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3-[3-(4-Bromophenyl)-1-phenyl-1*H*-pyrazol-4-yl]-5-ethoxy-2-phenylisoxazolidine

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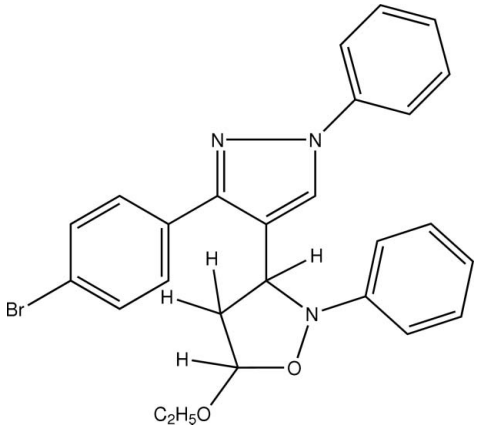
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.096; data-to-parameter ratio = 17.2.

In the title compound, $C_{26}H_{24}BrN_3O_2$, the isoxazolidine ring adopts an envelope conformation, the ring N atom deviating from the mean plane of the other four atoms by an angle of 0.286°. The orientation of the phenyl ring is +*sp* and the bromophenyl ring is +*sc* relative to the attached pyrazole ring; the dihedral angles between the least-squares planes of the pyrazole and the attached phenyl and bromophenyl rings are 21.8 (3) and 41.8 (3)°.

Related literature

For related literature, see: Allen *et al.* (1987); Gayathri *et al.* (2007); Frederickson (1997); Gothelf *et al.* (2002); Huisgen (1984); Kumar *et al.* (2003).



Experimental

Crystal data

$C_{26}H_{24}BrN_3O_2$
M_r = 490.39
Monoclinic, $C2/c$
a = 27.7493 (6) Å
b = 7.4254 (2) Å
c = 24.5230 (5) Å
β = 114.516 (1)°
V = 4597.41 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.82 mm^{-1}
T = 293 (2) K
0.26 × 0.23 × 0.22 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SAINT*; Bruker, 1999)
T_{min} = 0.650, T_{max} = 0.691
23867 measured reflections
4982 independent reflections
3038 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
S = 1.00
4982 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 1999); 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: *SHELXL97* and *PARST97* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2049).

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supplementary materials

Acta Cryst. (2008). E**64**, o342 [**doi:10.1107/S1600536807064938**]

3-[3-(4-Bromophenyl)-1-phenyl-1*H*-pyrazol-4-yl]-5-ethoxy-2-phenylisoxazolidine

S. Etti, K. Karthikeyan, G. Shanmugam and P. T. Perumal

Comment

The 1,3-dipolar cycloadditionof nitrones to alkenes provides a straight forward route to isoxazolidines(Frederickson, 1997, Gothelf *et al.*, 2002). The nitrone cycloadducts are attractive intermediates for the synthesis of several class of natural products and biologically active compounds such as b-aminoacids and alkaloids·(Huisgen, 1984)·The pyrazole unit is the core structure in a number of natural products. Many pyrazole derivatives are known to exhibit a wide range of biological properties such as anti-hyperglycemic, analgesic, anti-inflammatory, anti-pyretic, anti-bacterial, hypoglycemic, sedative, hypnotic activity, and anticoagulant activity. Particularly, arylpyrazoles are widely used in medicinal and pesticidal chemistry. Recently some arylpyrazoles were reported to display non-nucleoside HIV-1 reverse transcriptase inhibitory activity (Kumar *et al.*, 2003).

The isoxazolidine ring adopts envelope conformation with N as the flap, atom N7 deviates from the mean plane with a maximum deviation of 0.286 (2)°. The ethoxy group attached to the isoxazolidine adopts an extended conformation. The bond lengths and bond angles are comparable with literature values (Allen *et al.*,1987)·The dihedral angle between the LSQ planes of pyrazole and phenyl and bromo phenyl ring is 21.8 (3)° and 41.8 (3)°, which is lower than the reported value due to the simple substitution of a bromine to the phenyl ring (Gayathri *et al.*,2007). The phenyl ring is equatorially substituted to the isoxazolidine ring and slightly twisted due to the steric hinderance with the bromophenyl ring and the ethoxy group is substituted axailly to the isoxazolidine ring. The molecule iss stabilized by intra molecular C—H···O hydrogen bonds in the unit cell.

