IUCrData

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(*E*)-1-(4-Bromophenyl)-3-[3-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-1-phenyl-1*H*-pyrazol-4-yl]-prop-2-en-1-one

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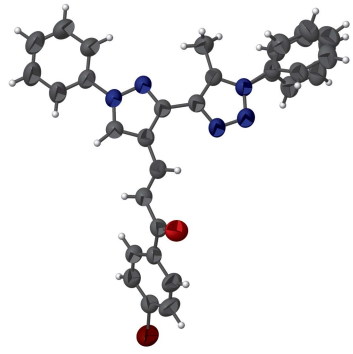
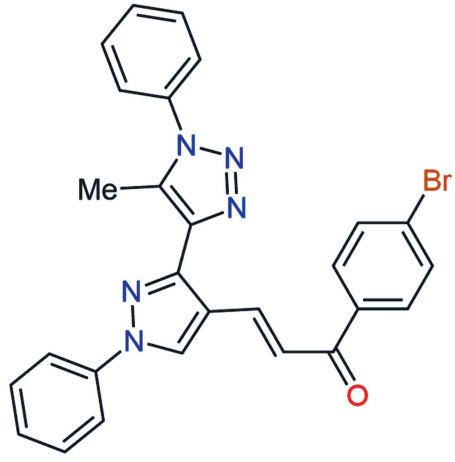
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{27}H_{20}BrN_5O$, the dihedral angle between the heterocyclic rings is 10.2 (2)°. The phenyl ring bound to the triazole ring is disordered over two orientations in a 0.808 (4):0.192 (4) ratio. In the crystal, C—H···O interactions form chains along [010]. π–π interactions are observed between the phenyl–pyrazolyl unit and the phenylene group of a neighbouring molecule.

3D view



Chemical scheme



Structure description

Pyrazolyltriazoles show some biological applications as antimicrobial (Abdel-Wahab *et al.*, 2017), anti-invasive and antimycobacterial agents (Kumar *et al.*, 2003). In addition, some pyrazolyltriazoles are useful as herbicides (Lang & Walworth, 1979).

The asymmetric unit comprises one molecule (Fig. 1). In the crystal, C—H···O hydrogen bonds link the molecules, forming chains along [010] (Table 1, Fig. 2). π–π interactions involving the phenyl–pyrazolyl group and the phenylene group of a neighbouring molecule are also observed [centroid-to-centroid distance = 3.887 (3) Å; symmetry operator for the phenylene group: $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$].

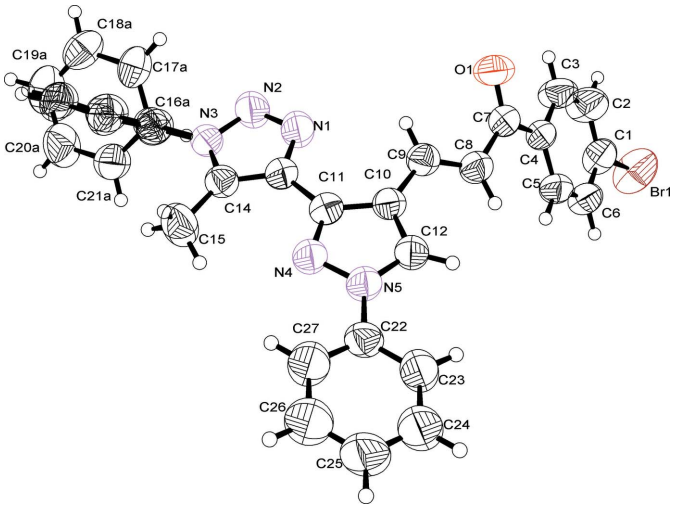


Figure 1
An *ORTEP* representation of the asymmetric unit showing 50% probability displacement ellipsoids.

Synthesis and crystallization

The title compound was synthesized based on a literature procedure by the reaction of a mixture of 3-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-1-phenyl-1*H*-pyrazole-4-carbaldehyde and 1-(4-bromophenyl)ethanone in aqueous ethanol in the presence of sodium hydroxide at room temperature for 5 h (Abdel-Wahab *et al.*, 2017). The solid obtained was collected by filtration, washed with cold water and recrystallized from dimethylformamide solution to obtain colourless crystals (86%), m.p 168–169°C (lit 168–169°C; Abdel-Wahab *et al.*, 2017).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C16–C21 phenyl ring is disordered with two components oriented approximately perpendicular to each other. The occupancies refined to 0.808 (4) and 0.192 (4). The components were restrained to have similar geometries (SAME command in *SHELXL*) and chemically equivalent bonds around the *ipso*-carbon atoms C16 and C16*A* were restrained to be similar (SADI commands of *SHELXL*, e.s.d. = 0.01 Å^2). ADPs of disordered atoms were restrained to be close to isotropic and U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Å were restrained to be similar (ISOR and SIMU restraints of *SHELXL*; e.s.d. = 0.01 Å^2 for SIMU N3, C16 and C16*A*, 0.1 Å^2 for all others).

