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Crystal structure of {(*E*)-4-[(1-allyl-1*H*-1,2,3-triazol-4-yl)methoxy]benzylidene}-[2-(morpholin-4-yl)ethyl]amine

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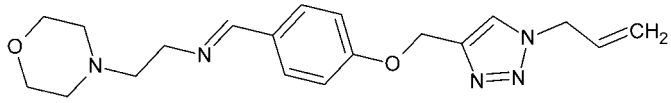
In the title compound, $C_{19}H_{25}N_5O_2$, the morpholine ring has a chair conformation. The plane of the central benzene ring makes dihedral angles of 88.75 (12) and 60.02 (7)°, respectively, with the mean plane formed by the four planar C atoms of the morpholine ring and with the plane of the triazole ring. In the crystal, molecules are linked *via* C—H$\cdots\pi$ interactions, forming slabs lying parallel to (10$\bar{1}$). The C atoms of the bridging ethylene group, between the morpholine and benzene rings, and the terminal ethene group of the prop-1-ene substituent attached to the triazole ring, are disordered over two sets of sites, with an occupancy ratio of 0.634 (13):0.366 (13).

Keywords: crystal structure; Schiff base; morpholine; 1,2,3-triazole; disorder.

CCDC reference: 1014976

1. Related literature

For information on Schiff bases, see: Vladimirova *et al.* (2001). For 1,2,3-triazole derivatives and the 'click' chemistry concept, see: Kolb *et al.* (2001); Wang *et al.* (2005). For the biological activity of 1,2,3-triazole derivatives, including their potential applications as antitumor, antibacterial, antifungal and antiviral agents, see: Yu *et al.* (2006). For the biological utility of molecules containing the morpholine moiety, see: Nelson *et al.* (2004).



2. Experimental

2.1. Crystal data

$C_{19}H_{25}N_5O_2$
M_r = 355.44
Monoclinic, $P2_1/c$
a = 22.3034 (10) Å
b = 5.2531 (3) Å
c = 16.5878 (8) Å
β = 93.051 (4)°
V = 1940.71 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.61 × 0.43 × 0.10 mm

2.2. Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.961, T_{max} = 0.993
25155 measured reflections
3610 independent reflections
1769 reflections with $I > 2\sigma(I)$
R_{int} = 0.191

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.130
S = 0.93
3610 reflections
272 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

Cg is the centroid of the 1,2,3-triazole ring N3–N5/C15/C16.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C6*A*—H6*A*1$\cdots Cg^{i}$	0.97	2.90	3.617 (8)	132

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU2753).

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supporting information

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Crystal structure of {(*E*)-4-[(1-allyl-1*H*-1,2,3-triazol-4-yl)methoxy]benzylidene}[2-(morpholin-4-yl)ethyl]amine

Sevim Türktekin Çelikesir, Mehmet Akkurt, Aliasghar Jarrahpour, Mehdi Mohammadi Chermahini, Pezhman Shiri and Orhan Büyükgüngör

S1. Synthesis and crystallization

Reaction of 4-((1-allyl-1H-1,2,3-triazol-4-yl)methoxy)benzaldehyde (1.0 mmol) with 2-morpholinoethanamine (1.0 mmol) in refluxing ethanol gave the title compound. Recrystallization from ethanol gave light brown crystals in 75% yield. m.p. 385 - 387 K. IR (KBr, cm^{-1}): 1635 (C=N). ^{1}H-NMR (250 MHz, $CDCl_3$), δ (ppm): 2.48 (CH_2—N morpholine, t, 4H, J=5 Hz), 2.62 (morpholine-CH_2—CH_2, t, 2H, J=7.5 Hz), 3.65 (CH_2—O morpholine and morpholine-CH_2—CH_2, t, 6H, J=5 Hz), 4.92 (d, 2H, J=7.5 Hz), 5.17 (s, 2H), 5.29 (m, 2H), 5.98 (m, 1H), 6.92 (aromatic H, d, 2H, J=10 Hz), 7.56 (aromatic H, d, 2H, J= Hz 5), 7.6 (H triazole, s, 1H), 8.15 (HC═N, s, 1H). ^{13}CNMR (62.9 MHz, $CDCl_3$), δ (p.p.m): 53.9 (CH_2—N morpholine), 58.8, 59.3 (N—CH_2—CH_2, and CH_2—N), 61.9 (CH_2—O), 66.9 (CH_2—O morpholine), 114.7-143.9 (aromatic carbons and C=C triazole), 161.1 (C=N).