Experimental

A solution of pyrazole nitrone (0.5 mmol) and ethyl vinyl ether (5 mmol) was refluxed in dry toluene (10 mL) at 60°C until the completion of the reaction as evidenced by thin-layer chromatography. The solvent was evaporated under reduced pressure. The crude was purified by column chromatography using ethyl acetate-petroleum ether (3:97) as eluent, to afford the pure isoxazolidine (68%) as a white solid. Single crystals were obtained by crystallization from petroleum ether and ethyl acetate mixture.

Figures

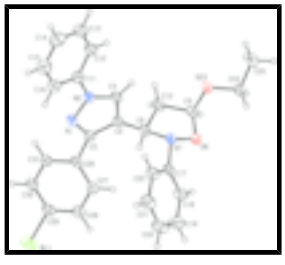

Fig. 1. The *ORTEP* diagram of the title compound with 30% probability displacement ellipsoids.

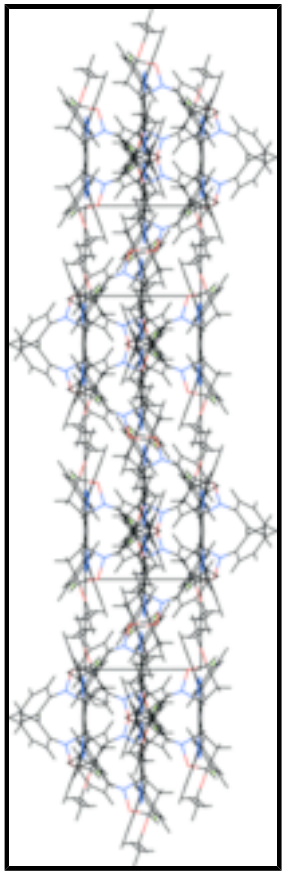

Fig. 2. Packing of the molecules viewed down *c* axis.

3-[3-(4-Bromophenyl)-1-phenyl-1*H*-pyrazol-4-yl]- 5-ethoxy-2-phenylisoxazolidine

Crystal data

$C_{26}H_{24}BrN_3O_2$	F_{000} = 2016
M_r = 490.39	D_x = 1.417 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4982 reflections
a = 27.7493 (6) Å	θ = 2.9–27.0º
b = 7.4254 (2) Å	μ = 1.82 mm^{-1}
c = 24.5230 (5) Å	*T* = 293 (2) K
β = 114.516 (1)º	Cubic, yellow
V = 4597.41 (18) Å^3	0.26 × 0.23 × 0.22 mm
Z = 8	

Data collection

Bruker Kappa APEXII diffractometer	R_{int} = 0.041
Radiation source: fine-focus sealed tube	θ_{max} = 27.0º
Monochromator: graphite	θ_{min} = 2.9º

T = 293(2) K
ω and φ scans
Absorption correction: multi-scan (SAINT; Bruker, 1999)
T_{min} = 0.650, T_{max} = 0.691
23867 measured reflections
4982 independent reflections
3038 reflections with $I > 2\sigma(I)$

$h = -35 \rightarrow 35$
$k = -9 \rightarrow 9$
$l = -31 \rightarrow 31$
Standard reflections: ?;
every ? reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.096$
S = 1.00
4982 reflections
289 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 2.7695P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}
Extinction correction: SHELXL
Extinction coefficient: 0.0028 (11)

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}
Br1	1.015166 (12)	0.61394 (5)	0.097949 (17)	0.09166 (16)
N1	0.76772 (7)	0.4888 (2)	0.08475 (8)	0.0420 (4)
N2	0.72795 (7)	0.4783 (2)	0.10324 (8)	0.0412 (4)
C3	0.74697 (9)	0.4845 (3)	0.16353 (10)	0.0436 (5)
H3	0.7268	0.4794	0.1857	0.052*
C4	0.80068 (9)	0.4996 (3)	0.18641 (9)	0.0388 (5)
C5	0.81190 (9)	0.5021 (3)	0.13506 (9)	0.0381 (5)
C11	0.67491 (9)	0.4517 (3)	0.06083 (10)	0.0419 (5)
C16	0.66488 (10)	0.3876 (3)	0.00433 (11)	0.0531 (6)

