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(1*Z*)-1-[(2*E*)-3-(4-Bromophenyl)-1-(4-fluorophenyl)prop-2-en-1-ylidene]-2-(2,4-dinitrophenyl)hydrazine

Rajni Kant,[a]* Vivek K. Gupta,[a] Kamini Kapoor,[a] M. Sapnakumari,[b] B. K. Sarojini[c] and B. Narayana[b]

[a]X-ray Crystallography Laboratory, Post-Graduate Department of Physics & Electronics, University of Jammu, Jammu Tawi 180 006, India, [b]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [c]Department of Chemistry, P.A. College of Engineering, Nadupadavu, Mangalore 574 153, India
Correspondence e-mail: rkvk.paper11@gmail.com

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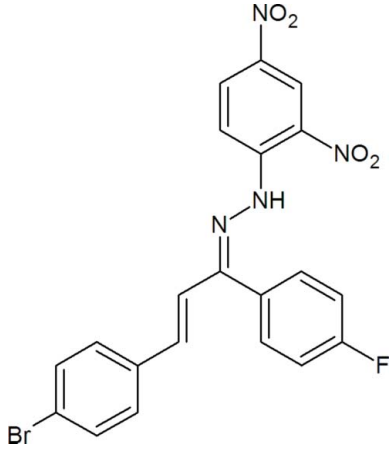
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.051; wR factor = 0.141; data-to-parameter ratio = 14.5.

In the title molecule, $C_{21}H_{14}BrFN_4O_4$, the mean planes of the two nitro groups form dihedral angles of 3.1 (2) and 7.1 (5)° with the benzene ring to which they are attached. The dinitro-substituted ring forms dihedral angles of 8.6 (2) and 71.9 (2)° with the bromo- and fluoro-substituted benzene rings, respectively. The dihedral angle between the bromo- and fluoro-substituted benzene rings is 80.6 (2)°. There is an intramolecular N—H···O hydrogen bond. In the crystal, pairs of weak C—H···O hydrogen bonds form inversion dimers. In addition, π–π stacking interactions between the bromo- and dinitro-substituted rings [centroid–centroid separation = 3.768 (2) Å] are observed.

Related literature

For applications of hydrazone derivatives, see: Rollas *et al.* (2007); Singh *et al.* (1982). For the synthesis, see: Jasinski *et al.* (2010). For a related structure, see: Yin *et al.* (2009).



Experimental

Crystal data

$C_{21}H_{14}BrFN_4O_4$
M_r = 485.27
Monoclinic, $P2_1/c$
a = 15.0738 (12) Å
b = 10.6511 (5) Å
c = 14.3353 (8) Å
β = 116.010 (9)°
V = 2068.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.03 mm^{-1}
T = 293 K
0.3 × 0.2 × 0.1 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.889, T_{max} = 1.000
15619 measured reflections
4058 independent reflections
2232 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.141
S = 1.01
4058 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21···O1	0.86	1.95	2.584 (4)	130
C11—H11···O4^{i}	0.93	2.45	3.316 (7)	154

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5491).

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supplementary materials

Acta Cryst. (2012). E**68**, o2193 [doi:10.1107/S1600536812027328]

(1*Z*)-1-[(2*E*)-3-(4-Bromophenyl)-1-(4-fluorophenyl)prop-2-en-1-ylidene]-2-(2,4-dinitrophenyl)hydrazine

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Comment

Hydrazone derivatives are important biologically active compounds which have received attention from the synthetic community (Rollas *et al.*, 2007). Hydrazone derivatives are also used as analytical reagents (Singh *et al.*, 1982). The crystal structure of 1-(but-2-enylidene)-2-(2-nitrophenyl)hydrazine has been reported (Yin *et al.*, 2009). In order to prepare a pyrazoline derivative, (2E)-3-(4-bromophenyl) -1-(4-fluorophenyl)prop-2-en-1-one was reacted with 2,4-dinitrophenyl hydrazine as for the method of Jasinski *et al.* (2010). But, instead of a pyrazoline derivative a 2,4-dintrophenylhydrazone compound (I) was obtained and its crystal structure is reported herein.