S2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were included in calculated positions and treated as riding atoms: C—H = 0.93 - 0.97 Å with U_{iso}(H) = 1.2U_{eq}(C). Reflections (1 2 0), (1 3 0) and (0 4 1) were omitted owing to bad agreement. Atoms C5A/C5B, C6A/C6B, C18A/C18B and C19A/C19B are disordered over two sites with an occupancy ratio of 0.634 (13):0.366 (13). Owing to the poor quality of the crystal the value of R_{int} is high (0.191).

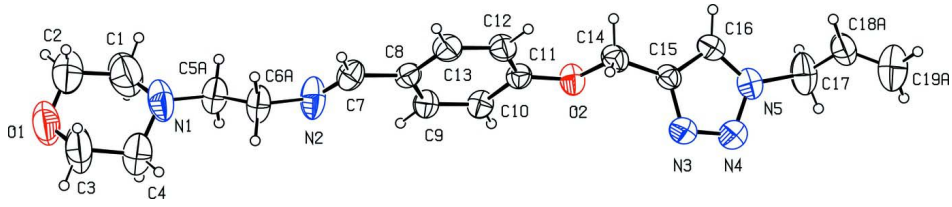

Figure 1

The molecular structure of the title molecule, with atom labelling. The displacement ellipsoids are drawn at the 30% probability level. For clarity only the major disordered components are shown.