H7	0.6926	0.3660	−0.0067	0.064*
C15	0.61347 (11)	0.3559 (3)	−0.03539 (13)	0.0661 (7)
H8	0.6066	0.3131	−0.0736	0.079*
C14	0.57219 (11)	0.3861 (4)	−0.01980 (14)	0.0699 (8)
H9	0.5376	0.3615	−0.0468	0.084*
C13	0.58227 (10)	0.4529 (4)	0.03587 (14)	0.0650 (7)
H10	0.5543	0.4749	0.0465	0.078*
C12	0.63349 (10)	0.4881 (3)	0.07642 (11)	0.0524 (6)
H11	0.6400	0.5359	0.1139	0.063*
C6	0.83710 (9)	0.5082 (3)	0.25106 (9)	0.0400 (5)
H6	0.8732	0.5337	0.2555	0.048*
N7	0.83638 (7)	0.3344 (2)	0.28223 (7)	0.0396 (4)
O8	0.86261 (6)	0.3879 (2)	0.34526 (6)	0.0474 (4)
C9	0.83812 (9)	0.5532 (3)	0.34867 (10)	0.0446 (5)
H9A	0.8637	0.6299	0.3798	0.054*
C10	0.82134 (10)	0.6428 (3)	0.28798 (10)	0.0497 (6)
H10A	0.8396	0.7565	0.2916	0.060*
H10B	0.7834	0.6642	0.2698	0.060*
C17	0.86907 (9)	0.1977 (3)	0.27316 (10)	0.0412 (5)
C22	0.84549 (10)	0.0922 (3)	0.22259 (11)	0.0521 (6)
H18	0.8098	0.1067	0.1976	0.062*
C21	0.87546 (12)	−0.0354 (3)	0.20937 (13)	0.0642 (7)
H19	0.8600	−0.1039	0.1746	0.077*
C20	0.92747 (13)	−0.0614 (4)	0.24692 (15)	0.0718 (8)
H20	0.9473	−0.1480	0.2380	0.086*
C19	0.95026 (11)	0.0402 (4)	0.29764 (14)	0.0718 (8)
H21	0.9856	0.0217	0.3234	0.086*
C18	0.92128 (10)	0.1703 (3)	0.31106 (12)	0.0573 (6)
H22	0.9371	0.2391	0.3457	0.069*
O23	0.79337 (6)	0.5295 (2)	0.35987 (6)	0.0468 (4)
C24	0.80487 (10)	0.4624 (3)	0.41873 (10)	0.0504 (6)
H24A	0.8319	0.5358	0.4486	0.060*
H24B	0.8177	0.3395	0.4226	0.060*
C25	0.75456 (11)	0.4695 (4)	0.42755 (12)	0.0703 (8)
H25A	0.7610	0.4249	0.4667	0.106*
H25B	0.7281	0.3964	0.3977	0.106*
H25C	0.7423	0.5917	0.4238	0.106*
C26	0.86227 (9)	0.5288 (3)	0.12921 (9)	0.0387 (5)
C31	0.86189 (9)	0.6344 (3)	0.08219 (10)	0.0456 (5)
H27	0.8305	0.6888	0.0564	0.055*
C30	0.90731 (10)	0.6599 (3)	0.07315 (11)	0.0522 (6)
H28	0.9065	0.7291	0.0412	0.063*
C29	0.95350 (9)	0.5817 (3)	0.11189 (11)	0.0513 (6)
C28	0.95552 (10)	0.4791 (3)	0.15916 (11)	0.0544 (6)
H30	0.9873	0.4282	0.1854	0.065*
C27	0.90973 (9)	0.4523 (3)	0.16740 (10)	0.0463 (6)
H31	0.9108	0.3815	0.1992	0.056*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0616 (2)	0.1079 (3)	0.1308 (3)	0.00190 (17)	0.0650 (2)	0.0236 (2)
N1	0.0463 (11)	0.0463 (10)	0.0442 (11)	−0.0036 (9)	0.0296 (10)	−0.0001 (8)
N2	0.0440 (11)	0.0436 (10)	0.0436 (11)	−0.0031 (8)	0.0258 (9)	0.0021 (8)
