 mmol) and 4-chlorobenzenamine (1.0 g, 7.8 mmol) in i-PrOH(15.0 ml) was stirred and heated at reflux for 6 h under N_2 atmosphere resulting in the precipitation of a colorless solid. After stirring at room temperature overnight the precipitation was filtered, washed with hot i-PrOH and dried on the air to afford the crude hydrochloride product (yield; 2.7 g, 94%). To isolate the free base, the crude product (0.5 g) was dissolved in water (10 ml) and basified using conc. aq. ammonia (5 ml). Extraction with dichloromethane (4 *x* 20 ml), gave after drying and evaporation, the title compound as colorless crystals. Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

Refinement

H atoms were positioned geometrically, with O—H = 0.85 Å (for H_2O), N—H = 0.86 Å (for NH) and C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*N*,*O*), where *x* = 1.5 for methyl H, and *x* = 1.2 for all other H atoms.

Figures

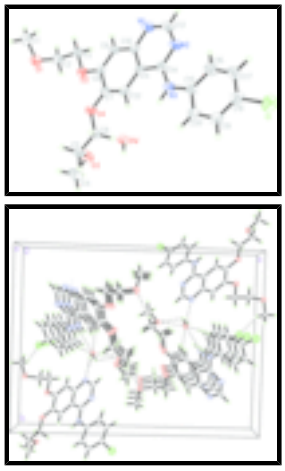

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

N-(4-chlorophenyl)-6,7-bis(2-methoxyethoxy)quinazolin-4-amine monohydrate

Crystal data

$C_{20}H_{22}ClN_3O_4 \cdot H_2O$	F_{000} = 888
M_r = 421.87	D_x = 1.354 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 411(2) K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 5.8850 (12) Å	Cell parameters from 25 reflections
b = 16.231 (3) Å	θ = 10–13º
c = 21.723 (4) Å	μ = 0.22 mm^{-1}
β = 93.93 (3)º	T = 298 (2) K
V = 2070.1 (7) Å^3	Block, colorless
Z = 4	0.30 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.036
Radiation source: fine-focus sealed tube	θ_{max} = 26.0º
Monochromator: graphite	θ_{min} = 1.6º
T = 298(2) K	h = −7→7
ω/2θ scans	k = 0→20
Absorption correction: ψ scan (North *et al.*, 1968)	l = 0→26
T_{min} = 0.937, T_{max} = 0.978	3 standard reflections
4474 measured reflections	every 120 min
4064 independent reflections	intensity decay: none
1956 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.067$	H-atom parameters constrained
$wR(F^2) = 0.179$	$w = 1/[\sigma^2(F_o^2) + (0.070P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} < 0.001$
4064 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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}
Cl	0.28318 (19)	0.54760 (8)	0.08634 (6)	0.0852 (4)
OW	2.2216 (5)	0.58666 (15)	0.30954 (12)	0.0652 (8)
HWB	2.3512	0.6041	0.3004	0.078*
HWA	2.1409	0.6263	0.3214	0.078*
O1	2.2847 (5)	0.23685 (18)	0.48805 (14)	0.0734 (8)
O2	2.0330 (5)	0.31921 (15)	0.38367 (12)	0.0610 (7)
O3	2.0406 (5)	0.60395 (19)	0.42442 (13)	0.0790 (9)
O4	1.8136 (5)	0.45376 (15)	0.39496 (12)	0.0634 (8)
N1	1.5256 (6)	0.23193 (19)	0.21452 (16)	0.0678 (10)
N2	1.2049 (6)	0.3156 (2)	0.18159 (16)	0.0699 (10)
N3	1.1257 (5)	0.43964 (18)	0.22824 (13)	0.0520 (8)
H3A	1.1693	0.4744	0.2565	0.062*
C1	2.1970 (9)	0.1593 (3)	0.5006 (2)	0.0893 (15)
H1B	2.1511	0.1582	0.5422	0.134*
H1C	2.3119	0.1182	0.4959	0.134*
H1D	2.0678	0.1481	0.4725	0.134*
C2	2.3533 (7)	0.2472 (3)	0.4277 (2)	0.0675 (12)
H2B	2.4608	0.2039	0.4195	0.081*

