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Crystal structure of ethyl 2-{4-[(2-oxo-3-phenyl-1,2-dihydroquinoxalin-1-yl)methyl]-1*H*-1,2,3-triazol-1-yl}acetate

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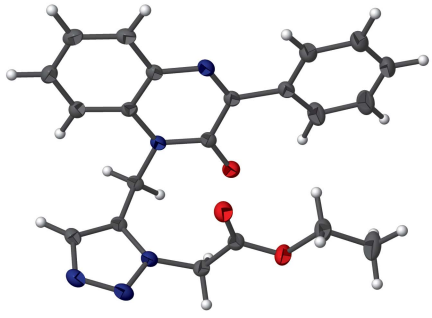
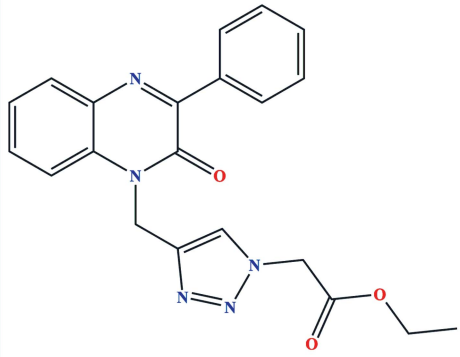
Structural data: full structural data are available from iucrdata.iucr.org

The quinoxaline portion of the title molecule, $C_{21}H_{19}N_5O_3$, is not quite planar as indicated by a dihedral angle of 3.38 (7)° between the constituent rings. The molecule is 'U-shaped', which is consolidated by an intramolecular antiparallel carbonyl electrostatic interaction with C··O distances of 2.8905 (16) and 3.0221 (15) Å, in the crystal forms corrugated layers through C—H···O and C—H···N hydrogen bonds and C—H···π(ring) and π-stacking interactions.

3D view



Chemical scheme



Structure description

Quinoxaline derivatives exhibit a wide range of biological applications including antimicrobial (Teja *et al.*, 2016), anti-inflammatory (Guirado *et al.*, 2012), anticancer (Abbas *et al.*, 2015), antidiabetic (Kulkarni *et al.*, 2012) and antihistaminic (Sridevi *et al.*, 2010) effects. As a continuation of our research on the synthesis and biological properties of quinoxaline derivatives (Missioui *et al.*, 2022*a*,*b*,*c*), the title compound was prepared and its crystal structure is reported here.

The quinoxaline portion is not quite planar as indicated by a dihedral angle of 3.38 (7)° between the constituent rings. The dihedral angle between the C9–C14 and C1/C6/N1/C7/C8/N2 rings is 9.05 (8)° while that between the latter ring and the triazole ring is 78.47 (3)°. The molecule adopts a 'U-shaped' conformation, which is consolidated by an intramolecular antiparallel carbonyl electrostatic interaction (Allen *et al.*, 1998) between the C8═O1 and C19═O2 groups with C19···O1 = 2.890 Å and C8···O2 = 3.022 Å. In the crystal, C12—H12···N3 hydrogen bonds (Table 1) lead to the formation of chains

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

*Cg*1 is the centroid of the triazole ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···N4^{i}	0.973 (16)	2.462 (16)	3.2183 (17)	134.3 (12)
C12—H12···N3^{ii}	0.988 (19)	2.572 (19)	3.4094 (18)	142.5 (15)
C15—H15*A*···*Cg*1^{iii}	0.997 (16)	2.657 (15)	3.3580 (14)	127.5 (10)
C15—H15*B*···O2^{iv}	0.986 (15)	2.464 (15)	3.2459 (16)	135.9 (11)

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{1}{2}, -y+1, z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, y, -z-\frac{1}{2}$; (iv) $x+\frac{1}{2}, y, -z+\frac{1}{2}$.

extending along the *c*-axis direction, which are linked into corrugated layers by C5—H5···N4 and C15—H15*B*···O2 hydrogen bonds and by C15—15A···*Cg*1 interactions (Table 1 and Fig. 2). These are accompanied by weak π-stacking interactions between C1/C6/N1/C7/C8/N2 and C1–C6 rings related by the symmetry operation $x-\frac{1}{2}, y, -z-\frac{1}{2}$ [centroid–centroid distance = 3.8105 (7) Å, dihedral angle = 6.13 (6)°].