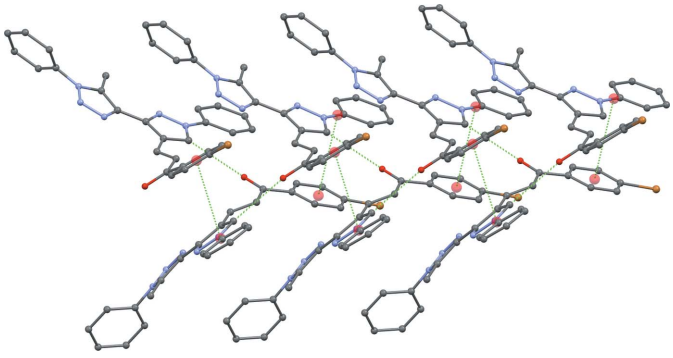


Figure 2
A segment of the crystal structure showing C—H···O and π–π interactions.

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1^{i}	0.93	2.28	3.201 (4)	172

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{27}H_{20}BrN_5O$
M_r	510.39
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	15.0387 (12), 6.8105 (3), 24.385 (2)
β (°)	106.473 (8)
V (Å^3)	2395.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.75
Crystal size (mm)	0.32 × 0.18 × 0.08
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku Oxford Diffraction, 2015)
T_{min}, T_{max}	0.540, 0.874
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22293, 5994, 2916
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.702
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.188, 1.03
No. of reflections	5994
No. of parameters	363
No. of restraints	271
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.56, −0.72

Computer programs: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015), *SHELXS* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

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full crystallographic data

IUCrData (2018). **3**, x180069 [https://doi.org/10.1107/S241431461800069X]

(*E*)-1-(4-Bromophenyl)-3-[3-(5-methyl-1-phenyl-1*H*-1,2,3-triazol-4-yl)-1-phenyl-1*H*-pyrazol-4-yl]prop-2-en-1-one

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Crystal data

$C_{27}H_{20}BrN_5O$
M_r = 510.39
Monoclinic, $P2_1/n$
a = 15.0387 (12) Å
b = 6.8105 (3) Å
c = 24.385 (2) Å
β = 106.473 (8)°
V = 2395.0 (3) Å^3
Z = 4
$F(000)$ = 1040
D_x = 1.415 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4138 reflections
θ = 3.3–22.8°
μ = 1.75 mm^{-1}
T = 293 K
Block, colourless
0.32 × 0.18 × 0.08 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku Oxford Diffraction, 2015)
T_{min} = 0.540, T_{max} = 0.874
22293 measured reflections
5994 independent reflections
2916 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 29.9°, θ_{min} = 3.1°
h = −19→20
k = −9→9
l = −33→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.188
S = 1.03
5994 reflections
363 parameters
271 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.077P)^2 + 1.0166P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}