C3	0.0515 (14)	0.0448 (12)	0.0477 (14)	−0.0017 (11)	0.0339 (12)	0.0042 (10)
C4	0.0502 (13)	0.0355 (11)	0.0404 (13)	0.0000 (10)	0.0285 (11)	0.0015 (9)
C5	0.0443 (13)	0.0354 (11)	0.0412 (13)	0.0000 (10)	0.0244 (11)	−0.0008 (9)
C11	0.0444 (13)	0.0365 (11)	0.0470 (14)	−0.0043 (10)	0.0211 (11)	0.0043 (10)
C16	0.0518 (15)	0.0544 (14)	0.0553 (16)	−0.0006 (12)	0.0246 (13)	−0.0019 (12)
C15	0.0646 (18)	0.0661 (17)	0.0582 (17)	−0.0037 (14)	0.0160 (15)	−0.0105 (13)
C14	0.0498 (16)	0.0674 (17)	0.080 (2)	−0.0050 (14)	0.0147 (15)	0.0006 (15)
C13	0.0474 (16)	0.0686 (17)	0.085 (2)	0.0019 (13)	0.0329 (16)	0.0117 (15)
C12	0.0518 (15)	0.0547 (14)	0.0589 (15)	−0.0013 (12)	0.0311 (13)	0.0020 (12)
C6	0.0496 (13)	0.0389 (11)	0.0418 (13)	−0.0025 (10)	0.0291 (11)	−0.0011 (10)
N7	0.0501 (11)	0.0415 (9)	0.0329 (10)	0.0028 (8)	0.0231 (9)	0.0001 (8)
O8	0.0559 (10)	0.0548 (9)	0.0356 (9)	0.0104 (8)	0.0229 (8)	−0.0017 (7)
C9	0.0498 (14)	0.0482 (13)	0.0425 (13)	−0.0005 (11)	0.0258 (11)	−0.0080 (10)
C10	0.0710 (16)	0.0422 (12)	0.0487 (14)	0.0039 (11)	0.0377 (13)	0.0000 (10)
C17	0.0507 (14)	0.0369 (11)	0.0472 (13)	0.0000 (10)	0.0314 (12)	0.0036 (10)
C22	0.0604 (15)	0.0440 (13)	0.0570 (16)	−0.0029 (11)	0.0296 (13)	−0.0065 (11)
C21	0.081 (2)	0.0482 (14)	0.0740 (19)	−0.0064 (14)	0.0422 (17)	−0.0176 (13)
C20	0.080 (2)	0.0531 (16)	0.100 (2)	0.0077 (15)	0.055 (2)	−0.0111 (16)
C19	0.0570 (17)	0.0723 (18)	0.086 (2)	0.0146 (15)	0.0292 (16)	−0.0078 (17)
C18	0.0571 (16)	0.0554 (14)	0.0623 (17)	0.0067 (12)	0.0276 (14)	−0.0070 (12)
O23	0.0522 (10)	0.0572 (9)	0.0387 (9)	0.0068 (8)	0.0266 (8)	0.0029 (7)
C24	0.0676 (16)	0.0511 (13)	0.0409 (13)	0.0092 (12)	0.0310 (12)	0.0044 (11)
C25	0.080 (2)	0.0892 (19)	0.0590 (17)	0.0074 (16)	0.0456 (16)	0.0151 (15)
C26	0.0464 (13)	0.0383 (11)	0.0402 (12)	−0.0014 (10)	0.0268 (11)	−0.0049 (10)
C31	0.0464 (13)	0.0485 (13)	0.0481 (14)	0.0030 (11)	0.0259 (11)	0.0058 (11)
C30	0.0579 (16)	0.0517 (14)	0.0611 (16)	−0.0013 (12)	0.0388 (14)	0.0091 (12)
C29	0.0469 (14)	0.0543 (14)	0.0665 (16)	−0.0033 (12)	0.0372 (13)	−0.0011 (12)
C28	0.0444 (14)	0.0663 (16)	0.0545 (16)	0.0064 (12)	0.0224 (13)	0.0017 (13)
C27	0.0536 (15)	0.0515 (13)	0.0419 (13)	0.0042 (11)	0.0277 (12)	0.0037 (10)