In (I) (Fig. 1), all bond lengths and angles are normal and correspond to those which are related in a reported structure (Yin *et al.*, 2009). The two nitro groups form dihedral angles of 3.1 (2) and 7.1 (5)° with the C16-C21 ring. The dinitro substituted ring (C16-C21) forms dihedral angles of 8.6 (2)° and 71.9 (2) ° with bromo (C1-C6) and fluoro (C10-C15) substituted benzene rings, respectively. The dihedral angle between the bromo and fluoro substituted benzene rings is 80.6 (2)°. There is an intramolecular N—H···O hydrogen bond and in the crystal, pairs of weak C—H···O hydrogen bonds form inversion dimers (Table 1, Fig. 2). In addition, π–π stacking interactions between the bromophenyl ring and dinitro phenyl ring are observed [centroid separation = 3.768 (2) Å, interplanar spacing =3.410 Å, centroid shift = 1.60 Å, Symmetry = x, 1 + y, z].

Experimental

A mixture of (2E)-3-(4-bromophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (3.05 g, 0.01 mol) and 2,4-dinitrophenylhydrazine (1.98 g, 0.01 mol) in 50 ml of glacial acetic acid was refluxed for 6 hrs. The reaction mixture was cooled to produce red crystals (m.p. 414–416 K). X-ray quality crystals were obtained by slow evaporation of an acetic acid solution of (I) at room temperature.

Refinement

All H atoms were positioned geometrically and were treated as riding on their parent C/N atoms, with N—H distance of 0.86 Å and C—H distances of 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C,N).

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

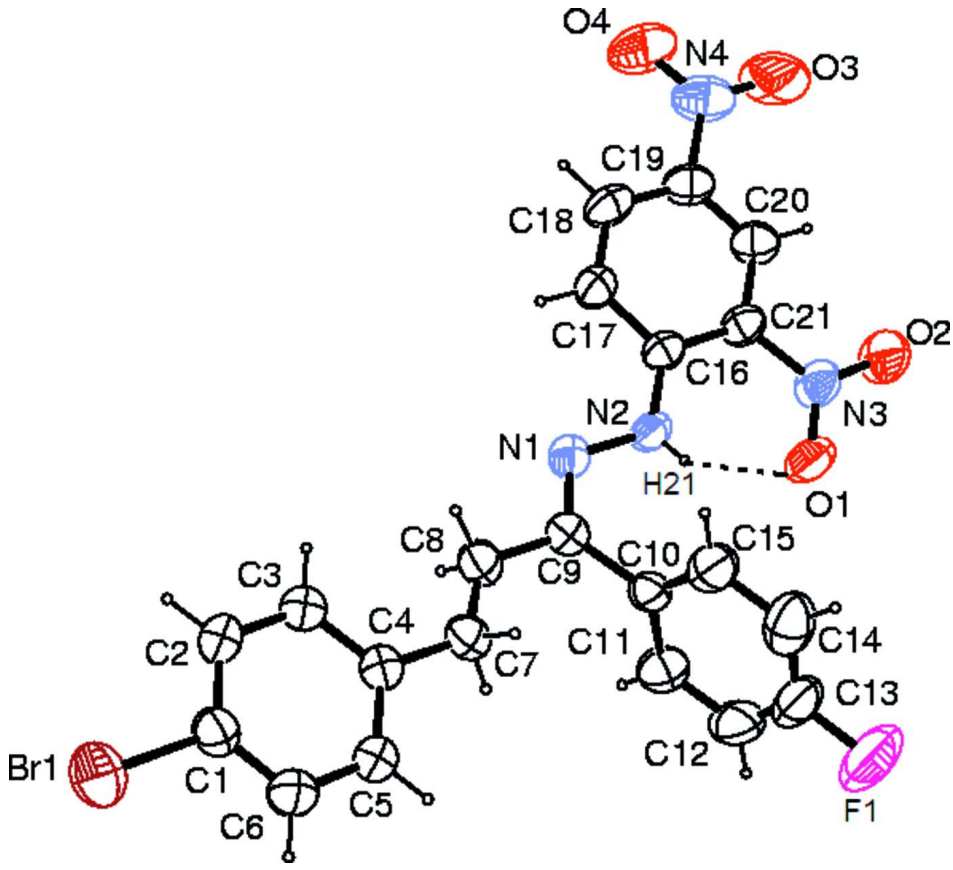

Figure 1

The molecular structure of (I) with ellipsoids drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii. The dashed line indicates a hydrogen bond.