H2C	2.4330	0.2994	0.4257	0.081*
C3	2.1656 (7)	0.2459 (2)	0.37812 (19)	0.0614 (11)
H3B	2.2280	0.2440	0.3379	0.074*
H3C	2.0710	0.1976	0.3824	0.074*
C4	2.1759 (7)	0.6585 (3)	0.4609 (2)	0.0865 (15)
H4A	2.3114	0.6712	0.4406	0.130*
H4B	2.2169	0.6334	0.5002	0.130*
H4C	2.0922	0.7083	0.4671	0.130*
C5	1.8353 (7)	0.5800 (2)	0.44938 (18)	0.0596 (11)
H5A	1.7497	0.6285	0.4599	0.071*
H5B	1.8683	0.5481	0.4867	0.071*
C6	1.6987 (7)	0.5297 (2)	0.40302 (18)	0.0604 (11)
H6A	1.5485	0.5195	0.4172	0.072*
H6B	1.6810	0.5590	0.3641	0.072*
C7	1.7244 (7)	0.4023 (2)	0.34991 (17)	0.0497 (9)
C8	1.8498 (7)	0.3282 (2)	0.34302 (17)	0.0500 (9)
C9	1.7805 (7)	0.2744 (2)	0.29797 (17)	0.0542 (10)
H9A	1.8631	0.2263	0.2931	0.065*
C10	1.5872 (7)	0.2897 (2)	0.25873 (17)	0.0534 (10)
C11	1.4585 (6)	0.3615 (2)	0.26580 (16)	0.0475 (9)
C12	1.5328 (6)	0.4175 (2)	0.31264 (17)	0.0502 (9)
H12A	1.4501	0.4654	0.3182	0.060*
C13	1.3404 (9)	0.2501 (3)	0.1796 (2)	0.0801 (14)
H13A	1.2983	0.2116	0.1492	0.096*
C14	1.2607 (6)	0.3716 (2)	0.22432 (17)	0.0506 (9)
C15	0.9255 (6)	0.4610 (2)	0.19267 (17)	0.0490 (9)
C16	0.8334 (7)	0.4174 (3)	0.1424 (2)	0.0710 (12)
H16A	0.9033	0.3693	0.1303	0.085*
C17	0.6390 (8)	0.4448 (3)	0.1103 (2)	0.0782 (14)
H17A	0.5801	0.4155	0.0760	0.094*
C18	0.5306 (7)	0.5149 (3)	0.1279 (2)	0.0598 (11)
C19	0.6159 (7)	0.5582 (2)	0.17804 (19)	0.0608 (11)
H19A	0.5421	0.6053	0.1906	0.073*
C20	0.8115 (7)	0.5316 (2)	0.20973 (18)	0.0601 (11)
H20A	0.8699	0.5617	0.2437	0.072*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0616 (7)	0.0858 (9)	0.1056 (10)	−0.0049 (6)	−0.0127 (6)	0.0152 (7)
OW	0.0705 (18)	0.0484 (16)	0.0770 (19)	−0.0015 (14)	0.0064 (15)	−0.0136 (14)
O1	0.081 (2)	0.066 (2)	0.072 (2)	0.0037 (17)	0.0000 (17)	−0.0073 (16)
O2	0.0661 (18)	0.0464 (16)	0.0693 (18)	0.0151 (14)	−0.0037 (15)	−0.0044 (13)
O3	0.077 (2)	0.087 (2)	0.074 (2)	−0.0186 (18)	0.0123 (17)	−0.0290 (17)
O4	0.0768 (18)	0.0420 (15)	0.0692 (18)	0.0147 (14)	−0.0109 (15)	−0.0117 (14)
N1	0.088 (3)	0.045 (2)	0.069 (2)	0.0070 (19)	−0.004 (2)	−0.0126 (17)
N2	0.090 (3)	0.045 (2)	0.072 (2)	0.0072 (19)	−0.011 (2)	−0.0171 (18)
N3	0.057 (2)	0.0486 (19)	0.0499 (19)	−0.0026 (16)	−0.0017 (16)	−0.0052 (15)

