Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(4-Fluorophenyl)-2-morpholinoquinazolin-4(3*H*)-one

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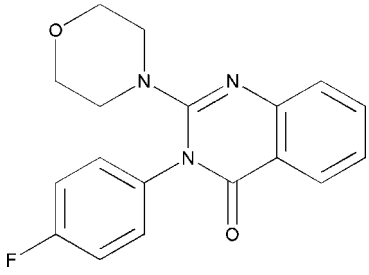
Received 1 June 2007; accepted 5 June 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.059; wR factor = 0.158; data-to-parameter ratio = 16.9.

The title compound, $C_{18}H_{16}FN_3O_2$, was obtained *via* the aza-Wittig reaction. The quinazolinone ring system is almost planar and makes a dihedral angle of 67.09 (8)° with the substituent benzene ring. The structure is stabilized by a weak C—H···O hydrogen bond and C—H···π interactions.

Related literature

Biological and pharmaceutical activities have been described by Shiba *et al.* (1997) and the preparation of potentially active heterocycles has been described by Ding *et al.* (2000). For ring-puckering analysis, see Cremer & Pople (1975).



Experimental

Crystal data

$C_{18}H_{16}FN_3O_2$
M_r = 325.34
Tetragonal, $I4_1/a$
a = 22.9526 (7) Å
c = 12.7318 (7) Å
V = 6707.4 (5) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 291 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
37145 measured reflections
3665 independent reflections
3033 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.158
S = 1.06
3665 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O1^{i}	0.93	2.57	3.306 (2)	137
C9—H9A···$Cg3^{i}$	0.97	2.85	3.673 (2)	143
C11—H11A···$Cg2^{ii}$	0.97	2.96	3.759 (2)	141
C12—H12A···$Cg1^{iii}$	0.97	2.72	3.548 (2)	143
C12—H12B···$Cg1^{ii}$	0.97	2.68	3.492 (2)	141

Symmetry codes: (i) $y+\frac{1}{4}, -x+\frac{5}{4}, z+\frac{1}{4}$; (ii) $-x+1, -y+1, -z$; (iii) $y-\frac{1}{4}, -x+\frac{5}{4}, -z+\frac{1}{4}$. Notes: $Cg1$, $Cg2$, $Cg3$ are the centroids of rings C1–C6, N1/C7/C15/C16/N2/C8 and C13–C18, respectively.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

We thank Dr Xiang-Gao Meng for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2172).

References

Bruker (2001). *SMART* (Version 5.628) and *SAINT* (Version 6.45). Bruker AXS Inc., Madison, Wisconsin, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Ding, M. W., Zeng, G. P. & Wu, T. J. (2000). *Synth. Commun.* **30**, 1599–1604.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SHELXTL* (Version 5.0). Bruker AXS Inc., Madison, Wisconsin, USA.
Shiba, S. A., El-Khamry, A. A., Shaban, M. E. & Atia, K. S. (1997). *Pharmazie*, **52**, 189–194.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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supplementary materials

Acta Cryst. (2007). E**63**, o3196 [**doi:10.1107/S1600536807027535**]

3-(4-Fluorophenyl)-2-morpholinoquinazolin-4(3*H*)-one

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Comment

Quinazolinones are important heterocyclic compounds which exhibit good biological and pharmaceutical activities, including anti-inflammotory, antifunga, anticancer and AMPA-receptor antagonistic properties (Shiba *et al.*, 1997). As part of our work on the preparation of potentially active heterocycles (Ding *et al.*, 2000), we have obtained the title compound, (I).

Within the molecule of (I), the bond lengths and angles present no unusual features. In (I), the quinazolinone ring system is approximately planar, with a maximum deviation of 0.060 (1) and 0.028 (1) Å for atoms N1 and N2, respectively; the C13—C18 benzene ring is twisted with respect to it, with a dihedral angle of 67.09 (8)°. The morpholine ring shows a distorted chair conformation [φ = 341.64 (1)° and θ = 176.25 (1)°, Puckering Amplitude = 0.586 (1) Å] (Cremer & Pople, 1975). The structure is stabilized by a weak C—H···O hydrogen bond and C—H···π interactions (Table 1); *Cg*1, *Cg*2 and *Cg*3 are the centroids of C1—C6, N1/C7/C5/C6/N2/C8 and C13—C18 rings, respectively..