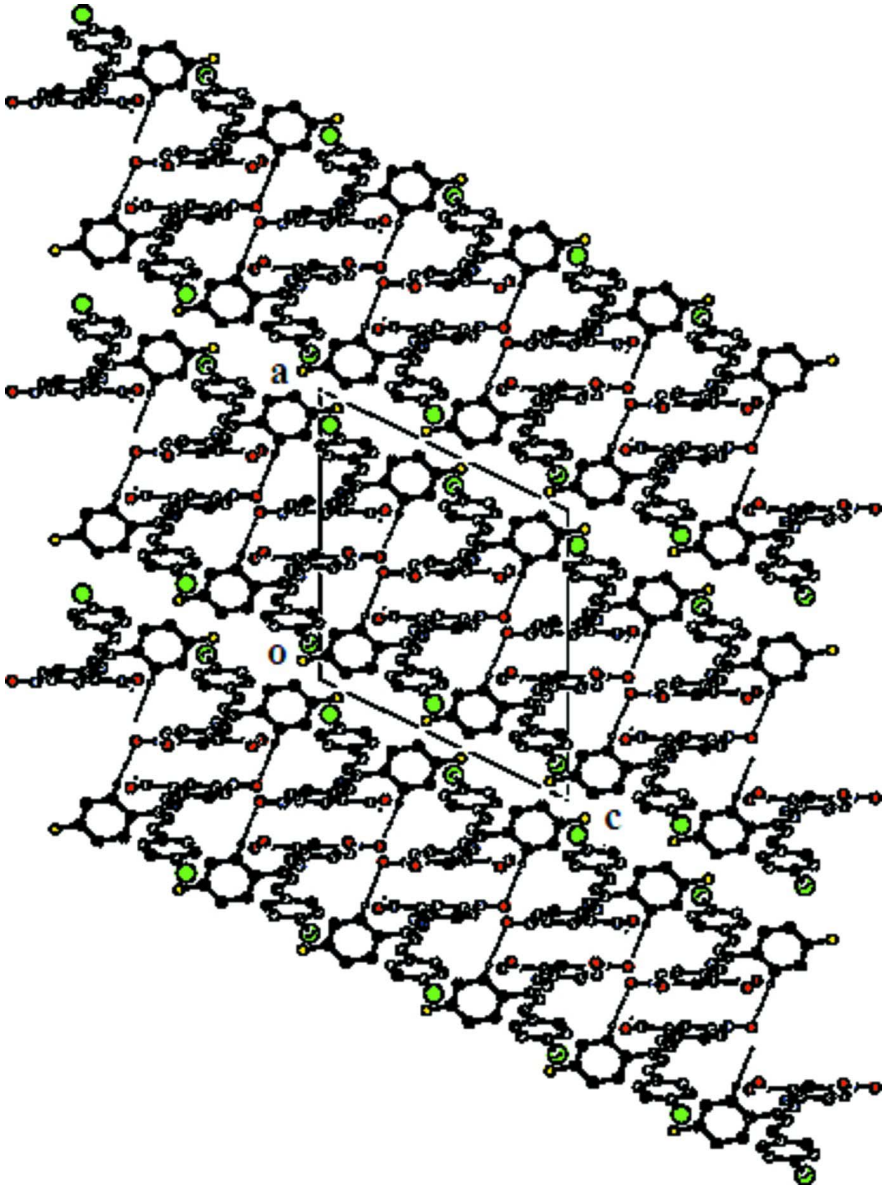

Figure 2

The packing arrangement of molecules viewed along the *b* axis. The broken lines show intermolecular C—H···O interactions.

