Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-[(1*E*)-(4-Fluorophenyl)methylene]-6-methoxy-2-naphthohydrazide

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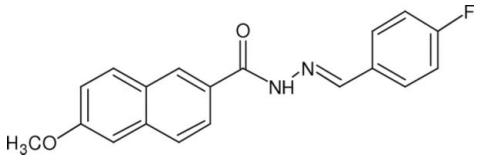
Received 5 April 2007; accepted 12 April 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.007 Å; R factor = 0.063; wR factor = 0.127; data-to-parameter ratio = 7.1.

The title compound, $C_{19}H_{15}FN_2O_2$, is a Schiff base which has been synthesized by a condensation reaction of 6-methoxy-2-naphthohydrazide and 4-fluorobenzaldehyde. The molecule is almost planar with the C=N double bond in a *trans* configuration. The crystal packing is stabilized by N—H···O hydrogen bonds that link molecules into chains running along the *c* axis. There are also weak C—H···O hydrogen bonds as well as C—H···π-ring interactions in the crystal structure.

Related literature

Some related structures of hydrazides such as 2′-(4-dimethylaminobenzylidene)pyrazine-2-carbohydrazide (Shi & Yuan, 2006), *N*′-(3-ethoxy-4-hydroxybenzylidene)isonicotinohydrazide (Qian *et al.*, 2006) and 2′-(1,3-benzodioxol-5-ylmethylene)-2-methoxybenzo-hydrazide (Jing & Yu, 2007) and a Schiff base (Yathirajan *et al.*, 2007) have been reported.



Experimental

Crystal data

$C_{19}H_{15}FN_2O_2$
M_r = 322.33
Monoclinic, *Pc*
a = 15.681 (2) Å
b = 5.6574 (7) Å
c = 9.2758 (10) Å
β = 104.746 (9)°
V = 795.79 (17) Å^3
Z = 2
Mo *K*α radiation
μ = 0.10 mm^{-1}
T = 173 (2) K
0.24 × 0.09 × 0.08 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: none
9090 measured reflections
1531 independent reflections
1246 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.127
S = 1.57
1531 reflections
217 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	2.11	2.778 (4)	132
C23—H23···O2^{ii}	0.95	2.55	3.428 (6)	154
C26—H26···O1^{iii}	0.95	2.50	3.403 (6)	158
C14—H14···*Cg*1^{i}	0.98	2.89	3.666 (5)	140
C19—H19···*Cg*2^{iv}	0.93	2.95	3.697 (5)	136

Symmetry codes: (i) $x, -y+1, z-\frac{1}{2}$; (ii) $x-1, y-1, z$; (iii) $x, -y, z-\frac{1}{2}$; (iv) $x, -y+2, z+\frac{1}{2}$. *Cg*1 and *Cg*2 are the centroids of the rings C11/C12/C13/C18/C19/C20 and C13/C14/C15/C16/C17/C18, respectively

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

BN thanks Mangalore University for research facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FB2048).

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 doi:10.1107/S160053680701820X

supplementary materials

Acta Cryst. (2007). E**63**, o2565 [**doi:10.1107/S160053680701820X**]

N'-[(1*E*)-(4-Fluorophenyl)methylene]-6-methoxy-2-naphthohydrazide

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Comment

The title compound, $C_{19}H_{15}FN_2O_2$, is a Schiff base which has been synthesized by a condensation reaction of 6-methoxy-2-naphthohydrazide and 4-fluorobenzaldehyde.

A view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Crystallographic Database, Version 5.28, November 2006; updated January 2007 (Allen, 2002); Mogul Version 1.1 (Bruno *et al.*, 2004). The molecule is almost planar (r.m.s. deviation for all non-H atoms = 0.123 Å) with the C=N double bond in a trans configuration. The crystal packing is stabilized by N—H···O hydrogen bonds that link molecules into chains running along the c-axis (Tab. 1 and Fig. 2). There are also C—H···O weak hydrogen bonds (Tab. 1) as well as C—H···π-ring interactions in the structure (Tab. 2).

Experimental

A mixture of 6-methoxy-2-naphthohydrazide (1.08 g, 0.005 mol) and 4-fluorobenzaldehyde (0.62 ml, 0.005 mol) in 15 ml of absolute ethanol containing 2 drops of 4 M sulfuric acid was refluxed for about 3 hours. On cooling to room temperature, a solid precipitated. The solid was filtered off, redissolved in 10 ml of a mixture (1:1) of dimethylformamide and acetone, and then recrystallized. (M. p.: 492-494 K). Analysis for $C_{19}H_{15}FN_2O_2$: Found (Calculated): C: 70.68 (70.80); H: 4.63 (4.69); N: 8.62 (8.69) weight %.