Experimental

To a solution of iminophosphorane (1.45 g, 3 mmol) in anhydrous dichloromethane (15 ml) was added 4-fluorophenyl isocyanate (3 mmol) under dry nitrogen at room temperature. The reaction mixture was left unstirred for 8 h at room temperature and then the solvent was removed under reduced pressure and ether-petroleum ether (1:2 *v*/*v*, 20 ml) was added to precipitate triphenylphosphine oxide. After filtration, the solution of carbodiimide was added to a solution of diethyl-amine in anhydrous dichloromethane. After stirring the reaction mixture for 8 h, the solvent was removed under reduced pressure and the residue was recrystallized from ethanol to give the title compound, (I), in a yield of 90% (m.p. 394–396 K). Single crystals suitable for X-ray diffraction were obtained by recrystallization from a mixed solvent of hexane and dichloromethane (1:3 *v*/*v*) at room temperature.

Refinement

H atoms were placed at calculated positions (C—H = 0.97 or 0.93 Å) and were refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

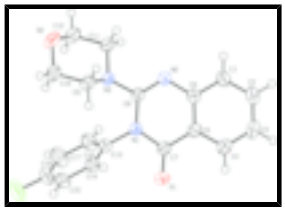

Fig. 1. The molecular structure of (I), showing the atom labelling scheme and with displacement ellipsoids drawn at the 50% probability level.

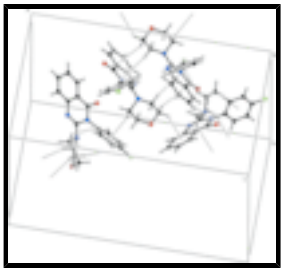

Fig. 2. A partial packing view of (I). Dashed lines indicate the C—H···π interactions.

3-(4-Fluorophenyl)-2-morpholinoquinazolin-4(3*H*)-one

Crystal data

$C_{18}H_{16}FN_3O_2$	$Z = 16$
$M_r = 325.34$	$F_{000} = 2720$
Tetragonal, $I4_1/a$	$D_x = 1.289$ Mg m^{-3}
Hall symbol: -I 4ad	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 22.9526$ (7) Å	Cell parameters from 8691 reflections
$b = 22.9526$ (7) Å	$\theta = 2.5$–24.9º
$c = 12.7318$ (7) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 90$º	$T = 291$ (2) K
$\beta = 90$º	Plate, colourless
$\gamma = 90$º	0.30 × 0.20 × 0.20 mm
$V = 6707.4$ (5) Å^3	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	3033 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.081$
Monochromator: graphite	$\theta_{max} = 27.0$º
$T = 292(2)$ K	$\theta_{min} = 1.8$º
φ and ω scans	$h = -29\rightarrow29$
Absorption correction: none	$k = -29\rightarrow29$
37145 measured reflections	$l = -16\rightarrow16$
3665 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0883P)^2 + 2.6139P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.059$	$(\Delta/\sigma)_{max} = 0.009$
$wR(F^2) = 0.158$	$\Delta\rho_{max} = 0.29$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.34$ e Å^{-3}
3665 reflections	Extinction correction: none

