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3-(4-Bromophenyl)-5-(4-fluorophenyl)-1-phenyl-4,5-dihydro-1*H*-pyrazole

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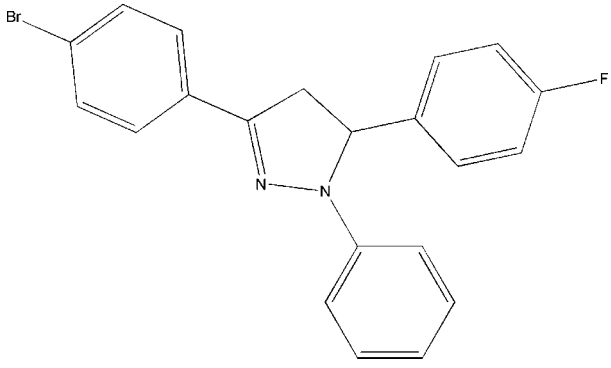
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.043; wR factor = 0.107; data-to-parameter ratio = 13.7.

In the title compound, $C_{21}H_{16}BrFN_2$, the pyrazoline ring forms dihedral angles of 8.1 (2), 14.2 (2) and 71.4 (2)° with the phenyl, 4-bromophenyl and 4-fluorophenyl substituents, respectively.

Related literature

For information on arylpyrazolines, see: Manna *et al.* (2002); Wiley *et al.* (1958). For the crystal structure of a similar triarylpyrazoline derivative, see: Guo *et al.* (2006).



Experimental

Crystal data

$C_{21}H_{16}BrFN_2$
M_r = 395.27
Monoclinic, $P2_1/c$
a = 15.271 (3) Å
b = 11.245 (2) Å
c = 10.727 (2) Å
β = 108.321 (3)°
V = 1748.8 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.37 mm^{-1}
T = 298 (2) K
0.35 × 0.31 × 0.09 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.492, T_{max} = 0.815
7203 measured reflections
3096 independent reflections
1957 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.107
S = 1.01
3096 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2085).

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supplementary materials

Acta Cryst. (2007). E**63**, o3499 [**doi:10.1107/S1600536807033120**]

3-(4-Bromophenyl)-5-(4-fluorophenyl)-1-phenyl-4,5-dihydro-1*H*-pyrazole

H. Li

Comment

Pyrazolines are important five-membered heterocyclic compounds. 1-Acetyl-3,5-diaryl-2-pyrazolines have been found to inhibit the monoamine oxidases (Manna *et al.*, 2002). 1,3,5-Triaryl-2-pyrazolines were also used as scintillation solutes (Wiley *et al.*,1958). Here we report the crystal strucutre of the title triaryl-2-pyrazoline. The title molecule is shown in Fig. 1; all bond lengths and bond angles are normal (Guo *et al.*, 2006). The mean plane of pyrazoline ring N1/N2/C7—C9 is inclined to the best planes of the phenyl, 4-bromophenyl and 4-fluorophenyl substituents by 14.2 (2), 8.1 (2) and 71.4 (2)°, respectively.

Experimental

1-(4-Bromophenyl)-3-(4-fluorophenyl)-2-propenyl-1-ketone (0.02 mol) and phenylhydrazine (0.02 mol) were added to 99.5% acetic acid (40 ml) and stirred with refluxing for 6 h. The mixture was poured into ice-water to afford yellow solid. The solid was filtrated and washed with water until pH of the solution was about 7.0. Finally, the yellow solid was dried at room temperature. Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H distances of 0.93–0.96 Å and U_{iso}=1.2–1.5U_{eq} of the parent atoms.

Figures

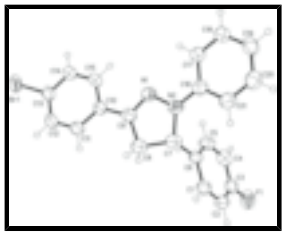


Fig. 1. The molecular structure with displacement ellipsoids drawn at the 30% probability level.