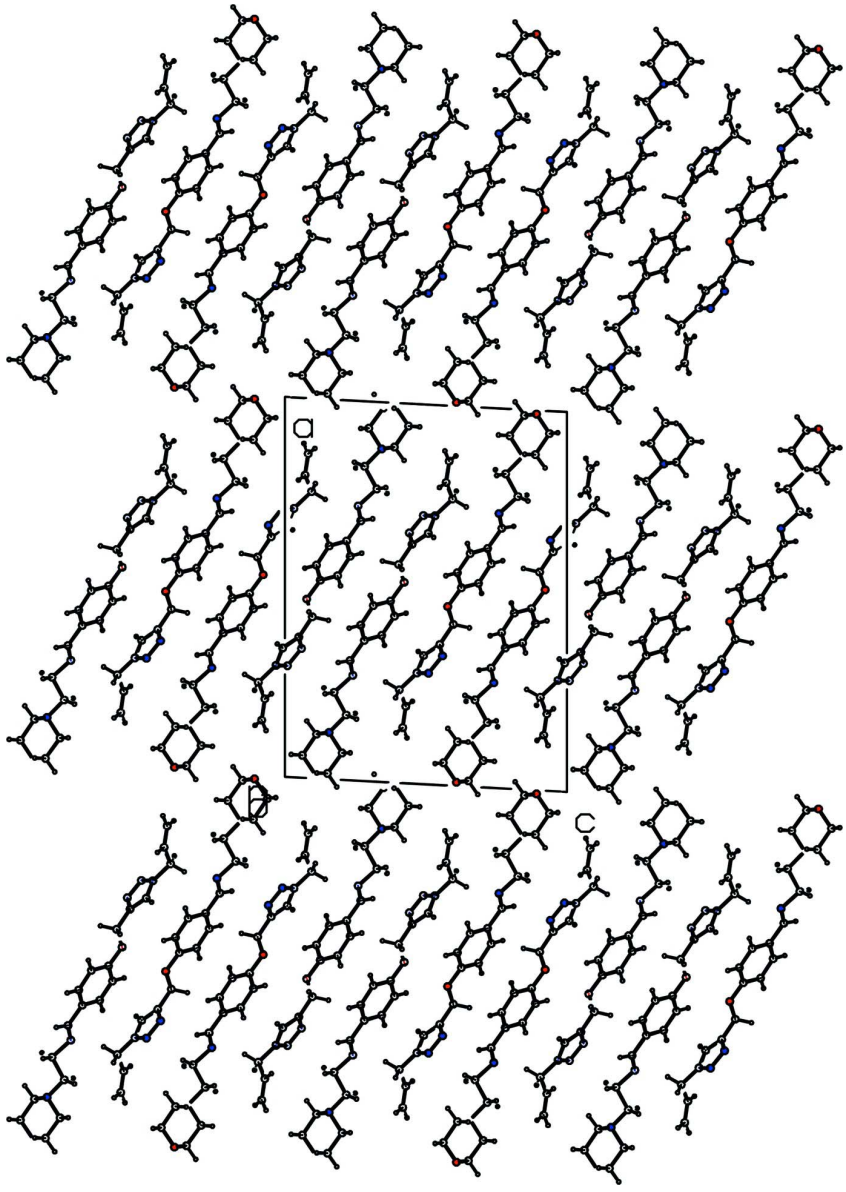

Figure 2

Crystal packing diagram of the title compound viewed along the *b* axis. For clarity only the major disordered components are shown.

{(*E*)-4-[(1-Allyl-1*H*-1,2,3-triazol-4-yl)methoxy]benzylidene}[2-(morpholin-4-yl)ethyl]amine

Crystal data

$C_{19}H_{25}N_5O_2$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 22.3034 (10) Å
b = 5.2531 (3) Å
c = 16.5878 (8) Å
β = 93.051 (4)°
V = 1940.71 (17) Å^3
Z = 4
$F(000)$ = 760
D_x = 1.217 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 15061 reflections
θ = 1.5–27.1°
μ = 0.08 mm^{-1}

T = 296 K
Block, light brown

0.61 × 0.43 × 0.10 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)

T_{min} = 0.961, T_{max} = 0.993
25155 measured reflections
3610 independent reflections
1769 reflections with $I > 2\sigma(I)$
R_{int} = 0.191
θ_{max} = 25.5°, θ_{min} = 1.8°
h = −26→26
k = −6→6
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.130
S = 0.93
3610 reflections
272 parameters
7 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -R-factor-obs *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}	Occ. (<1)
O1	0.00977 (10)	0.1772 (6)	0.1080 (2)	0.1613 (15)	
O2	0.52892 (6)	0.7614 (3)	0.42272 (9)	0.0777 (6)	
N1	0.12323 (13)	0.3855 (6)	0.15681 (19)	0.1249 (11)	
N2	0.27681 (10)	0.5151 (6)	0.24066 (15)	0.1151 (10)	
N3	0.65963 (9)	0.6517 (4)	0.44128 (13)	0.0839 (8)	
N4	0.70715 (9)	0.6485 (4)	0.49113 (14)	0.0923 (9)	
N5	0.70797 (8)	0.8676 (4)	0.53186 (12)	0.0807 (8)	
C1	0.0707 (2)	0.4126 (9)	0.2028 (3)	0.172 (2)	
C2	0.01503 (16)	0.4008 (10)	0.1505 (3)	0.179 (3)	
C3	0.05926 (16)	0.1478 (10)	0.0616 (3)	0.180 (2)	
C4	0.11659 (13)	0.1510 (8)	0.1120 (2)	0.1436 (18)	
C5A	0.1714 (3)	0.4194 (16)	0.2175 (5)	0.096 (2)	0.634 (13)
C6A	0.2293 (3)	0.482 (2)	0.1740 (5)	0.096 (3)	0.634 (13)
C7	0.31518 (10)	0.6820 (5)	0.23080 (15)	0.0809 (10)	
C8	0.37040 (9)	0.7061 (4)	0.28150 (13)	0.0658 (8)	