Synthesis and crystallization

To a solution of 3-phenyl-1-(prop-2-yn-1-yl)quinoxalin-2(1*H*)-one (0.68 mmol) in ethanol (15 ml) was added ethyl 2-azidoacetate (1.03 mmol). The reaction mixture was stirred under reflux for 72 h. After completion of the reaction (monitored by TLC), the solution was concentrated and the residue was purified by column chromatography on silica gel by using a hexane/ethyl acetate mixture (9:1) as eluent. The solid product obtained was crystallized from ethanol solution to afford colorless crystals. Yield 80%, m.p. = 408–410 K. ^{1}H MNR (300 MHz, $CDCl_3$) δ (p.p.m.):1.22–1.26 (*t*, 3H, CH_3, J = 6 Hz); 4.12-4.19 (*q*, 2H, *O*—CH_2, J = 6 Hz); 5.57 (*s*, 2H, N—CH_2CO_2); 5.60 (s, 2*H*, *N*—CH_2); 7.72 (*s*, H,$CH_{triazole}$); 7.44–8.31 (*m*, 9H_{arom}); ^{13}C MNR (75 MHz,$CDCl_3$) δ (p.p.m.):13.95 (CH_3); 34.99 (O—CH_2); 50.01(N—CH_2C═O); 62.48 (N—CH_2); 113.48, 124.61, 128.19 (traizole), 129.52, 130.70, 130.85, 131.16, 131.79, (CH_{arom}); 132.79, 133.53, 134.34, 135.52, 153.69 (C_q);154.32 (C═O_{arom});166.80 (C═$O_{acetate}$)

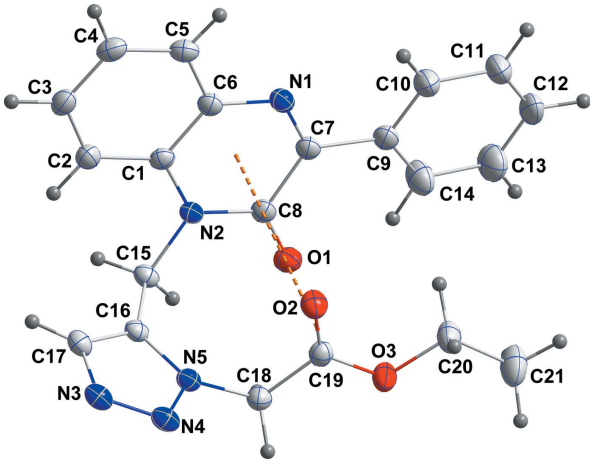

Figure 1
The title molecule with the labeling scheme and 50% probability ellipsoids. The π interaction between the C19═O2 carbonyl group and the C1/C6/N1/C7/C8/N2 ring is shown by an orange dashed line.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{19}N_5O_3$
M_r	389.41
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	150
a, *b*, *c* (Å)	8.8585 (3), 18.0405 (5), 23.1961 (7)
V (Å^3)	3707.0 (2)
Z	8
Radiation type	Cu *Kα*
μ (mm^{-1})	0.79
Crystal size (mm)	0.21 × 0.10 × 0.02
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.89, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26694, 3662, 3086
R_{int}	0.047
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.087, 1.05
No. of reflections	3662
No. of parameters	339
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.21

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

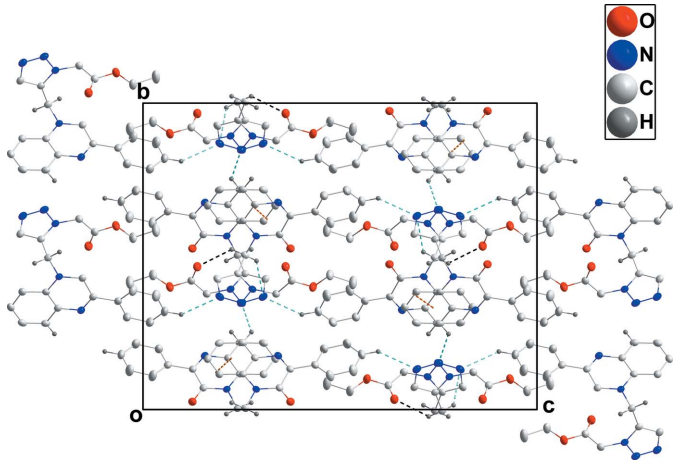

Figure 2
Packing viewed along the *a*-axis direction. C—H···O and C—H···N hydrogen bonds are shown, respectively, by black and light-blue dashed lines while the π-stacking interactions are shown by orange dashed lines.