Geometric parameters (Å, °)

Br1—C29	1.894 (2)	C10—H10A	0.9700
N1—C5	1.334 (3)	C10—H10B	0.9700
N1—N2	1.358 (2)	C17—C18	1.374 (3)
N2—C3	1.349 (3)	C17—C22	1.381 (3)
N2—C11	1.420 (3)	C22—C21	1.385 (3)
C3—C4	1.362 (3)	C22—H18	0.9300
C3—H3	0.9300	C21—C20	1.366 (4)
C4—C5	1.417 (3)	C21—H19	0.9300
C4—C6	1.486 (3)	C20—C19	1.365 (4)
C5—C26	1.476 (3)	C20—H20	0.9300

C11—C16	1.380 (3)	C19—C18	1.381 (3)
C11—C12	1.380 (3)	C19—H21	0.9300
C16—C15	1.373 (4)	C18—H22	0.9300
C16—H7	0.9300	O23—C24	1.432 (2)
C15—C14	1.369 (4)	C24—C25	1.500 (3)
C15—H8	0.9300	C24—H24A	0.9700
C14—C13	1.368 (4)	C24—H24B	0.9700
C14—H9	0.9300	C25—H25A	0.9600
C13—C12	1.380 (3)	C25—H25B	0.9600
C13—H10	0.9300	C25—H25C	0.9600
C12—H11	0.9300	C26—C27	1.382 (3)
C6—N7	1.504 (3)	C26—C31	1.391 (3)
C6—C10	1.529 (3)	C31—C30	1.380 (3)
C6—H6	0.9800	C31—H27	0.9300
N7—C17	1.439 (3)	C30—C29	1.368 (3)
N7—O8	1.464 (2)	C30—H28	0.9300
O8—C9	1.422 (3)	C29—C28	1.369 (3)
C9—O23	1.390 (2)	C28—C27	1.381 (3)
C9—C10	1.516 (3)	C28—H30	0.9300
C9—H9A	0.9800	C27—H31	0.9300
C5—N1—N2	104.94 (16)	C6—C10—H10B	110.9
C3—N2—N1	111.19 (17)	H10A—C10—H10B	108.9
C3—N2—C11	128.51 (17)	C18—C17—C22	119.8 (2)
N1—N2—C11	120.16 (17)	C18—C17—N7	123.8 (2)
N2—C3—C4	108.54 (17)	C22—C17—N7	116.4 (2)
N2—C3—H3	125.7	C17—C22—C21	119.4 (2)
C4—C3—H3	125.7	C17—C22—H18	120.3
C3—C4—C5	103.97 (18)	C21—C22—H18	120.3
C3—C4—C6	125.90 (18)	C20—C21—C22	120.5 (3)
C5—C4—C6	130.13 (19)	C20—C21—H19	119.7
N1—C5—C4	111.36 (18)	C22—C21—H19	119.7
N1—C5—C26	117.65 (17)	C19—C20—C21	119.8 (2)
C4—C5—C26	130.8 (2)	C19—C20—H20	120.1
C16—C11—C12	120.1 (2)	C21—C20—H20	120.1
C16—C11—N2	119.9 (2)	C20—C19—C18	120.5 (3)
C12—C11—N2	119.9 (2)	C20—C19—H21	119.7
C15—C16—C11	119.3 (2)	C18—C19—H21	119.7
C15—C16—H7	120.4	C17—C18—C19	119.8 (2)
C11—C16—H7	120.4	C17—C18—H22	120.1
C14—C15—C16	121.2 (3)	C19—C18—H22	120.1
C14—C15—H8	119.4	C9—O23—C24	113.54 (17)
C16—C15—H8	119.4	O23—C24—C25	107.5 (2)
C13—C14—C15	119.3 (3)	O23—C24—H24A	110.2
C13—C14—H9	120.3	C25—C24—H24A	110.2
C15—C14—H9	120.3	O23—C24—H24B	110.2
C14—C13—C12	120.7 (2)	C25—C24—H24B	110.2
C14—C13—H10	119.6	H24A—C24—H24B	108.5
C12—C13—H10	119.6	C24—C25—H25A	109.5
C13—C12—C11	119.4 (2)	C24—C25—H25B	109.5