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. All hydrogen atoms were placed in calculated positions and refined using a riding model. Aromatic C—H distances were set to 0.93 Å and their U_{iso} set to 1.2 times the U_{eq} for the atoms to which they are bonded. Methyl C—H distances were set to 0.96 Å and their U(iso) set to 1.5 times the U_{eq} for the C atoms to which they are bonded. Methyl H atoms were allowed to rotate, but not to tip.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	1.0981 (3)	1.0213 (5)	0.29653 (17)	0.0785 (10)	
C2	1.1082 (3)	0.8522 (7)	0.2687 (2)	0.0975 (13)	
H2	1.160233	0.833696	0.255904	0.117*	
C3	1.0414 (3)	0.7107 (6)	0.25995 (18)	0.0824 (11)	
H3	1.048966	0.595122	0.241468	0.099*	
C4	0.9628 (2)	0.7353 (4)	0.27788 (13)	0.0589 (8)	
C5	0.9540 (2)	0.9098 (5)	0.30512 (14)	0.0666 (8)	
H5	0.901407	0.930524	0.317247	0.080*	
C6	1.0209 (3)	1.0526 (5)	0.31461 (15)	0.0738 (9)	
H6	1.014007	1.168818	0.333022	0.089*	
C7	0.8946 (2)	0.5723 (5)	0.27006 (13)	0.0631 (8)	
C8	0.8192 (2)	0.5821 (5)	0.29743 (13)	0.0635 (8)	
H8	0.794382	0.703269	0.302706	0.076*	
C9	0.7861 (2)	0.4182 (5)	0.31482 (12)	0.0604 (8)	
H9	0.812808	0.299858	0.308945	0.072*	
C10	0.7120 (2)	0.4097 (4)	0.34206 (12)	0.0573 (7)	
C11	0.6926 (2)	0.2637 (4)	0.37887 (13)	0.0578 (7)	
C12	0.6418 (2)	0.5441 (5)	0.33655 (13)	0.0612 (8)	
H12	0.633770	0.659109	0.315142	0.073*	
C13	0.7493 (2)	0.0945 (4)	0.40400 (13)	0.0606 (8)	
C14	0.7407 (2)	−0.0346 (5)	0.44564 (13)	0.0596 (8)	
C15	0.6705 (3)	−0.0557 (7)	0.47706 (19)	0.0974 (13)	
H15A	0.620946	−0.138020	0.455656	0.146*	
H15B	0.646317	0.071308	0.482227	0.146*	
H15C	0.698566	−0.113972	0.513735	0.146*	
C16	0.8531 (4)	−0.2993 (6)	0.49653 (19)	0.0611 (15)	0.808 (4)
C17	0.7985 (3)	−0.4578 (6)	0.49705 (18)	0.0747 (13)	0.808 (4)
H17	0.738202	−0.464135	0.473091	0.090*	0.808 (4)
C18	0.8355 (5)	−0.6100 (7)	0.5344 (2)	0.0883 (16)	0.808 (4)
H18	0.799400	−0.719533	0.536034	0.106*	0.808 (4)
C19	0.9245 (6)	−0.5999 (11)	0.5689 (2)	0.088 (2)	0.808 (4)
H19	0.949225	−0.703796	0.593216	0.105*	0.808 (4)
C20	0.9776 (4)	−0.4372 (9)	0.5679 (2)	0.0929 (16)	0.808 (4)
H20	1.037732	−0.430199	0.591985	0.112*	0.808 (4)
C21	0.9421 (3)	−0.2827 (7)	0.53099 (19)	0.0770 (13)	0.808 (4)