Acknowledgements

Author contributions are as follows. Conceptualization, YR and NA; methodology, MM and AS; investigation, NA and MM; writing (original draft), JTM and YR; writing (review and editing of the manuscript), YR; formal analysis, AA and YR; supervision, YR and EME; crystal-structure determination and validation, JTM; synthesis, NA.

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full crystallographic data

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Crystal structure of ethyl 2-{4-[(2-oxo-3-phenyl-1,2-dihydroquinoxalin-1-yl)methyl]-1*H*-1,2,3-triazol-1-yl}acetate

Nadeem Abad, Mohcine Missioui, Abdulsalam Alsubari, Joel T. Mague, El Mokhtar Essassi and Youssef Ramli

2-{4-[(2-Oxo-3-phenyl-1,2-dihydroquinoxalin-1-yl)methyl]-1*H*-1,2,3-triazol-1-yl}acetate

Crystal data

$C_{21}H_{19}N_5O_3$
M_r = 389.41
Orthorhombic, *Pbca*
a = 8.8585 (3) Å
b = 18.0405 (5) Å
c = 23.1961 (7) Å
V = 3707.0 (2) Å^3
Z = 8
$F(000)$ = 1632
D_x = 1.395 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9932 reflections
θ = 3.8–72.3°
μ = 0.79 mm^{-1}
T = 150 K
Plate, colourless
0.21 × 0.10 × 0.02 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.89, T_{max} = 0.98
26694 measured reflections
3662 independent reflections
3086 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 72.5°, θ_{min} = 3.8°
h = −10→10
k = −22→22
l = −28→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.087
S = 1.05
3662 reflections
339 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 1.2273P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL 2018/1* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00064 (5)

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. 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.

All H atom positional and Uiso values were freely refined.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.43111 (11)	0.52576 (5)	0.37440 (4)	0.0275 (2)
O2	0.09359 (10)	0.46632 (5)	0.36206 (4)	0.0270 (2)
O3	0.20937 (11)	0.40033 (5)	0.43166 (4)	0.0303 (2)
N1	0.18289 (12)	0.67590 (6)	0.34317 (5)	0.0226 (2)
N2	0.34767 (11)	0.56638 (5)	0.28730 (4)	0.0193 (2)
N3	0.16535 (13)	0.36820 (6)	0.19501 (5)	0.0252 (2)
N4	0.16515 (13)	0.34789 (6)	0.24943 (5)	0.0250 (2)
N5	0.26117 (12)	0.39291 (6)	0.27772 (5)	0.0208 (2)
C1	0.26318 (14)	0.61609 (6)	0.25427 (5)	0.0195 (3)
C2	0.26183 (16)	0.61555 (7)	0.19390 (6)	0.0238 (3)
H2	0.3228 (19)	0.5802 (9)	0.1724 (7)	0.034 (4)*
C3	0.17264 (16)	0.66602 (7)	0.16465 (6)	0.0264 (3)
H3	0.1743 (18)	0.6650 (9)	0.1222 (7)	0.033 (4)*
C4	0.08259 (16)	0.71695 (7)	0.19408 (6)	0.0260 (3)
H4	0.0164 (19)	0.7523 (9)	0.1731 (7)	0.034 (4)*
C5	0.08467 (15)	0.71842 (7)	0.25326 (6)	0.0236 (3)
H5	0.0237 (18)	0.7530 (9)	0.2755 (7)	0.031 (4)*
C6	0.17717 (14)	0.66902 (7)	0.28405 (5)	0.0207 (3)
C7	0.26837 (14)	0.63234 (7)	0.37345 (5)	0.0211 (3)
C8	0.35681 (14)	0.57104 (7)	0.34670 (5)	0.0208 (3)
C9	0.27185 (16)	0.64586 (7)	0.43697 (6)	0.0248 (3)
C10	0.1715 (2)	0.69806 (8)	0.45951 (6)	0.0356 (3)
H10	0.101 (2)	0.7214 (11)	0.4333 (8)	0.053 (6)*
C11	0.1707 (2)	0.71453 (9)	0.51787 (7)	0.0435 (4)
H11	0.098 (2)	0.7522 (12)	0.5330 (9)	0.062 (6)*
C12	0.2704 (2)	0.67988 (9)	0.55500 (6)	0.0408 (4)
H12	0.268 (2)	0.6896 (11)	0.5969 (8)	0.050 (5)*
C13	0.3689 (2)	0.62824 (10)	0.53366 (7)	0.0434 (4)
H13	0.442 (2)	0.6034 (12)	0.5596 (9)	0.063 (6)*
C14	0.37072 (19)	0.61077 (9)	0.47502 (7)	0.0369 (4)
H14	0.443 (2)	0.5717 (11)	0.4606 (8)	0.051 (5)*
C15	0.42864 (14)	0.50430 (7)	0.25935 (6)	0.0206 (3)
H15A	0.5028 (17)	0.4856 (8)	0.2882 (6)	0.025 (4)*
H15B	0.4831 (17)	0.5225 (8)	0.2251 (6)	0.022 (4)*