3-(4-Bromophenyl)-5-(4-fluorophenyl)-1-phenyl-4,5-dihydro-1*H*-pyrazole

Crystal data

$C_{21}H_{16}BrFN_2$	F_{000} = 800
M_r = 395.27	D_x = 1.501 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation

	λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1936 reflections
a = 15.271 (3) Å	θ = 2.3–20.6º
b = 11.245 (2) Å	μ = 2.37 mm^{-1}
c = 10.727 (2) Å	T = 298 (2) K
β = 108.321 (3)º	Plate, yellow
V = 1748.8 (6) $Å^3$	0.35 × 0.31 × 0.09 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	3096 independent reflections
Radiation source: fine-focus sealed tube	1957 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
T = 298(2) K	θ_{max} = 25.0º
π and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -17 \rightarrow 18$
T_{min} = 0.492, T_{max} = 0.815	$k = -13 \rightarrow 11$
7203 measured reflections	$l = -12 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H-atom parameters constrained
$wR(F^2)$ = 0.107	$w = 1/[\sigma^2(F_o^2) + (0.0175P)^2 + 1.2354P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
3096 reflections	$\Delta\rho_{max}$ = 0.50 e $Å^{-3}$
226 parameters	$\Delta\rho_{min}$ = −0.63 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.7173 (3)	0.3506 (4)	0.5661 (4)	0.0687 (10)
H1	0.7611	0.3543	0.6489	0.082*
C2	0.6527 (3)	0.4398 (4)	0.5276 (4)	0.0749 (11)
H2	0.6525	0.5035	0.5828	0.090*
C3	0.5896 (3)	0.4319 (4)	0.4071 (5)	0.0738 (11)
C4	0.5879 (3)	0.3412 (4)	0.3239 (4)	0.0792 (12)
H4	0.5437	0.3386	0.2413	0.095*
C5	0.6531 (3)	0.2524 (4)	0.3638 (4)	0.0740 (11)
H5	0.6524	0.1891	0.3078	0.089*
C6	0.7190 (2)	0.2564 (3)	0.4854 (3)	0.0598 (9)
C7	0.7940 (3)	0.1637 (3)	0.5307 (4)	0.0715 (10)
H7	0.8071	0.1486	0.6247	0.086*
C8	0.8841 (3)	0.1979 (4)	0.5025 (4)	0.0820 (12)
H8A	0.8796	0.2763	0.4635	0.098*
H8B	0.9366	0.1959	0.5821	0.098*
C9	0.8916 (3)	0.1039 (3)	0.4082 (3)	0.0633 (9)
C10	0.9613 (2)	0.0970 (3)	0.3421 (4)	0.0611 (9)
C11	1.0370 (3)	0.1734 (3)	0.3722 (4)	0.0723 (11)
H11	1.0435	0.2310	0.4367	0.087*
C12	1.1024 (3)	0.1657 (4)	0.3085 (4)	0.0762 (12)
H12	1.1523	0.2176	0.3298	0.091*
C13	1.0933 (2)	0.0813 (4)	0.2141 (4)	0.0723 (11)
C14	1.0200 (3)	0.0046 (4)	0.1822 (4)	0.0785 (11)
H14	1.0143	−0.0530	0.1178	0.094*
C15	0.9549 (3)	0.0129 (4)	0.2456 (4)	0.0753 (11)
H15	0.9051	−0.0393	0.2231	0.090*
C16	0.7075 (3)	−0.0327 (3)	0.4722 (4)	0.0658 (10)