H21	0.977627	−0.171783	0.529759	0.092*	0.808 (4)
C16A	0.842 (2)	−0.323 (2)	0.4904 (7)	0.061 (4)	0.192 (4)
C17A	0.8740 (12)	−0.489 (2)	0.4700 (7)	0.075 (5)	0.192 (4)
H17A	0.876268	−0.489626	0.432317	0.090*	0.192 (4)
C18A	0.9034 (15)	−0.657 (2)	0.5034 (8)	0.085 (6)	0.192 (4)
H18A	0.926993	−0.764690	0.488634	0.102*	0.192 (4)
C19A	0.897 (3)	−0.660 (4)	0.5577 (11)	0.103 (9)	0.192 (4)
H19A	0.907791	−0.775943	0.578652	0.123*	0.192 (4)
C20A	0.8737 (18)	−0.492 (3)	0.5819 (8)	0.100 (6)	0.192 (4)
H20A	0.878799	−0.486441	0.620762	0.120*	0.192 (4)
C21A	0.8425 (15)	−0.329 (3)	0.5468 (6)	0.081 (6)	0.192 (4)
H21A	0.821092	−0.219898	0.562233	0.098*	0.192 (4)
C22	0.5037 (2)	0.5660 (5)	0.37391 (14)	0.0695 (9)	
C23	0.4761 (4)	0.7453 (7)	0.3505 (2)	0.1097 (17)	
H23	0.511457	0.811621	0.330734	0.132*	
C24	0.3955 (4)	0.8283 (9)	0.3563 (2)	0.130 (2)	
H24	0.376608	0.950212	0.340013	0.156*	
C25	0.3440 (4)	0.7356 (8)	0.3852 (2)	0.1119 (16)	
H25	0.290541	0.794225	0.389495	0.134*	
C26	0.3705 (4)	0.5559 (9)	0.4081 (3)	0.132 (2)	
H26	0.334345	0.490100	0.427467	0.158*	
C27	0.4514 (3)	0.4700 (7)	0.4029 (2)	0.1058 (15)	
H27	0.469785	0.347546	0.418977	0.127*	
N1	0.8288 (2)	0.0556 (5)	0.39076 (14)	0.0853 (9)	
N2	0.8712 (2)	−0.0915 (5)	0.42212 (14)	0.0855 (9)	
N3	0.81813 (19)	−0.1461 (4)	0.45570 (10)	0.0615 (6)	
N4	0.6169 (2)	0.3054 (4)	0.39428 (11)	0.0646 (7)	
N5	0.58666 (18)	0.4796 (4)	0.36765 (11)	0.0635 (7)	
Br1	1.19258 (4)	1.21670 (8)	0.31164 (3)	0.1228 (3)	
O1	0.9048 (2)	0.4247 (4)	0.24355 (11)	0.0885 (8)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.067 (2)	0.066 (2)	0.104 (3)	0.0020 (18)	0.027 (2)	0.008 (2)
C2	0.075 (3)	0.092 (3)	0.143 (4)	0.004 (2)	0.060 (3)	−0.006 (3)
C3	0.077 (3)	0.071 (2)	0.113 (3)	0.006 (2)	0.050 (2)	−0.011 (2)
C4	0.0616 (19)	0.0563 (17)	0.0609 (17)	0.0135 (15)	0.0207 (15)	0.0069 (14)
C5	0.066 (2)	0.0636 (19)	0.076 (2)	0.0103 (17)	0.0289 (17)	−0.0002 (16)
C6	0.074 (2)	0.0608 (19)	0.088 (2)	0.0070 (18)	0.0252 (19)	−0.0018 (17)
C7	0.070 (2)	0.0583 (18)	0.0641 (18)	0.0089 (16)	0.0238 (16)	0.0047 (15)
C8	0.063 (2)	0.0587 (18)	0.0707 (19)	0.0065 (15)	0.0227 (16)	0.0019 (15)
C9	0.0593 (19)	0.0625 (18)	0.0576 (17)	0.0068 (15)	0.0137 (14)	0.0005 (14)
C10	0.0582 (19)	0.0578 (17)	0.0550 (16)	0.0043 (14)	0.0148 (14)	−0.0016 (14)
C11	0.0558 (18)	0.0559 (17)	0.0608 (17)	0.0019 (14)	0.0150 (14)	−0.0026 (14)
C12	0.0602 (19)	0.0616 (18)	0.0631 (17)	0.0023 (15)	0.0195 (15)	0.0028 (15)
C13	0.064 (2)	0.0557 (17)	0.0652 (18)	0.0050 (15)	0.0231 (15)	0.0010 (15)
C14	0.0551 (18)	0.0623 (18)	0.0619 (17)	0.0037 (15)	0.0173 (14)	0.0008 (15)