217 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.59565 (8)	0.62432 (8)	−0.12006 (15)	0.0401 (4)
H1	0.5653	0.6505	−0.1093	0.048*
C2	0.63280 (9)	0.63192 (9)	−0.20375 (15)	0.0430 (5)
H2	0.6271	0.6630	−0.2495	0.052*
C3	0.67875 (9)	0.59369 (9)	−0.22054 (15)	0.0427 (5)
H3	0.7034	0.5990	−0.2777	0.051*
C4	0.68773 (8)	0.54821 (8)	−0.15293 (15)	0.0375 (4)
H4	0.7189	0.5230	−0.1637	0.045*
C5	0.65010 (7)	0.53949 (7)	−0.06747 (13)	0.0305 (4)
C6	0.60337 (7)	0.57732 (7)	−0.05088 (13)	0.0310 (4)
C7	0.65773 (7)	0.48957 (8)	0.00124 (13)	0.0319 (4)
C8	0.57321 (7)	0.52771 (7)	0.09563 (13)	0.0281 (4)
C9	0.56338 (8)	0.52223 (9)	0.28622 (13)	0.0356 (4)
H9A	0.5693	0.5627	0.3058	0.043*
H9B	0.6009	0.5028	0.2863	0.043*
C10	0.52302 (8)	0.49319 (10)	0.36305 (15)	0.0429 (5)
H10A	0.5182	0.4526	0.3439	0.051*
H10B	0.5399	0.4947	0.4328	0.051*
C11	0.48082 (8)	0.54901 (9)	0.18113 (14)	0.0383 (4)
H11A	0.4629	0.5465	0.1122	0.046*
H11B	0.4863	0.5898	0.1984	0.046*
C12	0.44237 (8)	0.52015 (10)	0.26214 (14)	0.0434 (5)
H12A	0.4051	0.5400	0.2642	0.052*
H12B	0.4354	0.4801	0.2416	0.052*
C13	0.61453 (7)	0.43071 (7)	0.14019 (13)	0.0311 (4)
C14	0.65930 (8)	0.41819 (8)	0.20947 (14)	0.0363 (4)
H14	0.6903	0.4440	0.2172	0.044*

C15	0.65774 (9)	0.36692 (9)	0.26745 (15)	0.0445 (5)
H15	0.6876	0.3577	0.3140	0.053*
C16	0.61141 (10)	0.33061 (9)	0.25439 (18)	0.0522 (6)
C17	0.56688 (10)	0.34217 (10)	0.1861 (2)	0.0601 (6)
H17	0.5358	0.3164	0.1796	0.072*
C18	0.56866 (9)	0.39266 (9)	0.12670 (17)	0.0449 (5)
H18	0.5394	0.4008	0.0784	0.054*
F1	0.60879 (7)	0.28091 (7)	0.31230 (15)	0.0853 (5)
N1	0.61561 (6)	0.48459 (6)	0.08071 (10)	0.0288 (3)
N2	0.56556 (6)	0.57138 (6)	0.03353 (11)	0.0338 (3)
N3	0.53697 (6)	0.51878 (6)	0.18116 (11)	0.0309 (3)
O1	0.69568 (6)	0.45289 (6)	−0.00868 (12)	0.0501 (4)
O2	0.46772 (6)	0.52110 (7)	0.36408 (10)	0.0459 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0392 (10)	0.0398 (10)	0.0414 (10)	0.0016 (8)	−0.0009 (8)	0.0097 (8)
C2	0.0477 (11)	0.0422 (11)	0.0390 (10)	−0.0081 (9)	−0.0020 (8)	0.0140 (8)
C3	0.0434 (11)	0.0512 (12)	0.0334 (9)	−0.0132 (9)	0.0089 (8)	0.0047 (8)
C4	0.0345 (9)	0.0406 (10)	0.0374 (10)	−0.0032 (8)	0.0064 (7)	−0.0011 (8)
C5	0.0290 (8)	0.0332 (9)	0.0292 (8)	−0.0039 (7)	0.0013 (6)	−0.0014 (7)
C6	0.0326 (9)	0.0315 (9)	0.0288 (8)	−0.0027 (7)	−0.0014 (7)	0.0021 (7)
C7	0.0278 (8)	0.0340 (9)	0.0340 (9)	0.0004 (7)	0.0030 (7)	−0.0003 (7)
C8	0.0251 (8)	0.0326 (8)	0.0266 (8)	−0.0002 (6)	−0.0007 (6)	−0.0003 (6)
C9	0.0293 (9)	0.0485 (11)	0.0291 (9)	0.0012 (8)	0.0000 (7)	−0.0041 (8)
C10	0.0418 (11)	0.0580 (12)	0.0289 (9)	0.0035 (9)	0.0033 (8)	0.0037 (8)
C11	0.0318 (9)	0.0481 (11)	0.0351 (9)	0.0099 (8)	0.0036 (7)	0.0015 (8)
C12	0.0317 (9)	0.0631 (13)	0.0354 (10)	0.0017 (9)	0.0043 (7)	−0.0038 (9)
C13	0.0328 (9)	0.0308 (9)	0.0298 (8)	0.0035 (7)	0.0020 (7)	0.0045 (7)
C14	0.0363 (9)	0.0380 (10)	0.0346 (9)	0.0050 (8)	−0.0031 (7)	0.0001 (7)
C15	0.0479 (11)	0.0508 (12)	0.0347 (10)	0.0151 (9)	−0.0043 (8)	0.0071 (8)
C16	0.0576 (13)	0.0409 (11)	0.0581 (13)	0.0072 (10)	0.0063 (11)	0.0215 (10)
C17	0.0500 (13)	0.0445 (12)	0.0859 (17)	−0.0114 (10)	−0.0091 (12)	0.0211 (12)
C18	0.0391 (10)	0.0405 (11)	0.0552 (12)	−0.0031 (8)	−0.0098 (9)	0.0106 (9)
F1	0.0905 (11)	0.0613 (9)	0.1042 (13)	0.0037 (8)	0.0010 (9)	0.0498 (9)
N1	0.0270 (7)	0.0314 (7)	0.0282 (7)	0.0016 (6)	0.0006 (5)	0.0029 (6)
N2	0.0335 (8)	0.0345 (8)	0.0333 (8)	0.0040 (6)	0.0053 (6)	0.0041 (6)
N3	0.0268 (7)	0.0390 (8)	0.0270 (7)	0.0042 (6)	0.0028 (5)	0.0029 (6)
O1	0.0454 (8)	0.0460 (8)	0.0591 (9)	0.0174 (6)	0.0204 (7)	0.0123 (7)
O2	0.0357 (7)	0.0717 (10)	0.0304 (7)	0.0037 (7)	0.0073 (5)	−0.0033 (6)