C16	0.32363 (14)	0.44361 (6)	0.24135 (5)	0.0191 (3)
H16	0.2784 (19)	0.4473 (9)	0.1516 (7)	0.036 (4)*
C17	0.26194 (15)	0.42622 (7)	0.18895 (6)	0.0226 (3)
C18	0.28965 (15)	0.37793 (7)	0.33815 (6)	0.0232 (3)
H18A	0.3932 (19)	0.3894 (9)	0.3470 (7)	0.030 (4)*
H18B	0.2764 (17)	0.3237 (9)	0.3441 (6)	0.026 (4)*
C19	0.18500 (14)	0.42063 (7)	0.37736 (5)	0.0221 (3)
C20	0.11923 (18)	0.43913 (9)	0.47469 (6)	0.0329 (3)
H20A	0.1346 (19)	0.4932 (10)	0.4678 (7)	0.036 (4)*
H20B	0.0111 (19)	0.4247 (9)	0.4681 (7)	0.032 (4)*
C21	0.1730 (2)	0.41458 (12)	0.53292 (7)	0.0456 (4)
H21A	0.165 (2)	0.3587 (12)	0.5382 (9)	0.062 (6)*
H21B	0.111 (2)	0.4381 (11)	0.5639 (9)	0.057 (6)*
H21C	0.277 (2)	0.4295 (11)	0.5392 (8)	0.052 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0328 (5)	0.0238 (5)	0.0258 (5)	0.0042 (4)	−0.0065 (4)	0.0000 (4)
O2	0.0241 (5)	0.0317 (5)	0.0251 (5)	0.0058 (4)	−0.0013 (4)	0.0000 (4)
O3	0.0350 (5)	0.0339 (5)	0.0219 (5)	0.0116 (4)	0.0037 (4)	0.0036 (4)
N1	0.0247 (5)	0.0210 (5)	0.0222 (5)	0.0002 (4)	−0.0005 (5)	−0.0029 (4)
N2	0.0204 (5)	0.0169 (5)	0.0204 (5)	−0.0001 (4)	−0.0007 (4)	−0.0021 (4)
N3	0.0228 (6)	0.0248 (6)	0.0280 (6)	0.0015 (4)	−0.0014 (5)	−0.0069 (4)
N4	0.0232 (5)	0.0218 (5)	0.0301 (6)	−0.0013 (4)	−0.0003 (5)	−0.0062 (4)
N5	0.0212 (5)	0.0189 (5)	0.0224 (5)	−0.0007 (4)	0.0010 (4)	−0.0026 (4)
C1	0.0197 (6)	0.0167 (5)	0.0222 (6)	−0.0030 (5)	−0.0013 (5)	0.0005 (5)
C2	0.0270 (7)	0.0221 (6)	0.0223 (6)	−0.0021 (5)	0.0022 (5)	−0.0002 (5)
C3	0.0328 (7)	0.0249 (6)	0.0215 (7)	−0.0052 (6)	−0.0021 (6)	0.0031 (5)
C4	0.0280 (7)	0.0198 (6)	0.0302 (7)	−0.0029 (5)	−0.0068 (6)	0.0041 (5)
C5	0.0230 (6)	0.0184 (6)	0.0295 (7)	−0.0002 (5)	−0.0029 (5)	−0.0013 (5)
C6	0.0219 (6)	0.0185 (6)	0.0216 (6)	−0.0028 (5)	−0.0010 (5)	−0.0014 (5)
C7	0.0231 (6)	0.0189 (6)	0.0213 (6)	−0.0031 (5)	−0.0003 (5)	−0.0013 (5)
C8	0.0217 (6)	0.0195 (6)	0.0213 (6)	−0.0032 (5)	−0.0016 (5)	−0.0012 (5)
C9	0.0306 (7)	0.0215 (6)	0.0225 (7)	−0.0046 (5)	−0.0001 (6)	−0.0022 (5)
C10	0.0537 (10)	0.0285 (7)	0.0246 (7)	0.0063 (7)	0.0022 (7)	−0.0013 (6)
C11	0.0717 (12)	0.0329 (8)	0.0260 (8)	0.0098 (8)	0.0073 (8)	−0.0043 (6)
C12	0.0684 (12)	0.0340 (8)	0.0201 (7)	−0.0059 (8)	0.0021 (7)	−0.0038 (6)
C13	0.0540 (10)	0.0499 (10)	0.0263 (8)	0.0030 (8)	−0.0102 (7)	−0.0036 (7)
C14	0.0395 (8)	0.0450 (9)	0.0263 (8)	0.0067 (7)	−0.0072 (6)	−0.0068 (6)
C15	0.0179 (6)	0.0198 (6)	0.0241 (6)	0.0009 (5)	0.0017 (5)	−0.0031 (5)
C16	0.0173 (5)	0.0178 (5)	0.0222 (6)	0.0026 (5)	0.0025 (5)	−0.0024 (5)
C17	0.0211 (6)	0.0240 (6)	0.0226 (6)	0.0029 (5)	0.0008 (5)	−0.0044 (5)
C18	0.0251 (7)	0.0219 (6)	0.0226 (7)	0.0024 (5)	0.0014 (5)	0.0008 (5)
C19	0.0219 (6)	0.0232 (6)	0.0212 (6)	−0.0020 (5)	0.0006 (5)	0.0004 (5)
C20	0.0366 (8)	0.0404 (8)	0.0218 (7)	0.0107 (7)	0.0051 (6)	0.0006 (6)
C21	0.0474 (10)	0.0652 (12)	0.0241 (8)	0.0154 (9)	0.0001 (7)	0.0041 (7)