C15	0.085 (3)	0.113 (3)	0.108 (3)	0.025 (2)	0.051 (2)	0.037 (3)
C16	0.065 (3)	0.062 (2)	0.054 (2)	0.007 (2)	0.012 (2)	−0.002 (2)
C17	0.083 (3)	0.066 (3)	0.069 (3)	−0.002 (2)	0.012 (2)	0.000 (2)
C18	0.121 (5)	0.065 (3)	0.081 (3)	0.004 (3)	0.031 (3)	0.010 (3)
C19	0.108 (6)	0.083 (4)	0.067 (3)	0.031 (4)	0.017 (3)	0.015 (3)
C20	0.084 (4)	0.106 (4)	0.076 (3)	0.025 (3)	0.002 (3)	0.003 (3)
C21	0.074 (3)	0.073 (3)	0.076 (3)	0.005 (2)	0.008 (2)	−0.001 (2)
C16A	0.062 (6)	0.060 (6)	0.056 (6)	0.007 (6)	0.011 (6)	0.001 (6)
C17A	0.067 (10)	0.068 (9)	0.080 (10)	−0.005 (8)	0.005 (8)	0.012 (8)
C18A	0.084 (12)	0.064 (10)	0.090 (11)	0.000 (9)	−0.001 (10)	−0.007 (9)
C19A	0.094 (16)	0.094 (15)	0.111 (15)	−0.015 (14)	0.014 (13)	0.019 (13)
C20A	0.107 (14)	0.111 (13)	0.078 (11)	0.024 (12)	0.021 (10)	0.036 (11)
C21A	0.093 (15)	0.079 (12)	0.071 (12)	0.015 (11)	0.022 (10)	0.007 (10)
C22	0.062 (2)	0.078 (2)	0.072 (2)	0.0145 (17)	0.0239 (17)	0.0045 (17)
C23	0.114 (4)	0.115 (3)	0.123 (3)	0.056 (3)	0.072 (3)	0.053 (3)
C24	0.127 (4)	0.143 (4)	0.146 (4)	0.075 (4)	0.080 (4)	0.061 (4)
C25	0.088 (3)	0.132 (4)	0.128 (4)	0.043 (3)	0.051 (3)	0.023 (3)
C26	0.106 (4)	0.126 (4)	0.196 (5)	0.034 (3)	0.095 (4)	0.039 (4)
C27	0.086 (3)	0.096 (3)	0.156 (4)	0.022 (2)	0.068 (3)	0.032 (3)
N1	0.089 (2)	0.081 (2)	0.103 (2)	0.0325 (18)	0.0543 (19)	0.0303 (18)
N2	0.085 (2)	0.086 (2)	0.100 (2)	0.0271 (18)	0.0492 (19)	0.0246 (18)
N3	0.0634 (17)	0.0619 (15)	0.0612 (14)	0.0084 (13)	0.0209 (13)	0.0052 (12)
N4	0.0609 (17)	0.0639 (16)	0.0716 (16)	0.0078 (13)	0.0230 (13)	0.0067 (13)
N5	0.0569 (16)	0.0639 (16)	0.0711 (15)	0.0086 (13)	0.0203 (13)	0.0048 (13)
Br1	0.0810 (4)	0.0904 (4)	0.1980 (7)	−0.0128 (2)	0.0410 (4)	0.0055 (3)
O1	0.111 (2)	0.0666 (15)	0.1043 (18)	−0.0025 (14)	0.0572 (16)	−0.0202 (14)

Geometric parameters (Å, º)

C1—C2	1.367 (6)	C17—H17	0.9300
C1—C6	1.370 (5)	C18—C19	1.366 (9)
C1—Br1	1.905 (4)	C18—H18	0.9300
C2—C3	1.364 (6)	C19—C20	1.370 (9)
C2—H2	0.9300	C19—H19	0.9300
C3—C4	1.382 (5)	C20—C21	1.389 (6)
C3—H3	0.9300	C20—H20	0.9300
C4—C5	1.386 (4)	C21—H21	0.9300
C4—C7	1.487 (5)	C16A—C17A	1.373 (8)
C5—C6	1.371 (5)	C16A—C21A	1.374 (8)
C5—H5	0.9300	C16A—N3	1.459 (9)
C6—H6	0.9300	C17A—C18A	1.403 (16)
C7—O1	1.228 (4)	C17A—H17A	0.9300
C7—C8	1.470 (4)	C18A—C19A	1.354 (19)
C8—C9	1.339 (4)	C18A—H18A	0.9300
C8—H8	0.9300	C19A—C20A	1.38 (2)
C9—C10	1.451 (4)	C19A—H19A	0.9300
C9—H9	0.9300	C20A—C21A	1.398 (16)
C10—C12	1.375 (4)	C20A—H20A	0.9300

C10—C11	1.423 (4)	C21A—H21A	0.9300
C11—N4	1.327 (4)	C22—C23	1.362 (5)
C11—C13	1.461 (4)	C22—C27	1.364 (5)
C12—N5	1.346 (4)	C22—N5	1.426 (4)
C12—H12	0.9300	C23—C24	1.381 (6)
C13—N1	1.350 (4)	C23—H23	0.9300
C13—C14	1.376 (4)	C24—C25	1.343 (7)
C14—N3	1.354 (4)	C24—H24	0.9300
C14—C15	1.477 (5)	C25—C26	1.357 (6)
C15—H15A	0.9600	C25—H25	0.9300
C15—H15B	0.9600	C26—C27	1.388 (6)
C15—H15C	0.9600	C26—H26	0.9300
C16—C17	1.359 (6)	C27—H27	0.9300
C16—C21	1.368 (6)	N1—N2	1.311 (4)
C16—N3	1.436 (5)	N2—N3	1.347 (4)
C17—C18	1.388 (7)	N4—N5	1.367 (4)