(1*Z*)-1-[(2*E*)-3-(4-Bromophenyl)-1-(4-fluorophenyl)prop-2-en-1- ylidene]-2-(2,4-dinitrophenyl)hydrazine

Crystal data

$C_{21}H_{14}BrFN_4O_4$
M_r = 485.27
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 15.0738 (12) Å
b = 10.6511 (5) Å
c = 14.3353 (8) Å
β = 116.010 (9)°
V = 2068.5 (2) Å^3
Z = 4
F(000) = 976
D_x = 1.558 Mg m^{-3}
Melting point = 416–414 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3762 reflections
θ = 3.6–29.0°

μ = 2.03 mm^{-1}
T = 293 K

Plate, red
0.3 × 0.2 × 0.1 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.1049 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
T_{min} = 0.889, T_{max} = 1.000

15619 measured reflections
4058 independent reflections
2232 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 26.0°, θ_{min} = 3.6°
h = −18→18
k = −13→13
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.141
S = 1.01
4058 reflections
280 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.8232P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Special details

Experimental. *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27–08-2010 CrysAlis171. NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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 $F^2 > \sigma(F^2)$ 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}
Br1	0.10475 (5)	1.47051 (5)	0.45912 (4)	0.1080 (3)
F1	0.0359 (3)	0.6564 (3)	−0.06938 (19)	0.1523 (14)
N2	0.3279 (2)	0.5513 (3)	0.3799 (2)	0.0541 (7)
H21	0.3030	0.5395	0.3139	0.065*
O1	0.3072 (2)	0.3913 (3)	0.23628 (19)	0.0930 (10)
O2	0.3459 (3)	0.1980 (3)	0.2728 (2)	0.0946 (10)
O3	0.4846 (3)	0.0425 (4)	0.6152 (3)	0.1316 (16)
O4	0.5243 (3)	0.1687 (4)	0.7432 (3)	0.1200 (13)
N3	0.3419 (3)	0.3052 (4)	0.2993 (2)	0.0700 (9)
N1	0.3238 (2)	0.6688 (3)	0.4176 (2)	0.0581 (8)
N4	0.4898 (3)	0.1471 (5)	0.6501 (4)	0.0932 (12)