C1	0.118 (4)	0.075 (3)	0.073 (3)	−0.002 (3)	−0.004 (3)	0.015 (3)
C2	0.065 (3)	0.056 (3)	0.083 (3)	0.006 (2)	0.010 (3)	−0.003 (2)
C3	0.068 (3)	0.049 (2)	0.067 (3)	0.012 (2)	0.008 (2)	0.005 (2)
C4	0.067 (3)	0.095 (4)	0.097 (4)	−0.011 (3)	0.003 (3)	−0.037 (3)
C5	0.064 (3)	0.054 (2)	0.060 (3)	0.007 (2)	0.001 (2)	−0.009 (2)
C6	0.067 (3)	0.044 (2)	0.069 (3)	0.007 (2)	−0.005 (2)	−0.010 (2)
C7	0.061 (2)	0.037 (2)	0.052 (2)	−0.0016 (19)	0.006 (2)	−0.0028 (18)
C8	0.058 (2)	0.040 (2)	0.051 (2)	0.0072 (19)	0.003 (2)	0.0046 (18)
C9	0.070 (3)	0.035 (2)	0.059 (2)	0.0044 (19)	0.011 (2)	−0.0046 (18)
C10	0.069 (3)	0.039 (2)	0.053 (2)	−0.001 (2)	0.008 (2)	−0.0019 (19)
C11	0.058 (2)	0.036 (2)	0.049 (2)	−0.0050 (18)	0.0080 (19)	0.0011 (17)
C12	0.057 (2)	0.037 (2)	0.056 (2)	0.0032 (19)	0.005 (2)	−0.0010 (18)
C13	0.113 (4)	0.051 (3)	0.073 (3)	0.003 (3)	−0.013 (3)	−0.021 (2)
C14	0.060 (3)	0.042 (2)	0.050 (2)	−0.006 (2)	0.005 (2)	0.0001 (18)
C15	0.051 (2)	0.046 (2)	0.049 (2)	−0.008 (2)	0.0041 (18)	−0.0016 (18)
C16	0.058 (3)	0.068 (3)	0.085 (3)	0.001 (2)	−0.003 (2)	−0.015 (2)
C17	0.070 (3)	0.083 (4)	0.079 (3)	−0.005 (3)	−0.013 (3)	−0.018 (3)
C18	0.052 (2)	0.059 (3)	0.069 (3)	−0.008 (2)	0.004 (2)	0.013 (2)
C19	0.067 (3)	0.050 (2)	0.066 (3)	0.004 (2)	0.005 (2)	0.006 (2)
C20	0.075 (3)	0.048 (2)	0.058 (3)	−0.006 (2)	0.000 (2)	0.003 (2)

Geometric parameters (Å, °)

Cl—C18	1.742 (4)	C4—H4B	0.9600
OW—HWB	0.8500	C4—H4C	0.9600
OW—HWA	0.8501	C5—C6	1.489 (5)
N1—C13	1.318 (5)	C5—H5A	0.9700
N1—C10	1.374 (4)	C5—H5B	0.9700
O1—C1	1.394 (5)	C6—H6A	0.9700
O1—C2	1.408 (5)	C6—H6B	0.9700
C1—H1B	0.9600	C7—C12	1.365 (5)
C1—H1C	0.9600	C7—C8	1.424 (5)
C1—H1D	0.9600	C8—C9	1.354 (5)
O2—C8	1.354 (4)	C9—C10	1.396 (5)
O2—C3	1.433 (4)	C9—H9A	0.9300
N2—C14	1.324 (4)	C10—C11	1.403 (5)
N2—C13	1.332 (5)	C11—C12	1.412 (5)
C2—C3	1.490 (5)	C11—C14	1.432 (5)
C2—H2B	0.9700	C12—H12A	0.9300
C2—H2C	0.9700	C13—H13A	0.9300
N3—C14	1.366 (4)	C15—C16	1.380 (5)
N3—C15	1.408 (4)	C15—C20	1.391 (5)
N3—H3A	0.8600	C16—C17	1.373 (5)
O3—C4	1.400 (5)	C16—H16A	0.9300
O3—C5	1.412 (5)	C17—C18	1.371 (6)
C3—H3B	0.9700	C17—H17A	0.9300
C3—H3C	0.9700	C18—C19	1.363 (5)
O4—C7	1.364 (4)	C19—C20	1.370 (5)
O4—C6	1.423 (4)	C19—H19A	0.9300