Geometric parameters (Å, º)

O1—C8	1.2301 (16)	C9—C14	1.395 (2)
O2—C19	1.2088 (16)	C9—C10	1.397 (2)
O3—C19	1.3293 (16)	C10—C11	1.386 (2)
O3—C20	1.4574 (17)	C10—H10	0.97 (2)
N1—C7	1.2978 (17)	C11—C12	1.383 (2)
N1—C6	1.3780 (16)	C11—H11	1.00 (2)
N2—C8	1.3827 (16)	C12—C13	1.369 (2)
N2—C1	1.3970 (16)	C12—H12	0.988 (19)
N2—C15	1.4797 (15)	C13—C14	1.396 (2)
N3—N4	1.3144 (16)	C13—H13	0.99 (2)
N3—C17	1.3592 (18)	C14—H14	1.01 (2)
N4—N5	1.3468 (15)	C15—C16	1.4962 (17)
N5—C16	1.3618 (16)	C15—H15A	0.997 (16)
N5—C18	1.4497 (17)	C15—H15B	0.986 (15)
C1—C2	1.4005 (18)	C16—C17	1.3691 (18)
C1—C6	1.4034 (17)	C17—H16	0.957 (17)
C2—C3	1.3832 (19)	C18—C19	1.5100 (18)
C2—H2	0.974 (17)	C18—H18A	0.963 (17)
C3—C4	1.395 (2)	C18—H18B	0.995 (16)
C3—H3	0.984 (16)	C20—C21	1.499 (2)
C4—C5	1.3732 (19)	C20—H20A	0.997 (18)
C4—H4	0.994 (17)	C20—H20B	1.005 (17)
C5—C6	1.4055 (18)	C21—H21A	1.02 (2)
C5—H5	0.973 (16)	C21—H21B	1.00 (2)
C7—C8	1.4905 (17)	C21—H21C	0.97 (2)
C7—C9	1.4937 (17)		
C19—O3—C20	115.32 (11)	C13—C12—C11	119.30 (14)
C7—N1—C6	120.37 (11)	C13—C12—H12	119.4 (11)
C8—N2—C1	122.62 (10)	C11—C12—H12	121.2 (11)
C8—N2—C15	117.02 (10)	C12—C13—C14	120.87 (16)
C1—N2—C15	120.34 (10)	C12—C13—H13	120.3 (12)
N4—N3—C17	108.35 (11)	C14—C13—H13	118.8 (12)
N3—N4—N5	107.40 (10)	C9—C14—C13	120.44 (15)
N4—N5—C16	111.08 (10)	C9—C14—H14	120.3 (11)
N4—N5—C18	117.95 (10)	C13—C14—H14	119.2 (11)
C16—N5—C18	130.82 (11)	N2—C15—C16	112.02 (10)
N2—C1—C2	123.27 (11)	N2—C15—H15A	106.4 (9)
N2—C1—C6	117.23 (11)	C16—C15—H15A	110.4 (9)
C2—C1—C6	119.49 (12)	N2—C15—H15B	109.8 (8)
C3—C2—C1	119.38 (12)	C16—C15—H15B	108.9 (8)
C3—C2—H2	119.8 (10)	H15A—C15—H15B	109.3 (12)
C1—C2—H2	120.8 (10)	N5—C16—C17	103.54 (11)
C2—C3—C4	121.35 (12)	N5—C16—C15	124.84 (11)
C2—C3—H3	118.0 (10)	C17—C16—C15	131.57 (12)
C4—C3—H3	120.7 (10)	N3—C17—C16	109.62 (12)