C13—C12—H11	120.3	H25A—C25—H25B	109.5
C11—C12—H11	120.3	C24—C25—H25C	109.5
C4—C6—N7	111.02 (16)	H25A—C25—H25C	109.5
C4—C6—C10	115.13 (18)	H25B—C25—H25C	109.5
N7—C6—C10	101.09 (15)	C27—C26—C31	118.09 (19)
C4—C6—H6	109.8	C27—C26—C5	123.58 (19)
N7—C6—H6	109.8	C31—C26—C5	118.3 (2)
C10—C6—H6	109.8	C30—C31—C26	121.1 (2)
C17—N7—O8	106.59 (15)	C30—C31—H27	119.4
C17—N7—C6	112.61 (15)	C26—C31—H27	119.4
O8—N7—C6	101.43 (14)	C29—C30—C31	119.0 (2)
C9—O8—N7	104.82 (14)	C29—C30—H28	120.5
O23—C9—O8	112.99 (18)	C31—C30—H28	120.5
O23—C9—C10	108.29 (19)	C30—C29—C28	121.4 (2)
O8—C9—C10	106.28 (16)	C30—C29—Br1	118.51 (17)
O23—C9—H9A	109.7	C28—C29—Br1	120.05 (19)
O8—C9—H9A	109.7	C29—C28—C27	119.2 (2)
C10—C9—H9A	109.7	C29—C28—H30	120.4
C9—C10—C6	104.34 (17)	C27—C28—H30	120.4
C9—C10—H10A	110.9	C28—C27—C26	121.1 (2)
C6—C10—H10A	110.9	C28—C27—H31	119.4
C9—C10—H10B	110.9	C26—C27—H31	119.4
C5—N1—N2—C3	−0.1 (2)	N7—O8—C9—C10	−29.9 (2)
C5—N1—N2—C11	−176.21 (17)	O23—C9—C10—C6	−119.66 (19)
N1—N2—C3—C4	0.0 (2)	O8—C9—C10—C6	2.0 (2)
C11—N2—C3—C4	175.68 (19)	C4—C6—C10—C9	145.05 (18)
N2—C3—C4—C5	0.1 (2)	N7—C6—C10—C9	25.3 (2)
N2—C3—C4—C6	−179.11 (18)	O8—N7—C17—C18	−18.5 (3)
N2—N1—C5—C4	0.2 (2)	C6—N7—C17—C18	91.9 (2)
N2—N1—C5—C26	−175.78 (17)	O8—N7—C17—C22	162.37 (17)
C3—C4—C5—N1	−0.2 (2)	C6—N7—C17—C22	−87.3 (2)
C6—C4—C5—N1	178.98 (19)	C18—C17—C22—C21	−2.7 (3)
C3—C4—C5—C26	175.1 (2)	N7—C17—C22—C21	176.5 (2)
C6—C4—C5—C26	−5.7 (4)	C17—C22—C21—C20	2.2 (4)
C3—N2—C11—C16	−157.4 (2)	C22—C21—C20—C19	−0.5 (4)
N1—N2—C11—C16	17.9 (3)	C21—C20—C19—C18	−0.6 (4)
C3—N2—C11—C12	21.8 (3)	C22—C17—C18—C19	1.6 (4)
N1—N2—C11—C12	−162.82 (19)	N7—C17—C18—C19	−177.5 (2)
C12—C11—C16—C15	−1.8 (3)	C20—C19—C18—C17	0.1 (4)
N2—C11—C16—C15	177.5 (2)	O8—C9—O23—C24	68.5 (2)
C11—C16—C15—C14	−0.3 (4)	C10—C9—O23—C24	−174.05 (17)
C16—C15—C14—C13	1.5 (4)	C9—O23—C24—C25	171.8 (2)
C15—C14—C13—C12	−0.7 (4)	N1—C5—C26—C27	−143.2 (2)
C14—C13—C12—C11	−1.4 (4)	C4—C5—C26—C27	41.8 (3)
C16—C11—C12—C13	2.6 (3)	N1—C5—C26—C31	35.7 (3)
N2—C11—C12—C13	−176.7 (2)	C4—C5—C26—C31	−139.3 (2)
C3—C4—C6—N7	65.4 (3)	C27—C26—C31—C30	1.1 (3)
C5—C4—C6—N7	−113.6 (2)	C5—C26—C31—C30	−177.9 (2)
C3—C4—C6—C10	−48.7 (3)	C26—C31—C30—C29	−1.0 (3)