C2—C1—C6	120.9 (4)	C18—C19—C20	120.2 (5)
C2—C1—Br1	120.2 (3)	C18—C19—H19	119.9
C6—C1—Br1	118.9 (3)	C20—C19—H19	119.9
C3—C2—C1	119.5 (4)	C19—C20—C21	120.4 (5)
C3—C2—H2	120.2	C19—C20—H20	119.8
C1—C2—H2	120.2	C21—C20—H20	119.8
C2—C3—C4	121.5 (3)	C16—C21—C20	117.6 (5)
C2—C3—H3	119.2	C16—C21—H21	121.2
C4—C3—H3	119.2	C20—C21—H21	121.2
C3—C4—C5	117.5 (3)	C17A—C16A—C21A	115.9 (11)
C3—C4—C7	119.3 (3)	C17A—C16A—N3	121.6 (12)
C5—C4—C7	123.1 (3)	C21A—C16A—N3	122.3 (12)
C6—C5—C4	121.6 (3)	C16A—C17A—C18A	123.1 (13)
C6—C5—H5	119.2	C16A—C17A—H17A	118.4
C4—C5—H5	119.2	C18A—C17A—H17A	118.4
C1—C6—C5	118.9 (3)	C19A—C18A—C17A	118.7 (17)
C1—C6—H6	120.5	C19A—C18A—H18A	120.7
C5—C6—H6	120.5	C17A—C18A—H18A	120.7
O1—C7—C8	120.2 (3)	C18A—C19A—C20A	120.2 (19)
O1—C7—C4	119.6 (3)	C18A—C19A—H19A	119.9
C8—C7—C4	120.0 (3)	C20A—C19A—H19A	119.9
C9—C8—C7	120.7 (3)	C19A—C20A—C21A	118.6 (17)
C9—C8—H8	119.7	C19A—C20A—H20A	120.7
C7—C8—H8	119.7	C21A—C20A—H20A	120.7
C8—C9—C10	125.6 (3)	C16A—C21A—C20A	122.7 (14)
C8—C9—H9	117.2	C16A—C21A—H21A	118.6
C10—C9—H9	117.2	C20A—C21A—H21A	118.6
C12—C10—C11	103.8 (3)	C23—C22—C27	119.6 (4)
C12—C10—C9	126.6 (3)	C23—C22—N5	119.8 (3)
C11—C10—C9	129.6 (3)	C27—C22—N5	120.6 (3)
N4—C11—C10	112.0 (3)	C22—C23—C24	119.8 (4)

N4—C11—C13	119.7 (3)	C22—C23—H23	120.1
C10—C11—C13	128.0 (3)	C24—C23—H23	120.1
N5—C12—C10	107.8 (3)	C25—C24—C23	121.0 (5)
N5—C12—H12	126.1	C25—C24—H24	119.5
C10—C12—H12	126.1	C23—C24—H24	119.5
N1—C13—C14	109.1 (3)	C24—C25—C26	119.6 (4)
N1—C13—C11	120.3 (3)	C24—C25—H25	120.2
C14—C13—C11	130.4 (3)	C26—C25—H25	120.2
N3—C14—C13	103.6 (3)	C25—C26—C27	120.3 (5)
N3—C14—C15	123.8 (3)	C25—C26—H26	119.8
C13—C14—C15	132.5 (3)	C27—C26—H26	119.8
C14—C15—H15A	109.5	C22—C27—C26	119.7 (4)
C14—C15—H15B	109.5	C22—C27—H27	120.2
H15A—C15—H15B	109.5	C26—C27—H27	120.2
C14—C15—H15C	109.5	N2—N1—C13	109.1 (3)
H15A—C15—H15C	109.5	N1—N2—N3	107.0 (3)
H15B—C15—H15C	109.5	N2—N3—C14	111.3 (2)
C17—C16—C21	123.3 (4)	N2—N3—C16	117.3 (3)
C17—C16—N3	118.7 (4)	C14—N3—C16	131.4 (3)
C21—C16—N3	117.9 (4)	N2—N3—C16A	119.3 (11)
C16—C17—C18	117.9 (5)	C14—N3—C16A	128.9 (13)
C16—C17—H17	121.0	C11—N4—N5	104.3 (2)
C18—C17—H17	121.0	C12—N5—N4	112.1 (3)
C19—C18—C17	120.5 (5)	C12—N5—C22	128.5 (3)
C19—C18—H18	119.8	N4—N5—C22	119.4 (3)
C17—C18—H18	119.8		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1^{i}	0.93	2.28	3.201 (4)	172

Symmetry code: (i) −*x*+3/2, *y*+1/2, −*z*+1/2.