C4—H4A	0.9600	C20—H20A	0.9300
HWB—OW—HWA	110.3	C5—C6—H6B	110.0
C13—N1—C10	114.7 (4)	H6A—C6—H6B	108.3
C1—O1—C2	115.1 (3)	O4—C7—C12	125.2 (3)
O1—C1—H1B	109.5	O4—C7—C8	114.6 (3)
O1—C1—H1C	109.5	C12—C7—C8	120.2 (3)
H1B—C1—H1C	109.5	C9—C8—O2	126.1 (3)
O1—C1—H1D	109.5	C9—C8—C7	119.2 (4)
H1B—C1—H1D	109.5	O2—C8—C7	114.7 (3)
H1C—C1—H1D	109.5	C8—C9—C10	121.3 (4)
C8—O2—C3	116.7 (3)	C8—C9—H9A	119.4
C14—N2—C13	116.8 (4)	C10—C9—H9A	119.4
O1—C2—C3	115.2 (3)	N1—C10—C9	118.0 (4)
O1—C2—H2B	108.5	N1—C10—C11	121.6 (4)
C3—C2—H2B	108.5	C9—C10—C11	120.3 (4)
O1—C2—H2C	108.5	C10—C11—C12	118.1 (4)
C3—C2—H2C	108.5	C10—C11—C14	116.6 (3)
H2B—C2—H2C	107.5	C12—C11—C14	125.3 (3)
C14—N3—C15	129.3 (3)	C7—C12—C11	120.9 (3)
C14—N3—H3A	115.3	C7—C12—H12A	119.5
C15—N3—H3A	115.3	C11—C12—H12A	119.5
C4—O3—C5	115.1 (3)	N1—C13—N2	129.3 (4)
O2—C3—C2	107.9 (3)	N1—C13—H13A	115.4
O2—C3—H3B	110.1	N2—C13—H13A	115.4
C2—C3—H3B	110.1	N2—C14—N3	118.7 (3)
O2—C3—H3C	110.1	N2—C14—C11	120.9 (4)
C2—C3—H3C	110.1	N3—C14—C11	120.3 (3)
H3B—C3—H3C	108.4	C16—C15—C20	117.6 (4)
C7—O4—C6	117.1 (3)	C16—C15—N3	125.2 (4)
O3—C4—H4A	109.5	C20—C15—N3	117.2 (3)
O3—C4—H4B	109.5	C17—C16—C15	120.3 (4)
H4A—C4—H4B	109.5	C17—C16—H16A	119.8
O3—C4—H4C	109.5	C15—C16—H16A	119.8
H4A—C4—H4C	109.5	C18—C17—C16	121.0 (4)
H4B—C4—H4C	109.5	C18—C17—H17A	119.5
O3—C5—C6	109.1 (3)	C16—C17—H17A	119.5
O3—C5—H5A	109.9	C19—C18—C17	119.8 (4)
C6—C5—H5A	109.9	C19—C18—Cl	120.4 (4)
O3—C5—H5B	109.9	C17—C18—Cl	119.8 (4)
C6—C5—H5B	109.9	C18—C19—C20	119.3 (4)
H5A—C5—H5B	108.3	C18—C19—H19A	120.3
O4—C6—C5	108.6 (3)	C20—C19—H19A	120.3
O4—C6—H6A	110.0	C19—C20—C15	122.0 (4)
C5—C6—H6A	110.0	C19—C20—H20A	119.0
O4—C6—H6B	110.0	C15—C20—H20A	119.0
C1—O1—C2—C3	67.2 (5)	C8—C7—C12—C11	−1.6 (5)
C8—O2—C3—C2	−178.6 (3)	C10—C11—C12—C7	0.0 (5)
O1—C2—C3—O2	69.4 (4)	C14—C11—C12—C7	−179.9 (3)