C1	0.1384 (3)	1.3158 (4)	0.4190 (3)	0.0624 (10)
C2	0.1915 (3)	1.2297 (4)	0.4951 (3)	0.0620 (10)
H2	0.2122	1.2492	0.5648	0.074*
C3	0.2135 (3)	1.1146 (4)	0.4666 (3)	0.0615 (10)
H3	0.2490	1.0559	0.5173	0.074*
C4	0.1829 (3)	1.0855 (3)	0.3623 (3)	0.0574 (9)
C5	0.1301 (3)	1.1750 (4)	0.2885 (3)	0.0655 (10)
H5	0.1090	1.1564	0.2186	0.079*
C6	0.1080 (3)	1.2911 (4)	0.3162 (3)	0.0692 (11)
H6	0.0732	1.3507	0.2660	0.083*
C7	0.2021 (3)	0.9630 (3)	0.3285 (3)	0.0621 (10)
H7	0.1672	0.9451	0.2581	0.074*
C8	0.2633 (3)	0.8747 (3)	0.3863 (3)	0.0613 (10)
H8	0.3046	0.8936	0.4553	0.074*
C9	0.2700 (3)	0.7506 (3)	0.3489 (3)	0.0560 (9)
C10	0.2108 (3)	0.7207 (3)	0.2368 (3)	0.0523 (9)
C11	0.2375 (4)	0.7628 (4)	0.1622 (3)	0.0780 (12)
H11	0.2958	0.8080	0.1816	0.094*
C12	0.1792 (5)	0.7388 (5)	0.0598 (4)	0.0965 (17)
H12	0.1981	0.7659	0.0095	0.116*
C13	0.0950 (5)	0.6765 (5)	0.0324 (3)	0.0895 (16)
C14	0.0659 (3)	0.6315 (5)	0.1030 (4)	0.0905 (14)
H14	0.0074	0.5864	0.0822	0.109*
C15	0.1253 (3)	0.6545 (4)	0.2068 (3)	0.0695 (11)
H15	0.1068	0.6246	0.2566	0.083*
C16	0.3702 (2)	0.4545 (3)	0.4448 (2)	0.0495 (8)
C17	0.4066 (3)	0.4703 (4)	0.5530 (2)	0.0565 (9)
H17	0.4031	0.5488	0.5797	0.068*
C18	0.4465 (3)	0.3722 (4)	0.6188 (3)	0.0643 (11)
H18	0.4705	0.3840	0.6900	0.077*
C19	0.4517 (3)	0.2545 (4)	0.5802 (3)	0.0614 (10)
C20	0.4187 (3)	0.2341 (4)	0.4765 (3)	0.0614 (10)
H20	0.4231	0.1549	0.4516	0.074*
C21	0.3786 (2)	0.3336 (4)	0.4092 (2)	0.0537 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1532 (6)	0.0716 (4)	0.1080 (4)	0.0292 (3)	0.0652 (4)	−0.0073 (3)
F1	0.197 (3)	0.147 (3)	0.0548 (16)	0.047 (3)	0.0025 (18)	−0.0091 (17)
N2	0.0666 (19)	0.0520 (18)	0.0393 (15)	0.0087 (15)	0.0193 (14)	0.0017 (14)
O1	0.145 (3)	0.077 (2)	0.0458 (15)	0.027 (2)	0.0320 (17)	0.0036 (16)
O2	0.142 (3)	0.073 (2)	0.079 (2)	0.022 (2)	0.0581 (19)	−0.0100 (16)
O3	0.181 (4)	0.087 (3)	0.122 (3)	0.061 (3)	0.062 (3)	0.047 (2)
O4	0.114 (3)	0.140 (3)	0.074 (2)	0.031 (2)	0.0118 (19)	0.046 (2)
N3	0.085 (2)	0.072 (2)	0.058 (2)	0.015 (2)	0.0360 (18)	−0.0049 (19)
N1	0.0656 (19)	0.0526 (18)	0.0520 (17)	0.0019 (16)	0.0219 (15)	−0.0028 (16)
N4	0.084 (3)	0.099 (3)	0.086 (3)	0.026 (3)	0.028 (2)	0.040 (3)
C1	0.072 (3)	0.051 (2)	0.068 (2)	0.001 (2)	0.034 (2)	−0.003 (2)
C2	0.073 (3)	0.060 (2)	0.050 (2)	−0.002 (2)	0.025 (2)	−0.0078 (19)

C3	0.070 (3)	0.054 (2)	0.054 (2)	0.002 (2)	0.0223 (19)	0.0022 (19)
C4	0.066 (2)	0.049 (2)	0.054 (2)	−0.0019 (19)	0.0235 (19)	−0.0034 (18)
C5	0.084 (3)	0.055 (2)	0.051 (2)	−0.001 (2)	0.024 (2)	−0.0016 (19)
C6	0.081 (3)	0.062 (3)	0.057 (2)	0.010 (2)	0.023 (2)	0.005 (2)
C7	0.079 (3)	0.051 (2)	0.055 (2)	−0.004 (2)	0.028 (2)	−0.0027 (19)
C8	0.072 (3)	0.050 (2)	0.056 (2)	−0.004 (2)	0.022 (2)	−0.0055 (19)
C9	0.062 (2)	0.051 (2)	0.057 (2)	−0.0016 (19)	0.0279 (19)	0.0011 (19)
C10	0.066 (2)	0.0431 (19)	0.050 (2)	0.0094 (18)	0.0277 (19)	0.0034 (16)
C11	0.102 (3)	0.075 (3)	0.069 (3)	−0.005 (3)	0.049 (3)	0.003 (2)
C12	0.165 (6)	0.078 (3)	0.064 (3)	0.017 (4)	0.066 (4)	0.011 (3)
C13	0.120 (4)	0.080 (3)	0.042 (3)	0.036 (3)	0.011 (3)	−0.003 (2)
C14	0.073 (3)	0.096 (4)	0.081 (3)	0.009 (3)	0.013 (3)	−0.014 (3)
C15	0.072 (3)	0.077 (3)	0.058 (2)	0.003 (2)	0.026 (2)	0.001 (2)
C16	0.045 (2)	0.057 (2)	0.0428 (19)	0.0024 (17)	0.0162 (16)	0.0023 (17)
C17	0.058 (2)	0.061 (2)	0.046 (2)	−0.0004 (19)	0.0180 (18)	−0.0017 (18)
C18	0.051 (2)	0.091 (3)	0.0410 (19)	−0.002 (2)	0.0110 (17)	0.006 (2)
C19	0.050 (2)	0.071 (3)	0.058 (2)	0.013 (2)	0.0180 (19)	0.019 (2)
C20	0.058 (2)	0.061 (2)	0.065 (2)	0.0100 (19)	0.0274 (19)	0.007 (2)
C21	0.054 (2)	0.062 (2)	0.047 (2)	0.0077 (19)	0.0236 (17)	0.0017 (18)