C9	0.38592 (9)	0.5339 (4)	0.34293 (14)	0.0711 (8)	
C10	0.43840 (9)	0.5580 (4)	0.38852 (14)	0.0695 (8)	
C11	0.47744 (9)	0.7556 (4)	0.37429 (13)	0.0646 (8)	
C12	0.46337 (10)	0.9286 (4)	0.31340 (14)	0.0774 (9)	
C13	0.40997 (11)	0.9006 (4)	0.26846 (15)	0.0805 (9)	
C14	0.57484 (10)	0.9369 (4)	0.40298 (15)	0.0775 (9)	
C15	0.63014 (9)	0.8731 (4)	0.45100 (13)	0.0644 (8)	
C16	0.66101 (11)	1.0086 (5)	0.50812 (15)	0.0795 (9)	
C17	0.75478 (13)	0.9218 (7)	0.59454 (18)	0.1190 (14)	
C18A	0.7974 (4)	1.113 (2)	0.5714 (7)	0.114 (3)	0.634 (13)
C19A	0.8541 (6)	1.080 (3)	0.5825 (11)	0.151 (5)	0.634 (13)
C5B	0.1961 (5)	0.338 (2)	0.1835 (7)	0.083 (4)	0.366 (13)
C6B	0.2144 (7)	0.590 (3)	0.2047 (9)	0.104 (5)	0.366 (13)
C18B	0.8105 (6)	0.998 (4)	0.5629 (12)	0.109 (6)	0.366 (13)
C19B	0.8417 (14)	1.199 (3)	0.579 (2)	0.153 (10)	0.366 (13)
H1A	0.07240	0.57420	0.23110	0.2060*	
H1B	0.07020	0.27810	0.24280	0.2060*	
H5A1	0.17700	0.26510	0.24920	0.1160*	0.634 (13)
H3A	0.05980	0.28410	0.02220	0.2160*	
H3B	0.05590	−0.01220	0.03260	0.2160*	
H6A2	0.22430	0.63690	0.14260	0.1150*	0.634 (13)
H5A2	0.16200	0.55730	0.25360	0.1160*	0.634 (13)
H2A	−0.01930	0.41900	0.18370	0.2150*	
H2B	0.01450	0.54230	0.11290	0.2150*	
H6A1	0.23960	0.34400	0.13840	0.1150*	0.634 (13)
H10	0.44790	0.44120	0.42930	0.0830*	
H12	0.48940	1.06130	0.30290	0.0930*	
H13	0.40040	1.01780	0.22780	0.0970*	
H14A	0.56250	1.10930	0.41490	0.0930*	
H14B	0.58190	0.92630	0.34590	0.0930*	
H16	0.65130	1.16920	0.52710	0.0950*	
H17A	0.73600	0.97870	0.64280	0.1430*	
H17B	0.77630	0.76560	0.60780	0.1430*	
H18A	0.78320	1.26370	0.54790	0.1370*	0.634 (13)
H19A	0.86880	0.93050	0.60600	0.1820*	0.634 (13)
H19B	0.88050	1.20590	0.56710	0.1820*	0.634 (13)
H4A	0.11720	0.00870	0.14930	0.1720*	
H4B	0.15010	0.13150	0.07760	0.1720*	
H7	0.30840	0.79780	0.18890	0.0970*	
H9	0.36010	0.40000	0.35310	0.0850*	
H5B1	0.20110	0.22290	0.22900	0.0990*	0.366 (13)
H5B2	0.21790	0.27290	0.13880	0.0990*	0.366 (13)
H6B1	0.18950	0.66640	0.24420	0.1250*	0.366 (13)
H6B2	0.21640	0.70040	0.15800	0.1250*	0.366 (13)
H18B	0.82620	0.88730	0.52550	0.1310*	0.366 (13)
H19C	0.82840	1.31630	0.61640	0.1840*	0.366 (13)