Refinement

All the H atoms were found in a difference Fourier map. Nevertheless, the hydrogens were refined using a riding model with N—H = 0.88 Å, C—H = 0.95Å or C_{methyl}—H = 0.96Å and U_{iso}(H) = 1.2U_{eq}(C,*N*) or U_{iso}(H) = 1.5U_{eq}(C_{methyl}). In the absence of anomalous scatterers 1517 Friedel pairs have been merged prior to refinement.

Figures

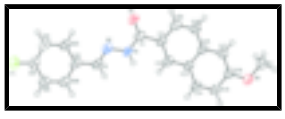

Fig. 1. A view of the title compound with the atom numbering. The displacement ellipsoids are at the 50% probability level.

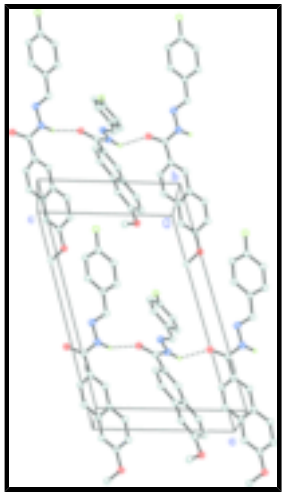

Fig. 2. Packing diagram of the title compound. H atoms bonded to C are not shown. The N—H···O hydrogen bonds are shown as dashed lines.

_N_'-[(1E)-(4-Fluorophenyl)methylene]-6-methoxy-2-naphthohydrazide

Crystal data

$C_{19}H_{15}FN_2O_2$	F_{000} = 336
M_r = 322.33	D_x = 1.345 Mg m^{-3}
Monoclinic, *Pc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P -2yc	Cell parameters from 6963 reflections
a = 15.681 (2) Å	θ = 3.7–25.3º
b = 5.6574 (7) Å	μ = 0.10 mm^{-1}
c = 9.2758 (10) Å	*T* = 173 (2) K
β = 104.746 (9)º	Needle, colourless
V = 795.79 (17) Å^3	0.24 × 0.09 × 0.08 mm
Z = 2	

Data collection

Stoe IPDSII two-circle diffractometer	1246 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.069
Monochromator: graphite	θ_{max} = 25.9º
T = 173(2) K	θ_{min} = 3.6º
ω scans	*h* = −19→19
Absorption correction: none	*k* = −6→6
9090 measured reflections	*l* = −11→11
1531 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained

$R[F^2 > 2\sigma(F^2)] = 0.063$

$wR(F^2) = 0.127$

$S = 1.57$

1531 reflections

217 parameters

2 restraints

60 constraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.0088P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.23$ e Å^{-3}

$\Delta\rho_{min} = -0.25$ e Å^{-3}

Extinction correction: none

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}
F1	0.3049 (2)	−0.5672 (6)	0.2289 (4)	0.0710 (10)
N1	0.6850 (2)	0.3354 (7)	0.3540 (4)	0.0459 (10)
H1	0.7100	0.3124	0.2803	0.055*
N2	0.6140 (2)	0.1982 (8)	0.3648 (4)	0.0454 (10)
O1	0.6834 (2)	0.5483 (7)	0.5623 (3)	0.0560 (10)
O2	1.1811 (2)	0.9463 (7)	0.3792 (4)	0.0596 (10)
C1	0.7163 (3)	0.5057 (9)	0.4572 (4)	0.0451 (12)
C2	0.5913 (3)	0.0397 (9)	0.2636 (5)	0.0443 (11)
H2	0.6241	0.0238	0.1909	0.053*
C3	1.2147 (4)	1.1340 (11)	0.4833 (7)	0.0630 (15)
H3A	1.1768	1.2735	0.4573	0.095*
H3B	1.2748	1.1740	0.4791	0.095*
H3C	1.2152	1.0822	0.5844	0.095*
C11	0.7977 (3)	0.6295 (9)	0.4426 (4)	0.0417 (11)
C12	0.8549 (3)	0.5335 (9)	0.3667 (5)	0.0426 (11)
H12	0.8393	0.3898	0.3136	0.051*
C13	0.9355 (3)	0.6423 (9)	0.3658 (5)	0.0402 (11)
C14	0.9964 (3)	0.5461 (9)	0.2891 (5)	0.0446 (11)
H14	0.9813	0.4052	0.2327	0.054*
C15	1.0744 (3)	0.6503 (9)	0.2950 (5)	0.0478 (12)
H15	1.1129	0.5842	0.2416	0.057*