Geometric parameters (Å, °)

C1—C2	1.376 (3)	C10—H10A	0.9700
C1—C6	1.404 (2)	C10—H10B	0.9700
C1—H1	0.9300	C11—N3	1.464 (2)
C2—C3	1.388 (3)	C11—C12	1.510 (3)
C2—H2	0.9300	C11—H11A	0.9700

C3—C4	1.369 (3)	C11—H11B	0.9700
C3—H3	0.9300	C12—O2	1.423 (2)
C4—C5	1.404 (2)	C12—H12A	0.9700
C4—H4	0.9300	C12—H12B	0.9700
C5—C6	1.396 (2)	C13—C18	1.379 (3)
C5—C7	1.452 (2)	C13—C14	1.384 (2)
C6—N2	1.388 (2)	C13—N1	1.450 (2)
C7—O1	1.218 (2)	C14—C15	1.390 (3)
C7—N1	1.404 (2)	C14—H14	0.9300
C8—N2	1.289 (2)	C15—C16	1.361 (3)
C8—N3	1.386 (2)	C15—H15	0.9300
C8—N1	1.401 (2)	C16—F1	1.360 (2)
C9—N3	1.471 (2)	C16—C17	1.368 (3)
C9—C10	1.503 (3)	C17—C18	1.384 (3)
C9—H9A	0.9700	C17—H17	0.9300
C9—H9B	0.9700	C18—H18	0.9300
C10—O2	1.422 (2)		
C2—C1—C6	120.34 (18)	N3—C11—H11A	110.1
C2—C1—H1	119.8	C12—C11—H11A	110.1
C6—C1—H1	119.8	N3—C11—H11B	110.1
C1—C2—C3	120.66 (17)	C12—C11—H11B	110.1
C1—C2—H2	119.7	H11A—C11—H11B	108.5
C3—C2—H2	119.7	O2—C12—C11	112.17 (16)
C4—C3—C2	119.97 (17)	O2—C12—H12A	109.2
C4—C3—H3	120.0	C11—C12—H12A	109.2
C2—C3—H3	120.0	O2—C12—H12B	109.2
C3—C4—C5	120.24 (17)	C11—C12—H12B	109.2
C3—C4—H4	119.9	H12A—C12—H12B	107.9
C5—C4—H4	119.9	C18—C13—C14	120.98 (16)
C6—C5—C4	120.09 (16)	C18—C13—N1	119.23 (15)
C6—C5—C7	119.49 (15)	C14—C13—N1	119.79 (15)
C4—C5—C7	120.35 (16)	C13—C14—C15	119.68 (18)
N2—C6—C5	122.43 (15)	C13—C14—H14	120.2
N2—C6—C1	118.84 (16)	C15—C14—H14	120.2
C5—C6—C1	118.68 (16)	C16—C15—C14	118.28 (18)
O1—C7—N1	120.72 (16)	C16—C15—H15	120.9
O1—C7—C5	124.69 (16)	C14—C15—H15	120.9
N1—C7—C5	114.54 (14)	F1—C16—C15	118.8 (2)
N2—C8—N3	121.03 (15)	F1—C16—C17	118.3 (2)
N2—C8—N1	124.13 (14)	C15—C16—C17	122.85 (18)
N3—C8—N1	114.77 (14)	C16—C17—C18	119.2 (2)
N3—C9—C10	108.30 (14)	C16—C17—H17	120.4
N3—C9—H9A	110.0	C18—C17—H17	120.4
C10—C9—H9A	110.0	C13—C18—C17	119.01 (19)
N3—C9—H9B	110.0	C13—C18—H18	120.5
C10—C9—H9B	110.0	C17—C18—H18	120.5
H9A—C9—H9B	108.4	C8—N1—C7	121.23 (14)
O2—C10—C9	110.88 (16)	C8—N1—C13	121.31 (13)
O2—C10—H10A	109.5	C7—N1—C13	117.23 (13)