H19D	0.87750	1.22610	0.55460	0.1840*	0.366 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0905 (16)	0.195 (3)	0.196 (3)	−0.0408 (17)	−0.0134 (17)	−0.031 (2)
O2	0.0721 (9)	0.0850 (10)	0.0749 (11)	−0.0148 (8)	−0.0063 (8)	0.0196 (8)
N1	0.1009 (18)	0.141 (2)	0.127 (2)	−0.0382 (17)	−0.0480 (18)	0.0348 (19)
N2	0.0763 (14)	0.164 (2)	0.1018 (18)	−0.0213 (15)	−0.0260 (13)	0.0395 (17)
N3	0.0847 (13)	0.0753 (13)	0.0906 (16)	0.0021 (11)	−0.0044 (12)	−0.0121 (11)
N4	0.0861 (14)	0.0884 (15)	0.1015 (17)	0.0078 (12)	−0.0030 (13)	−0.0022 (13)
N5	0.0753 (13)	0.0914 (14)	0.0747 (14)	−0.0147 (12)	−0.0029 (11)	0.0018 (12)
C1	0.147 (3)	0.194 (4)	0.171 (4)	−0.033 (3)	−0.022 (3)	−0.030 (3)
C2	0.101 (3)	0.206 (5)	0.227 (5)	−0.006 (3)	−0.021 (3)	−0.035 (4)
C3	0.090 (2)	0.266 (5)	0.180 (4)	−0.035 (3)	−0.021 (3)	−0.065 (4)
C4	0.090 (2)	0.183 (4)	0.156 (3)	−0.008 (2)	−0.011 (2)	−0.001 (3)
C5A	0.066 (3)	0.141 (5)	0.082 (4)	−0.004 (3)	0.001 (3)	0.001 (3)
C6A	0.059 (3)	0.151 (7)	0.077 (5)	−0.011 (4)	0.000 (3)	−0.001 (4)
C7	0.0742 (15)	0.1012 (19)	0.0670 (16)	0.0125 (14)	0.0008 (13)	0.0074 (14)
C8	0.0673 (13)	0.0702 (14)	0.0597 (15)	0.0124 (11)	0.0007 (11)	−0.0038 (11)
C9	0.0664 (14)	0.0790 (14)	0.0680 (16)	−0.0028 (11)	0.0048 (12)	0.0050 (13)
C10	0.0686 (13)	0.0735 (14)	0.0664 (15)	−0.0002 (11)	0.0041 (12)	0.0155 (11)
C11	0.0681 (13)	0.0658 (13)	0.0594 (14)	0.0053 (11)	−0.0024 (11)	0.0016 (11)
C12	0.0843 (16)	0.0622 (14)	0.0844 (18)	−0.0044 (11)	−0.0085 (14)	0.0129 (12)
C13	0.0953 (17)	0.0662 (14)	0.0785 (18)	0.0044 (13)	−0.0104 (14)	0.0156 (12)
C14	0.0825 (15)	0.0649 (13)	0.0845 (18)	−0.0127 (11)	0.0003 (13)	0.0070 (12)
C15	0.0676 (13)	0.0558 (12)	0.0697 (15)	−0.0082 (11)	0.0032 (12)	0.0023 (11)
C16	0.0864 (16)	0.0665 (13)	0.0849 (18)	−0.0048 (13)	−0.0009 (14)	−0.0124 (13)
C17	0.0904 (19)	0.175 (3)	0.089 (2)	−0.029 (2)	−0.0193 (17)	0.002 (2)
C18A	0.094 (5)	0.092 (5)	0.152 (6)	−0.016 (5)	−0.042 (5)	−0.009 (5)
C19A	0.093 (6)	0.206 (13)	0.153 (7)	−0.026 (9)	−0.007 (5)	0.020 (11)
C5B	0.071 (7)	0.119 (7)	0.057 (6)	0.029 (5)	0.000 (5)	0.002 (5)
C6B	0.114 (10)	0.128 (10)	0.068 (8)	0.010 (8)	−0.008 (6)	0.006 (6)
C18B	0.066 (9)	0.125 (12)	0.134 (9)	0.009 (7)	−0.011 (6)	−0.027 (10)
C19B	0.116 (17)	0.127 (13)	0.217 (19)	−0.036 (11)	0.016 (14)	−0.018 (14)