C16	1.0994 (3)	0.8597 (9)	0.3811 (5)	0.0451 (12)
C17	1.0422 (3)	0.9647 (9)	0.4528 (5)	0.0467 (12)
H17	1.0585	1.1073	0.5068	0.056*
C18	0.9591 (3)	0.8602 (8)	0.4460 (5)	0.0408 (11)
C19	0.8981 (3)	0.9577 (9)	0.5207 (5)	0.0442 (11)
H19	0.9120	1.1021	0.5737	0.053*
C20	0.8208 (3)	0.8489 (9)	0.5175 (5)	0.0454 (12)
H20	0.7811	0.9205	0.5665	0.055*
C21	0.5165 (3)	−0.1173 (8)	0.2571 (4)	0.0415 (11)
C22	0.4518 (3)	−0.0650 (10)	0.3318 (5)	0.0470 (12)
H22	0.4567	0.0750	0.3899	0.056*
C23	0.3808 (3)	−0.2141 (10)	0.3223 (5)	0.0528 (13)
H23	0.3366	−0.1758	0.3719	0.063*
C24	0.3750 (3)	−0.4206 (10)	0.2395 (6)	0.0517 (13)
C25	0.4372 (3)	−0.4777 (10)	0.1636 (5)	0.0508 (12)
H25	0.4319	−0.6195	0.1071	0.061*
C26	0.5081 (3)	−0.3244 (9)	0.1707 (5)	0.0484 (12)
H26	0.5506	−0.3602	0.1170	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.065 (2)	0.074 (2)	0.079 (2)	−0.0181 (16)	0.0265 (17)	−0.0044 (18)
N1	0.043 (2)	0.071 (3)	0.030 (2)	−0.009 (2)	0.0204 (17)	−0.0011 (18)
N2	0.045 (2)	0.063 (3)	0.0297 (18)	0.0003 (18)	0.0123 (16)	0.0062 (18)
O1	0.060 (2)	0.083 (3)	0.0327 (17)	−0.0114 (18)	0.0258 (15)	−0.0084 (16)
O2	0.048 (2)	0.082 (3)	0.055 (2)	−0.0157 (19)	0.0231 (17)	−0.0125 (19)
C1	0.053 (3)	0.057 (3)	0.028 (2)	0.003 (2)	0.015 (2)	0.004 (2)
C2	0.036 (3)	0.069 (3)	0.031 (2)	0.002 (2)	0.0141 (19)	0.003 (2)
C3	0.058 (3)	0.074 (4)	0.059 (3)	−0.017 (3)	0.018 (3)	−0.013 (3)
C11	0.041 (3)	0.057 (3)	0.030 (2)	0.002 (2)	0.0143 (19)	0.004 (2)
C12	0.045 (3)	0.060 (3)	0.025 (2)	0.000 (2)	0.0127 (19)	0.004 (2)
C13	0.039 (3)	0.055 (3)	0.028 (2)	0.001 (2)	0.0111 (18)	0.002 (2)
C14	0.042 (3)	0.061 (3)	0.035 (2)	0.000 (2)	0.017 (2)	−0.004 (2)
C15	0.044 (3)	0.066 (3)	0.037 (3)	0.005 (3)	0.017 (2)	0.000 (2)
C16	0.043 (3)	0.061 (3)	0.033 (2)	−0.002 (2)	0.012 (2)	0.004 (2)
C17	0.056 (3)	0.050 (3)	0.036 (2)	−0.006 (2)	0.014 (2)	−0.005 (2)
C18	0.042 (3)	0.051 (3)	0.033 (2)	−0.002 (2)	0.0151 (19)	0.005 (2)
C19	0.051 (3)	0.052 (3)	0.033 (2)	0.000 (2)	0.018 (2)	−0.001 (2)
C20	0.049 (3)	0.060 (3)	0.030 (2)	0.007 (2)	0.015 (2)	0.007 (2)
C21	0.035 (2)	0.064 (3)	0.026 (2)	0.008 (2)	0.0078 (18)	0.006 (2)
C22	0.044 (3)	0.066 (3)	0.033 (2)	0.002 (2)	0.015 (2)	−0.001 (2)
C23	0.039 (3)	0.073 (4)	0.051 (3)	0.007 (2)	0.022 (2)	0.011 (3)
C24	0.038 (3)	0.068 (4)	0.049 (3)	−0.003 (3)	0.011 (2)	0.009 (3)
C25	0.051 (3)	0.059 (3)	0.042 (3)	0.002 (2)	0.011 (2)	0.000 (2)
C26	0.044 (3)	0.064 (3)	0.038 (2)	0.009 (2)	0.014 (2)	0.006 (2)