C5—C4—C6—C10	132.3 (2)	C31—C30—C29—C28	0.1 (4)
C4—C6—N7—C17	80.7 (2)	C31—C30—C29—Br1	178.75 (17)
C10—C6—N7—C17	−156.73 (18)	C30—C29—C28—C27	0.8 (4)
C4—C6—N7—O8	−165.78 (15)	Br1—C29—C28—C27	−177.84 (18)
C10—C6—N7—O8	−43.17 (19)	C29—C28—C27—C26	−0.8 (4)
C17—N7—O8—C9	164.37 (15)	C31—C26—C27—C28	−0.2 (3)
C6—N7—O8—C9	46.37 (17)	C5—C26—C27—C28	178.8 (2)
N7—O8—C9—O23	88.77 (19)		

Fig. 1

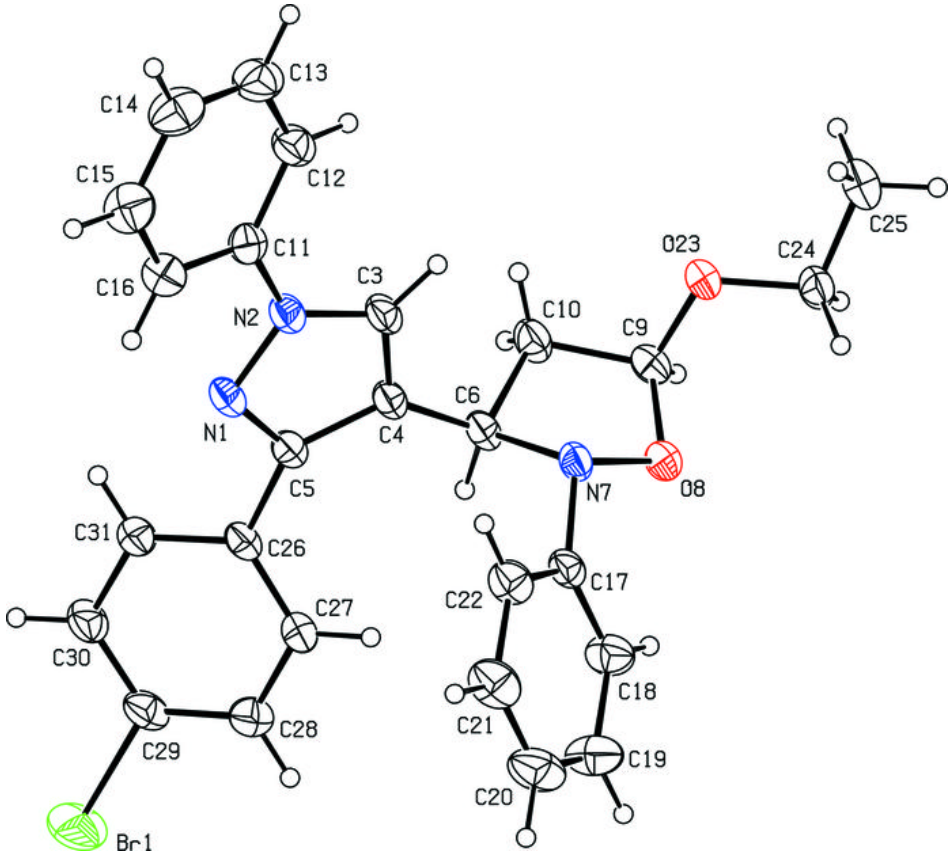
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Fig. 2