Geometric parameters (Å, º)

O1—C2	1.372 (6)	C1—H1A	0.9700
O1—C3	1.388 (5)	C1—H1B	0.9700
O2—C11	1.366 (2)	C2—H2A	0.9700
O2—C14	1.429 (3)	C2—H2B	0.9700
N1—C1	1.439 (5)	C3—H3A	0.9700
N1—C4	1.442 (5)	C3—H3B	0.9700
N1—C5A	1.444 (8)	C4—H4A	0.9700
N1—C5B	1.680 (12)	C4—H4B	0.9700
N2—C6A	1.500 (8)	C5A—H5A1	0.9700
N2—C7	1.242 (4)	C5A—H5A2	0.9700
N2—C6B	1.536 (16)	C5B—H5B1	0.9700
N3—N4	1.309 (3)	C5B—H5B2	0.9700

N3—C15	1.350 (3)	C6A—H6A2	0.9700
N4—N5	1.334 (3)	C6A—H6A1	0.9700
N5—C16	1.325 (3)	C6B—H6B2	0.9700
N5—C17	1.462 (4)	C6B—H6B1	0.9700
C1—C2	1.478 (6)	C7—H7	0.9300
C3—C4	1.490 (5)	C9—H9	0.9300
C5A—C6A	1.548 (10)	C10—H10	0.9300
C5B—C6B	1.424 (19)	C12—H12	0.9300
C7—C8	1.459 (3)	C13—H13	0.9300
C8—C9	1.392 (3)	C14—H14A	0.9700
C8—C13	1.375 (3)	C14—H14B	0.9700
C9—C10	1.365 (3)	C16—H16	0.9300
C10—C11	1.383 (3)	C17—H17A	0.9700
C11—C12	1.382 (3)	C17—H17B	0.9700
C12—C13	1.379 (3)	C18A—H18A	0.9300
C14—C15	1.471 (3)	C18B—H18B	0.9300
C15—C16	1.345 (3)	C19A—H19B	0.9300
C17—C18B	1.432 (15)	C19A—H19A	0.9300
C17—C18A	1.449 (10)	C19B—H19C	0.9300
C18A—C19A	1.280 (16)	C19B—H19D	0.9300
C18B—C19B	1.29 (3)		

C2—O1—C3	109.4 (3)	N1—C4—H4B	109.00
C11—O2—C14	118.02 (17)	C3—C4—H4A	109.00
C1—N1—C4	107.1 (3)	C3—C4—H4B	110.00
C1—N1—C5A	102.4 (4)	H4A—C4—H4B	108.00
C1—N1—C5B	132.7 (5)	N1—C5A—H5A1	110.00
C4—N1—C5A	121.1 (4)	N1—C5A—H5A2	110.00
C4—N1—C5B	94.6 (4)	C6A—C5A—H5A1	110.00
C6A—N2—C7	116.7 (4)	C6A—C5A—H5A2	110.00
C6B—N2—C7	112.6 (6)	H5A1—C5A—H5A2	108.00
N4—N3—C15	108.6 (2)	H5B1—C5B—H5B2	109.00
N3—N4—N5	107.31 (19)	N1—C5B—H5B2	112.00
N4—N5—C16	110.0 (2)	C6B—C5B—H5B1	112.00
N4—N5—C17	121.2 (2)	N1—C5B—H5B1	112.00
C16—N5—C17	128.7 (2)	C6B—C5B—H5B2	112.00
N1—C1—C2	111.5 (4)	N2—C6A—H6A2	111.00
O1—C2—C1	112.6 (4)	C5A—C6A—H6A1	111.00
O1—C3—C4	111.8 (4)	N2—C6A—H6A1	111.00
N1—C4—C3	111.1 (3)	C5A—C6A—H6A2	111.00
N1—C5A—C6A	108.0 (6)	H6A1—C6A—H6A2	109.00
N1—C5B—C6B	100.8 (9)	N2—C6B—H6B1	113.00
N2—C6A—C5A	104.8 (6)	C5B—C6B—H6B2	113.00
N2—C6B—C5B	95.7 (10)	N2—C6B—H6B2	113.00
N2—C7—C8	123.5 (2)	C5B—C6B—H6B1	113.00
C9—C8—C13	117.5 (2)	H6B1—C6B—H6B2	110.00
C7—C8—C9	122.3 (2)	N2—C7—H7	118.00
C7—C8—C13	120.2 (2)	C8—C7—H7	118.00