Geometric parameters (Å, °)

F1—C24	1.360 (6)	C14—H14	0.9500
N1—C1	1.359 (6)	C15—C16	1.427 (7)
N1—N2	1.381 (5)	C15—H15	0.9500
N1—H1	0.8800	C16—C17	1.379 (7)
N2—C2	1.281 (6)	C17—C18	1.417 (7)
O1—C1	1.238 (5)	C17—H17	0.9500
O2—C16	1.377 (6)	C18—C19	1.428 (6)
O2—C3	1.442 (7)	C19—C20	1.353 (7)
C1—C11	1.492 (7)	C19—H19	0.9500
C2—C21	1.460 (7)	C20—H20	0.9500
C2—H2	0.9500	C21—C22	1.399 (6)
C3—H3A	0.9800	C21—C26	1.407 (7)
C3—H3B	0.9800	C22—C23	1.381 (8)
C3—H3C	0.9800	C22—H22	0.9500
C11—C12	1.384 (6)	C23—C24	1.389 (7)
C11—C20	1.424 (7)	C23—H23	0.9500
C12—C13	1.408 (7)	C24—C25	1.378 (7)
C12—H12	0.9500	C25—C26	1.399 (8)
C13—C14	1.436 (6)	C25—H25	0.9500
C13—C18	1.439 (6)	C26—H26	0.9500
C14—C15	1.346 (7)		
C1—N1—N2	120.1 (3)	O2—C16—C15	114.3 (4)
C1—N1—H1	120.0	C17—C16—C15	120.5 (4)
N2—N1—H1	120.0	C16—C17—C18	120.1 (5)
C2—N2—N1	114.8 (4)	C16—C17—H17	119.9
C16—O2—C3	115.8 (4)	C18—C17—H17	119.9
O1—C1—N1	123.0 (4)	C17—C18—C19	122.6 (5)
O1—C1—C11	121.2 (4)	C17—C18—C13	119.6 (4)
N1—C1—C11	115.7 (4)	C19—C18—C13	117.7 (4)
N2—C2—C21	121.7 (4)	C20—C19—C18	121.4 (5)
N2—C2—H2	119.1	C20—C19—H19	119.3
C21—C2—H2	119.1	C18—C19—H19	119.3
O2—C3—H3A	109.5	C19—C20—C11	121.5 (4)
O2—C3—H3B	109.5	C19—C20—H20	119.3
H3A—C3—H3B	109.5	C11—C20—H20	119.3
O2—C3—H3C	109.5	C22—C21—C26	118.9 (4)
H3A—C3—H3C	109.5	C22—C21—C2	121.9 (4)
H3B—C3—H3C	109.5	C26—C21—C2	119.2 (4)
C12—C11—C20	118.2 (4)	C23—C22—C21	120.9 (5)
C12—C11—C1	122.8 (5)	C23—C22—H22	119.5
C20—C11—C1	118.8 (4)	C21—C22—H22	119.5
C11—C12—C13	122.0 (5)	C22—C23—C24	119.2 (4)
C11—C12—H12	119.0	C22—C23—H23	120.4
C13—C12—H12	119.0	C24—C23—H23	120.4
C12—C13—C14	123.3 (5)	F1—C24—C25	118.9 (5)
C12—C13—C18	119.0 (4)	F1—C24—C23	119.4 (4)