Geometric parameters (Å, º)

Br1—C1	1.886 (4)	C7—H7	0.9300
F1—C13	1.352 (5)	C8—C9	1.447 (5)
N2—C16	1.347 (4)	C8—H8	0.9300
N2—N1	1.376 (4)	C9—C10	1.491 (5)
N2—H21	0.8600	C10—C15	1.363 (5)
O1—N3	1.231 (4)	C10—C11	1.372 (5)
O2—N3	1.213 (4)	C11—C12	1.365 (6)
O3—N4	1.209 (5)	C11—H11	0.9300
O4—N4	1.223 (5)	C12—C13	1.330 (7)
N3—C21	1.455 (4)	C12—H12	0.9300
N1—C9	1.298 (4)	C13—C14	1.356 (7)
N4—C19	1.463 (5)	C14—C15	1.381 (5)
C1—C6	1.363 (5)	C14—H14	0.9300
C1—C2	1.381 (5)	C15—H15	0.9300
C2—C3	1.378 (5)	C16—C21	1.411 (5)
C2—H2	0.9300	C16—C17	1.411 (4)
C3—C4	1.393 (5)	C17—C18	1.359 (5)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.386 (5)	C18—C19	1.386 (5)
C4—C7	1.464 (5)	C18—H18	0.9300
C5—C6	1.384 (5)	C19—C20	1.361 (5)
C5—H5	0.9300	C20—C21	1.381 (5)
C6—H6	0.9300	C20—H20	0.9300
C7—C8	1.324 (5)		

C16—N2—N1	120.9 (3)	C15—C10—C11	118.9 (4)
C16—N2—H21	119.5	C15—C10—C9	119.1 (3)
N1—N2—H21	119.5	C11—C10—C9	121.9 (4)

O2—N3—O1	122.3 (3)	C12—C11—C10	120.4 (5)
O2—N3—C21	119.1 (3)	C12—C11—H11	119.8
O1—N3—C21	118.6 (3)	C10—C11—H11	119.8
C9—N1—N2	115.6 (3)	C13—C12—C11	119.6 (4)
O3—N4—O4	123.0 (4)	C13—C12—H12	120.2
O3—N4—C19	120.1 (4)	C11—C12—H12	120.2
O4—N4—C19	116.9 (5)	C12—C13—F1	119.3 (6)
C6—C1—C2	122.0 (4)	C12—C13—C14	122.3 (4)
C6—C1—Br1	119.4 (3)	F1—C13—C14	118.3 (6)
C2—C1—Br1	118.6 (3)	C13—C14—C15	118.2 (5)
C3—C2—C1	119.2 (3)	C13—C14—H14	120.9
C3—C2—H2	120.4	C15—C14—H14	120.9
C1—C2—H2	120.4	C10—C15—C14	120.6 (4)
C2—C3—C4	120.5 (3)	C10—C15—H15	119.7
C2—C3—H3	119.8	C14—C15—H15	119.7
C4—C3—H3	119.8	N2—C16—C21	122.7 (3)
C5—C4—C3	118.4 (3)	N2—C16—C17	120.4 (3)
C5—C4—C7	119.4 (3)	C21—C16—C17	116.9 (3)
C3—C4—C7	122.2 (3)	C18—C17—C16	120.8 (4)
C6—C5—C4	121.7 (3)	C18—C17—H17	119.6
C6—C5—H5	119.2	C16—C17—H17	119.6
C4—C5—H5	119.2	C17—C18—C19	120.3 (3)
C1—C6—C5	118.3 (4)	C17—C18—H18	119.9
C1—C6—H6	120.9	C19—C18—H18	119.9
C5—C6—H6	120.9	C20—C19—C18	121.5 (3)
C8—C7—C4	127.6 (3)	C20—C19—N4	118.0 (4)
C8—C7—H7	116.2	C18—C19—N4	120.5 (4)
C4—C7—H7	116.2	C19—C20—C21	118.6 (4)
C7—C8—C9	124.0 (3)	C19—C20—H20	120.7
C7—C8—H8	118.0	C21—C20—H20	120.7
C9—C8—H8	118.0	C20—C21—C16	122.0 (3)
N1—C9—C8	116.9 (3)	C20—C21—N3	116.1 (3)
N1—C9—C10	123.7 (3)	C16—C21—N3	121.9 (3)
C8—C9—C10	119.3 (3)		