C8—C9—C10	121.17 (19)	C10—C9—H9	119.00
C9—C10—C11	120.3 (2)	C8—C9—H9	119.00
O2—C11—C12	124.47 (19)	C9—C10—H10	120.00
C10—C11—C12	119.8 (2)	C11—C10—H10	120.00
O2—C11—C10	115.68 (19)	C11—C12—H12	121.00
C11—C12—C13	118.7 (2)	C13—C12—H12	121.00
C8—C13—C12	122.5 (2)	C8—C13—H13	119.00
O2—C14—C15	108.63 (18)	C12—C13—H13	119.00
C14—C15—C16	130.1 (2)	O2—C14—H14A	110.00
N3—C15—C14	122.10 (19)	O2—C14—H14B	110.00
N3—C15—C16	107.8 (2)	C15—C14—H14A	110.00
N5—C16—C15	106.3 (2)	C15—C14—H14B	110.00
N5—C17—C18A	113.6 (5)	H14A—C14—H14B	108.00
N5—C17—C18B	113.3 (8)	C15—C16—H16	127.00
C17—C18A—C19A	121.7 (11)	N5—C16—H16	127.00
C17—C18B—C19B	129 (2)	N5—C17—H17A	109.00
N1—C1—H1A	109.00	C18A—C17—H17B	109.00
N1—C1—H1B	109.00	N5—C17—H17B	109.00
C2—C1—H1A	109.00	C18A—C17—H17A	109.00
C2—C1—H1B	109.00	C18B—C17—H17B	84.00
H1A—C1—H1B	108.00	H17A—C17—H17B	108.00
O1—C2—H2A	109.00	C18B—C17—H17A	130.00
O1—C2—H2B	109.00	C19A—C18A—H18A	119.00
C1—C2—H2A	109.00	C17—C18A—H18A	119.00
C1—C2—H2B	109.00	C19B—C18B—H18B	116.00
H2A—C2—H2B	108.00	C17—C18B—H18B	116.00
O1—C3—H3A	109.00	C18A—C19A—H19B	120.00
O1—C3—H3B	109.00	H19A—C19A—H19B	120.00
C4—C3—H3A	109.00	C18A—C19A—H19A	120.00
C4—C3—H3B	109.00	C18B—C19B—H19C	120.00
H3A—C3—H3B	108.00	C18B—C19B—H19D	120.00
N1—C4—H4A	109.00	H19C—C19B—H19D	120.00

C2—O1—C3—C4	57.7 (5)	N4—N5—C16—C15	0.0 (3)
C3—O1—C2—C1	−57.7 (5)	N1—C1—C2—O1	58.5 (5)
C14—O2—C11—C12	−8.4 (3)	O1—C3—C4—N1	−58.5 (5)
C11—O2—C14—C15	−167.78 (18)	N1—C5A—C6A—N2	179.8 (6)
C14—O2—C11—C10	170.68 (19)	N2—C7—C8—C13	−178.0 (3)
C1—N1—C4—C3	55.4 (4)	N2—C7—C8—C9	3.4 (4)
C4—N1—C5A—C6A	79.1 (7)	C7—C8—C13—C12	−178.5 (2)
C4—N1—C1—C2	−55.3 (5)	C7—C8—C9—C10	178.8 (2)
C5A—N1—C1—C2	176.3 (5)	C9—C8—C13—C12	0.1 (3)
C1—N1—C5A—C6A	−161.9 (6)	C13—C8—C9—C10	0.1 (3)
C5A—N1—C4—C3	172.1 (5)	C8—C9—C10—C11	−0.1 (3)
C6A—N2—C7—C8	−167.7 (4)	C9—C10—C11—C12	−0.3 (3)
C7—N2—C6A—C5A	−143.5 (5)	C9—C10—C11—O2	−179.44 (19)
C15—N3—N4—N5	−0.4 (3)	C10—C11—C12—C13	0.6 (3)
N4—N3—C15—C14	179.4 (2)	O2—C11—C12—C13	179.6 (2)

N4—N3—C15—C16	0.4 (3)	C11—C12—C13—C8	−0.5 (3)
N3—N4—N5—C16	0.3 (3)	O2—C14—C15—N3	65.1 (3)
N3—N4—N5—C17	178.3 (2)	O2—C14—C15—C16	−116.2 (3)
C17—N5—C16—C15	−177.8 (2)	N3—C15—C16—N5	−0.3 (3)
N4—N5—C17—C18A	108.4 (5)	C14—C15—C16—N5	−179.1 (2)
C16—N5—C17—C18A	−74.0 (5)	N5—C17—C18A—C19A	−132.7 (12)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the 1,2,3-triazole ring N3–N5/C15/C16.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6*A*—H6*A*1···*Cg*^{i}	0.97	2.90	3.617 (8)	132

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