C4—O3—C5—C6	174.0 (3)	C10—N1—C13—N2	−0.8 (7)
C7—O4—C6—C5	−174.2 (3)	C14—N2—C13—N1	0.2 (8)
O3—C5—C6—O4	67.7 (4)	C13—N2—C14—N3	−179.6 (4)
C6—O4—C7—C12	−0.8 (5)	C13—N2—C14—C11	0.3 (6)
C6—O4—C7—C8	178.5 (3)	C15—N3—C14—N2	0.4 (6)
C3—O2—C8—C9	0.2 (5)	C15—N3—C14—C11	−179.6 (3)
C3—O2—C8—C7	−179.5 (3)	C10—C11—C14—N2	−0.2 (5)
O4—C7—C8—C9	−177.5 (3)	C12—C11—C14—N2	179.8 (4)
C12—C7—C8—C9	1.9 (5)	C10—C11—C14—N3	179.8 (3)
O4—C7—C8—O2	2.2 (5)	C12—C11—C14—N3	−0.3 (5)
C12—C7—C8—O2	−178.4 (3)	C14—N3—C15—C16	−4.6 (6)
O2—C8—C9—C10	179.6 (3)	C14—N3—C15—C20	175.2 (3)
C7—C8—C9—C10	−0.8 (6)	C20—C15—C16—C17	1.4 (6)
C13—N1—C10—C9	179.4 (4)	N3—C15—C16—C17	−178.8 (4)
C13—N1—C10—C11	0.9 (6)	C15—C16—C17—C18	−1.1 (7)
C8—C9—C10—N1	−179.3 (4)	C16—C17—C18—C19	−0.1 (7)
C8—C9—C10—C11	−0.8 (6)	C16—C17—C18—Cl	−179.6 (3)
N1—C10—C11—C12	179.6 (3)	C17—C18—C19—C20	0.9 (6)
C9—C10—C11—C12	1.1 (5)	Cl—C18—C19—C20	−179.6 (3)
N1—C10—C11—C14	−0.5 (5)	C18—C19—C20—C15	−0.6 (6)
C9—C10—C11—C14	−178.9 (3)	C16—C15—C20—C19	−0.5 (6)
O4—C7—C12—C11	177.8 (3)	N3—C15—C20—C19	179.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
OW—HWA···O3	0.85	2.38	2.794 (4)	110
C16—H16A···N2	0.93	2.21	2.825 (6)	123
N3—H3A···OW^{i}	0.86	2.17	2.999 (4)	163
C12—H12A···OW^{i}	0.93	2.38	3.299 (4)	168
C20—H20A···OW^{i}	0.93	2.47	3.257 (5)	143

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

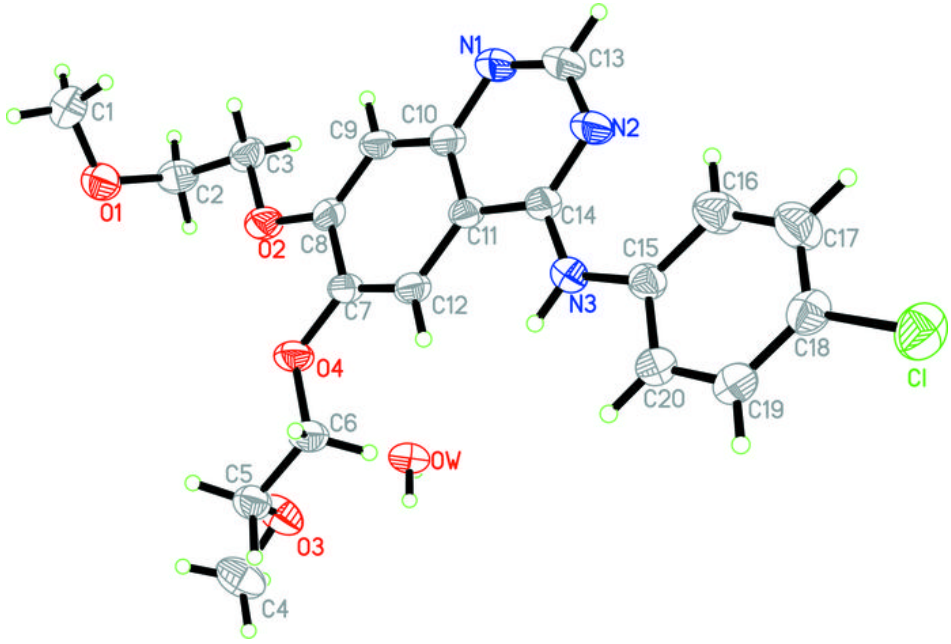
N1
C13
C1
C10
C9
N2
C3
C16
C2
C14
C17
O1
O2
C8
C11
C15
N3
C7
C12
C18
Cl
O4
C20
C19
C6
OW
C5
O3
C4

Fig. 2