C14—C13—C18	117.7 (4)	C25—C24—C23	121.6 (5)
C15—C14—C13	121.8 (5)	C24—C25—C26	119.2 (5)
C15—C14—H14	119.1	C24—C25—H25	120.4
C13—C14—H14	119.1	C26—C25—H25	120.4
C14—C15—C16	120.2 (4)	C25—C26—C21	120.1 (4)
C14—C15—H15	119.9	C25—C26—H26	120.0
C16—C15—H15	119.9	C21—C26—H26	120.0
O2—C16—C17	125.1 (5)		
C1—N1—N2—C2	−178.4 (4)	C16—C17—C18—C13	0.9 (7)
N2—N1—C1—O1	−0.9 (7)	C12—C13—C18—C17	176.5 (5)
N2—N1—C1—C11	175.0 (4)	C14—C13—C18—C17	−3.1 (6)
N1—N2—C2—C21	−178.8 (4)	C12—C13—C18—C19	−1.2 (5)
O1—C1—C11—C12	154.8 (5)	C14—C13—C18—C19	179.2 (5)
N1—C1—C11—C12	−21.2 (7)	C17—C18—C19—C20	−177.1 (4)
O1—C1—C11—C20	−21.0 (7)	C13—C18—C19—C20	0.5 (6)
N1—C1—C11—C20	162.9 (4)	C18—C19—C20—C11	1.5 (7)
C20—C11—C12—C13	2.0 (6)	C12—C11—C20—C19	−2.7 (6)
C1—C11—C12—C13	−173.9 (4)	C1—C11—C20—C19	173.4 (4)
C11—C12—C13—C14	179.5 (4)	N2—C2—C21—C22	17.9 (7)
C11—C12—C13—C18	−0.1 (6)	N2—C2—C21—C26	−163.6 (4)
C12—C13—C14—C15	−177.5 (4)	C26—C21—C22—C23	0.5 (6)
C18—C13—C14—C15	2.1 (7)	C2—C21—C22—C23	179.0 (4)
C13—C14—C15—C16	1.2 (7)	C21—C22—C23—C24	1.2 (7)
C3—O2—C16—C17	12.4 (8)	C22—C23—C24—F1	−179.5 (4)
C3—O2—C16—C15	−170.3 (4)	C22—C23—C24—C25	−1.6 (7)
C14—C15—C16—O2	179.2 (4)	F1—C24—C25—C26	178.2 (4)
C14—C15—C16—C17	−3.5 (7)	C23—C24—C25—C26	0.3 (7)
O2—C16—C17—C18	179.4 (4)	C24—C25—C26—C21	1.4 (7)
C15—C16—C17—C18	2.4 (7)	C22—C21—C26—C25	−1.8 (6)
C16—C17—C18—C19	178.5 (4)	C2—C21—C26—C25	179.7 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	2.11	2.778 (4)	132
C23—H23···O2^{ii}	0.95	2.55	3.428 (6)	154
C26—H26···O1^{iii}	0.95	2.50	3.403 (6)	158
C14—H14···Cg1^{i}	0.98	2.89	3.666 (5)	140
C19—H19···Cg2^{iv}	0.93	2.95	3.697 (5)	136

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

Fig. 1

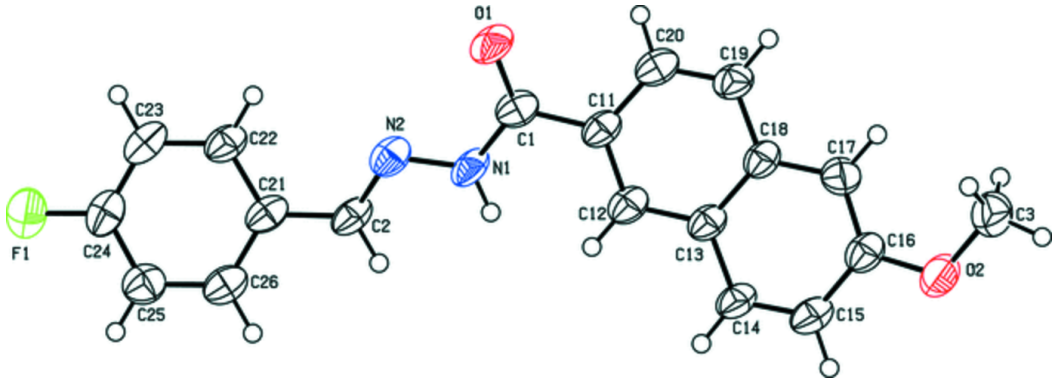
O1
C20
C19
C23
C22
N2
C1
C11
C18
C17
C21
N1
C12
C3
C2
C13
C16
F1
C24
O2
C26
C25
C14
C15

Fig. 2