C17	0.6978 (3)	−0.1413 (4)	0.4081 (4)	0.0710 (10)
H17	0.7320	−0.1576	0.3521	0.085*
C18	0.6379 (3)	−0.2246 (4)	0.4273 (4)	0.0801 (12)
H18	0.6315	−0.2969	0.3832	0.096*
C19	0.5869 (3)	−0.2037 (4)	0.5102 (4)	0.0831 (12)
H19	0.5475	−0.2617	0.5238	0.100*
C20	0.5951 (3)	−0.0962 (4)	0.5724 (4)	0.0834 (12)
H20	0.5604	−0.0808	0.6279	0.100*
C21	0.6544 (3)	−0.0102 (4)	0.5535 (4)	0.0770 (11)
H21	0.6588	0.0630	0.5954	0.092*
Br1	1.18176 (3)	0.06824 (5)	0.12420 (5)	0.0946 (2)
F1	0.52413 (17)	0.5188 (2)	0.3673 (3)	0.1060 (8)
N1	0.8282 (2)	0.0237 (3)	0.3876 (3)	0.0656 (8)
N2	0.7700 (2)	0.0519 (3)	0.4573 (3)	0.0780 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.077 (3)	0.068 (3)	0.062 (2)	−0.008 (2)	0.0222 (19)	−0.010 (2)
C2	0.085 (3)	0.062 (3)	0.087 (3)	−0.009 (2)	0.040 (3)	−0.015 (2)
C3	0.068 (3)	0.066 (3)	0.096 (3)	−0.001 (2)	0.040 (2)	0.010 (3)
C4	0.080 (3)	0.086 (3)	0.065 (3)	−0.011 (2)	0.015 (2)	0.010 (3)
C5	0.094 (3)	0.067 (3)	0.060 (3)	−0.009 (2)	0.024 (2)	−0.012 (2)
C6	0.073 (2)	0.053 (2)	0.059 (2)	−0.0068 (19)	0.0279 (19)	−0.0023 (19)
C7	0.088 (3)	0.060 (3)	0.068 (2)	−0.004 (2)	0.026 (2)	−0.004 (2)
C8	0.077 (3)	0.073 (3)	0.092 (3)	−0.004 (2)	0.021 (2)	−0.012 (2)
C9	0.066 (2)	0.055 (2)	0.063 (2)	0.0034 (19)	0.0113 (18)	0.0053 (19)
C10	0.053 (2)	0.052 (2)	0.069 (2)	0.0022 (17)	0.0070 (18)	0.0050 (19)
C11	0.061 (2)	0.061 (2)	0.083 (3)	−0.002 (2)	0.005 (2)	−0.004 (2)
C12	0.052 (2)	0.064 (3)	0.101 (3)	−0.0082 (19)	0.008 (2)	0.010 (2)
C13	0.054 (2)	0.066 (3)	0.091 (3)	0.0000 (19)	0.014 (2)	0.012 (2)
C14	0.071 (3)	0.066 (3)	0.103 (3)	−0.011 (2)	0.032 (2)	−0.010 (2)
C15	0.063 (2)	0.067 (3)	0.097 (3)	−0.018 (2)	0.026 (2)	−0.009 (2)
C16	0.067 (2)	0.058 (3)	0.071 (2)	0.0082 (19)	0.021 (2)	0.013 (2)
C17	0.068 (2)	0.061 (3)	0.088 (3)	0.002 (2)	0.029 (2)	−0.003 (2)
C18	0.075 (3)	0.062 (3)	0.106 (3)	−0.005 (2)	0.031 (2)	−0.004 (2)
C19	0.080 (3)	0.080 (3)	0.094 (3)	−0.008 (2)	0.033 (2)	0.012 (3)
C20	0.090 (3)	0.091 (4)	0.076 (3)	0.004 (3)	0.037 (2)	0.011 (3)
C21	0.095 (3)	0.067 (3)	0.075 (3)	0.003 (2)	0.036 (2)	0.001 (2)
Br1	0.0622 (3)	0.1061 (4)	0.1179 (4)	−0.0031 (2)	0.0318 (2)	0.0126 (3)
F1	0.0852 (17)	0.0916 (18)	0.148 (2)	0.0161 (15)	0.0462 (16)	0.0240 (17)
N1	0.072 (2)	0.0533 (19)	0.072 (2)	−0.0006 (16)	0.0236 (16)	0.0048 (16)
N2	0.092 (2)	0.053 (2)	0.102 (2)	−0.0041 (18)	0.050 (2)	−0.0085 (18)