C16—N2—N1—C9	−171.1 (3)	F1—C13—C14—C15	−178.6 (4)
C6—C1—C2—C3	−0.8 (6)	C11—C10—C15—C14	−0.8 (6)
Br1—C1—C2—C3	177.7 (3)	C9—C10—C15—C14	176.3 (4)
C1—C2—C3—C4	0.3 (6)	C13—C14—C15—C10	0.0 (6)
C2—C3—C4—C5	0.0 (6)	N1—N2—C16—C21	−178.0 (3)
C2—C3—C4—C7	−178.1 (4)	N1—N2—C16—C17	3.5 (5)
C3—C4—C5—C6	0.3 (6)	N2—C16—C17—C18	177.9 (3)
C7—C4—C5—C6	178.4 (4)	C21—C16—C17—C18	−0.7 (5)
C2—C1—C6—C5	1.1 (6)	C16—C17—C18—C19	−0.3 (5)
Br1—C1—C6—C5	−177.4 (3)	C17—C18—C19—C20	1.0 (6)
C4—C5—C6—C1	−0.9 (6)	C17—C18—C19—N4	−176.7 (3)
C5—C4—C7—C8	168.4 (4)	O3—N4—C19—C20	−5.6 (6)
C3—C4—C7—C8	−13.6 (6)	O4—N4—C19—C20	175.9 (4)
C4—C7—C8—C9	172.9 (4)	O3—N4—C19—C18	172.3 (5)

N2—N1—C9—C8	179.3 (3)	O4—N4—C19—C18	−6.3 (6)
N2—N1—C9—C10	3.5 (5)	C18—C19—C20—C21	−0.6 (6)
C7—C8—C9—N1	−171.1 (4)	N4—C19—C20—C21	177.2 (3)
C7—C8—C9—C10	4.9 (6)	C19—C20—C21—C16	−0.5 (5)
N1—C9—C10—C15	75.0 (5)	C19—C20—C21—N3	−178.2 (3)
C8—C9—C10—C15	−100.7 (4)	N2—C16—C21—C20	−177.4 (3)
N1—C9—C10—C11	−108.0 (4)	C17—C16—C21—C20	1.1 (5)
C8—C9—C10—C11	76.3 (5)	N2—C16—C21—N3	0.2 (5)
C15—C10—C11—C12	0.1 (6)	C17—C16—C21—N3	178.7 (3)
C9—C10—C11—C12	−176.9 (4)	O2—N3—C21—C20	1.9 (5)
C10—C11—C12—C13	1.4 (7)	O1—N3—C21—C20	−178.6 (3)
C11—C12—C13—F1	177.9 (4)	O2—N3—C21—C16	−175.8 (4)
C11—C12—C13—C14	−2.3 (8)	O1—N3—C21—C16	3.7 (5)
C12—C13—C14—C15	1.6 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H21···O1	0.86	1.95	2.584 (4)	130
C11—H11···O4^{i}	0.93	2.45	3.316 (7)	154

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