C9—C10—H10A	109.5	C8—N2—C6	117.79 (15)
O2—C10—H10B	109.5	C8—N3—C11	117.28 (14)
C9—C10—H10B	109.5	C8—N3—C9	117.35 (13)
H10A—C10—H10B	108.1	C11—N3—C9	109.72 (13)
N3—C11—C12	107.85 (15)	C10—O2—C12	110.48 (14)
C6—C1—C2—C3	−0.7 (3)	N2—C8—N1—C7	7.1 (2)
C1—C2—C3—C4	−0.6 (3)	N3—C8—N1—C7	−176.00 (14)
C2—C3—C4—C5	1.0 (3)	N2—C8—N1—C13	−167.20 (16)
C3—C4—C5—C6	−0.2 (3)	N3—C8—N1—C13	9.7 (2)
C3—C4—C5—C7	176.81 (17)	O1—C7—N1—C8	177.33 (17)
C4—C5—C6—N2	−178.68 (16)	C5—C7—N1—C8	−5.0 (2)
C7—C5—C6—N2	4.3 (3)	O1—C7—N1—C13	−8.2 (2)
C4—C5—C6—C1	−1.0 (3)	C5—C7—N1—C13	169.47 (14)
C7—C5—C6—C1	−178.05 (16)	C18—C13—N1—C8	64.6 (2)
C2—C1—C6—N2	179.18 (17)	C14—C13—N1—C8	−115.37 (18)
C2—C1—C6—C5	1.4 (3)	C18—C13—N1—C7	−109.90 (19)
C6—C5—C7—O1	177.26 (18)	C14—C13—N1—C7	70.1 (2)
C4—C5—C7—O1	0.3 (3)	N3—C8—N2—C6	−179.62 (15)
C6—C5—C7—N1	−0.3 (2)	N1—C8—N2—C6	−2.9 (2)
C4—C5—C7—N1	−177.26 (15)	C5—C6—N2—C8	−2.8 (2)
N3—C9—C10—O2	−59.7 (2)	C1—C6—N2—C8	179.56 (16)
N3—C11—C12—O2	57.9 (2)	N2—C8—N3—C11	17.8 (2)
C18—C13—C14—C15	−0.9 (3)	N1—C8—N3—C11	−159.21 (15)
N1—C13—C14—C15	179.11 (16)	N2—C8—N3—C9	−116.15 (18)
C13—C14—C15—C16	−0.5 (3)	N1—C8—N3—C9	66.8 (2)
C14—C15—C16—F1	−178.64 (19)	C12—C11—N3—C8	163.67 (15)
C14—C15—C16—C17	0.7 (4)	C12—C11—N3—C9	−59.11 (19)
F1—C16—C17—C18	179.8 (2)	C10—C9—N3—C8	−162.18 (16)
C15—C16—C17—C18	0.4 (4)	C10—C9—N3—C11	60.63 (19)
C14—C13—C18—C17	2.0 (3)	C9—C10—O2—C12	58.3 (2)
N1—C13—C18—C17	−177.98 (19)	C11—C12—O2—C10	−57.8 (2)
C16—C17—C18—C13	−1.8 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O1^{i}	0.93	2.57	3.306 (2)	137
C9—H9A···Cg3^{i}	0.97	2.85	3.673 (2)	143
C11—H11A···Cg2^{ii}	0.97	2.96	3.759 (2)	141
C12—H12A···Cg1^{iii}	0.97	2.72	3.548 (2)	143
C12—H12B···Cg1^{ii}	0.97	2.68	3.492 (2)	141