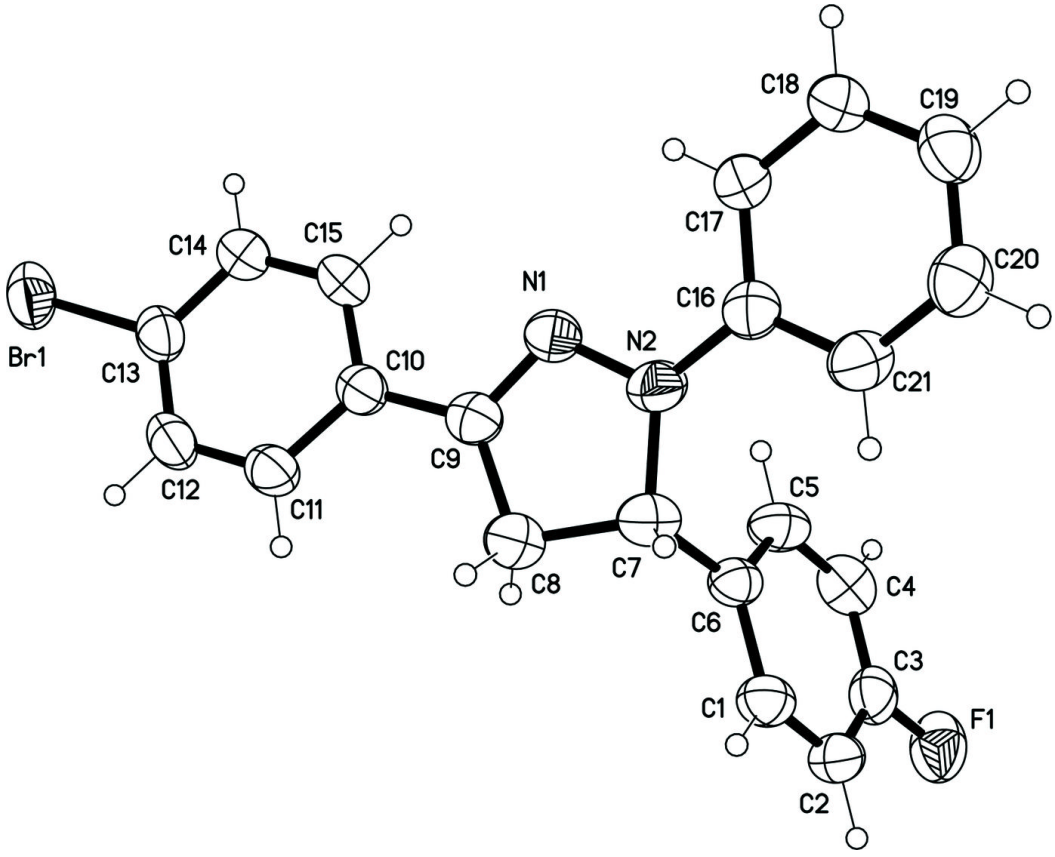
Geometric parameters (Å, °)