Symmetry codes: (i) *y*+1/4, −*x*+5/4, *z*+1/4; (ii) −*x*+1, −*y*+1, −*z*; (iii) *y*−1/4, −*x*+5/4, −*z*+1/4.

Fig. 1

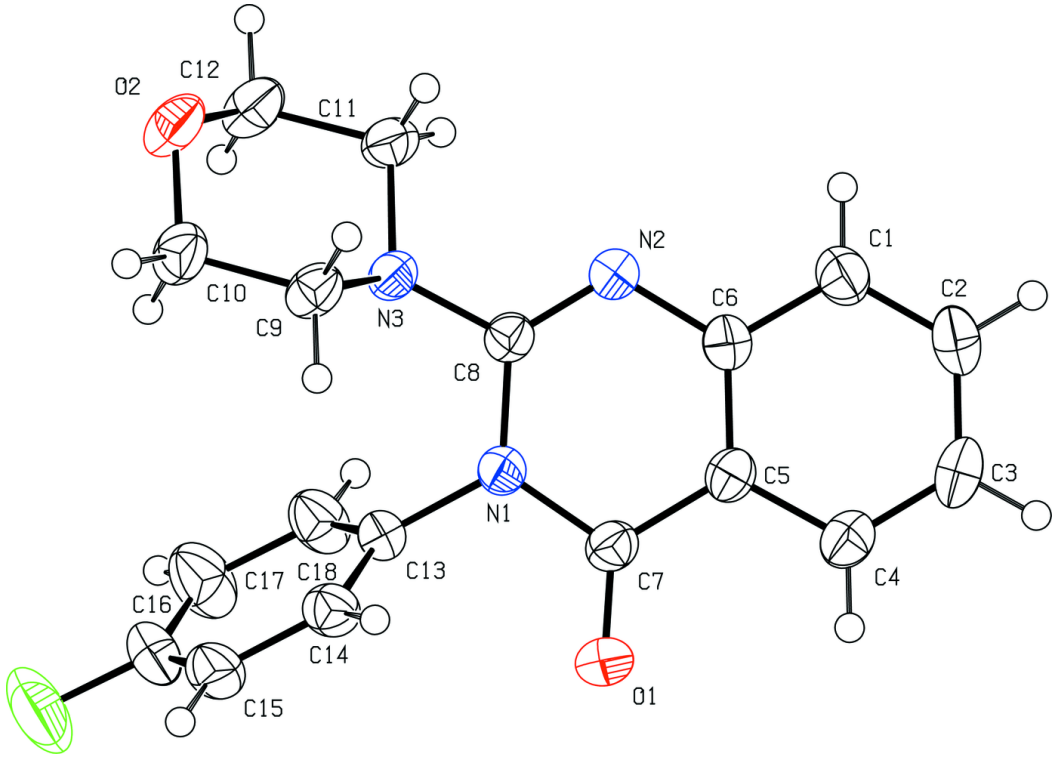
O2
C12
C11
C10
C9
N3
N2
C1
C6
C2
C8
C5
C3
N1
C13
C17
C18
C16
C7
C4
C14
O1
C15

Fig. 2