C1—C6	1.374 (5)	C11—C12	1.378 (5)
C1—C2	1.376 (5)	C11—H11	0.9300
C1—H1	0.9300	C12—C13	1.363 (5)
C2—C3	1.351 (6)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.369 (5)
C3—C4	1.350 (6)	C13—Br1	1.897 (4)
C3—F1	1.367 (5)	C14—C15	1.374 (5)
C4—C5	1.379 (6)	C14—H14	0.9300
C4—H4	0.9300	C15—H15	0.9300
C5—C6	1.376 (5)	C16—C17	1.386 (5)
C5—H5	0.9300	C16—C21	1.388 (5)
C6—C7	1.511 (5)	C16—N2	1.392 (5)
C7—N2	1.468 (5)	C17—C18	1.370 (5)
C7—C8	1.547 (5)	C17—H17	0.9300
C7—H7	0.9800	C18—C19	1.374 (5)
C8—C9	1.492 (5)	C18—H18	0.9300
C8—H8A	0.9700	C19—C20	1.367 (6)

C8—H8B	0.9700	C19—H19	0.9300
C9—N1	1.290 (4)	C20—C21	1.383 (6)
C9—C10	1.456 (5)	C20—H20	0.9300
C10—C15	1.382 (5)	C21—H21	0.9300
C10—C11	1.394 (5)	N1—N2	1.367 (4)
C6—C1—C2	121.8 (4)	C12—C11—H11	119.2
C6—C1—H1	119.1	C10—C11—H11	119.2
C2—C1—H1	119.1	C13—C12—C11	119.5 (4)
C3—C2—C1	117.9 (4)	C13—C12—H12	120.3
C3—C2—H2	121.0	C11—C12—H12	120.3
C1—C2—H2	121.0	C12—C13—C14	120.6 (4)
C4—C3—C2	122.8 (4)	C12—C13—Br1	120.6 (3)
C4—C3—F1	118.3 (4)	C14—C13—Br1	118.8 (4)
C2—C3—F1	118.9 (4)	C13—C14—C15	119.7 (4)
C3—C4—C5	118.7 (4)	C13—C14—H14	120.2
C3—C4—H4	120.7	C15—C14—H14	120.2
C5—C4—H4	120.7	C14—C15—C10	121.7 (4)
C6—C5—C4	120.9 (4)	C14—C15—H15	119.2
C6—C5—H5	119.6	C10—C15—H15	119.2
C4—C5—H5	119.6	C17—C16—C21	118.7 (4)
C1—C6—C5	118.0 (4)	C17—C16—N2	121.0 (4)
C1—C6—C7	119.4 (3)	C21—C16—N2	120.3 (4)
C5—C6—C7	122.6 (3)	C18—C17—C16	120.0 (4)
N2—C7—C6	112.4 (3)	C18—C17—H17	120.0
N2—C7—C8	101.3 (3)	C16—C17—H17	120.0
C6—C7—C8	113.4 (3)	C17—C18—C19	121.4 (4)
N2—C7—H7	109.8	C17—C18—H18	119.3
C6—C7—H7	109.8	C19—C18—H18	119.3
C8—C7—H7	109.8	C20—C19—C18	118.9 (4)
C9—C8—C7	102.6 (3)	C20—C19—H19	120.5
C9—C8—H8A	111.2	C18—C19—H19	120.5
C7—C8—H8A	111.2	C19—C20—C21	120.7 (4)
C9—C8—H8B	111.2	C19—C20—H20	119.7
C7—C8—H8B	111.2	C21—C20—H20	119.7
H8A—C8—H8B	109.2	C20—C21—C16	120.2 (4)
N1—C9—C10	120.2 (4)	C20—C21—H21	119.9
N1—C9—C8	113.5 (3)	C16—C21—H21	119.9
C10—C9—C8	126.2 (3)	C9—N1—N2	109.0 (3)
C15—C10—C11	117.0 (4)	N1—N2—C16	119.4 (3)
C15—C10—C9	120.7 (3)	N1—N2—C7	113.4 (3)
C11—C10—C9	122.3 (4)	C16—N2—C7	126.1 (3)
C12—C11—C10	121.5 (4)		
C6—C1—C2—C3	0.5 (6)	C11—C12—C13—Br1	179.9 (3)
C1—C2—C3—C4	−0.3 (6)	C12—C13—C14—C15	0.2 (6)
C1—C2—C3—F1	179.3 (3)	Br1—C13—C14—C15	−179.6 (3)
C2—C3—C4—C5	0.4 (6)	C13—C14—C15—C10	−0.3 (6)
F1—C3—C4—C5	−179.3 (3)	C11—C10—C15—C14	0.1 (6)
C3—C4—C5—C6	−0.6 (6)	C9—C10—C15—C14	−179.8 (4)

C2—C1—C6—C5	−0.7 (6)	C21—C16—C17—C18	−1.1 (6)
C2—C1—C6—C7	177.5 (3)	N2—C16—C17—C18	178.1 (4)
C4—C5—C6—C1	0.7 (6)	C16—C17—C18—C19	−0.5 (6)
C4—C5—C6—C7	−177.4 (4)	C17—C18—C19—C20	1.4 (6)
C1—C6—C7—N2	160.8 (3)	C18—C19—C20—C21	−0.7 (6)
C5—C6—C7—N2	−21.1 (5)	C19—C20—C21—C16	−0.8 (6)
C1—C6—C7—C8	−85.0 (4)	C17—C16—C21—C20	1.7 (6)
C5—C6—C7—C8	93.0 (4)	N2—C16—C21—C20	−177.4 (4)
N2—C7—C8—C9	4.5 (4)	C10—C9—N1—N2	−178.1 (3)
C6—C7—C8—C9	−116.2 (3)	C8—C9—N1—N2	1.9 (4)
C7—C8—C9—N1	−4.2 (4)	C9—N1—N2—C16	−167.0 (3)
C7—C8—C9—C10	175.8 (3)	C9—N1—N2—C7	1.5 (4)
N1—C9—C10—C15	7.4 (5)	C17—C16—N2—N1	−5.7 (5)
C8—C9—C10—C15	−172.7 (4)	C21—C16—N2—N1	173.4 (3)
N1—C9—C10—C11	−172.6 (3)	C17—C16—N2—C7	−172.7 (3)
C8—C9—C10—C11	7.4 (6)	C21—C16—N2—C7	6.5 (6)
C15—C10—C11—C12	0.1 (5)	C6—C7—N2—N1	117.4 (3)
C9—C10—C11—C12	−180.0 (3)	C8—C7—N2—N1	−3.9 (4)
C10—C11—C12—C13	−0.2 (6)	C6—C7—N2—C16	−75.0 (5)
C11—C12—C13—C14	0.0 (6)	C8—C7—N2—C16	163.7 (4)

Fig. 1


C18
C19
C17
C20
C14
C15
N1
C16
Br1
C13
C10
N2
C21
C9
C12
C11
C5
C8
C7
C4
C6
C3
C1
F1
C2