C5—C4—C3	119.61 (12)	N3—C17—H16	119.7 (10)
C5—C4—H4	119.1 (10)	C16—C17—H16	130.7 (10)
C3—C4—H4	121.3 (10)	N5—C18—C19	112.36 (11)
C4—C5—C6	120.24 (12)	N5—C18—H18A	109.3 (10)
C4—C5—H5	122.3 (9)	C19—C18—H18A	110.3 (10)
C6—C5—H5	117.4 (9)	N5—C18—H18B	107.3 (9)
N1—C6—C1	122.08 (11)	C19—C18—H18B	110.2 (9)
N1—C6—C5	118.04 (11)	H18A—C18—H18B	107.1 (13)
C1—C6—C5	119.86 (12)	O2—C19—O3	125.10 (12)
N1—C7—C8	122.05 (11)	O2—C19—C18	125.61 (12)
N1—C7—C9	116.55 (11)	O3—C19—C18	109.29 (11)
C8—C7—C9	121.40 (11)	O3—C20—C21	107.51 (13)
O1—C8—N2	120.76 (12)	O3—C20—H20A	106.6 (10)
O1—C8—C7	123.81 (12)	C21—C20—H20A	112.9 (10)
N2—C8—C7	115.41 (11)	O3—C20—H20B	107.1 (9)
C14—C9—C10	117.95 (13)	C21—C20—H20B	111.4 (9)
C14—C9—C7	124.25 (13)	H20A—C20—H20B	111.0 (14)
C10—C9—C7	117.79 (12)	C20—C21—H21A	112.3 (12)
C11—C10—C9	120.89 (15)	C20—C21—H21B	110.4 (12)
C11—C10—H10	121.1 (12)	H21A—C21—H21B	107.3 (16)
C9—C10—H10	118.0 (12)	C20—C21—H21C	110.8 (12)
C12—C11—C10	120.55 (16)	H21A—C21—H21C	108.7 (17)
C12—C11—H11	120.0 (12)	H21B—C21—H21C	107.2 (16)
C10—C11—H11	119.4 (12)		

C17—N3—N4—N5	0.03 (14)	N1—C7—C9—C14	−171.75 (14)
N3—N4—N5—C16	0.56 (13)	C8—C7—C9—C14	9.3 (2)
N3—N4—N5—C18	−175.36 (10)	N1—C7—C9—C10	6.99 (18)
C8—N2—C1—C2	175.04 (12)	C8—C7—C9—C10	−172.00 (13)
C15—N2—C1—C2	−6.76 (18)	C14—C9—C10—C11	0.2 (2)
C8—N2—C1—C6	−4.48 (17)	C7—C9—C10—C11	−178.63 (15)
C15—N2—C1—C6	173.72 (11)	C9—C10—C11—C12	0.5 (3)
N2—C1—C2—C3	178.84 (12)	C10—C11—C12—C13	−0.9 (3)
C6—C1—C2—C3	−1.65 (19)	C11—C12—C13—C14	0.6 (3)
C1—C2—C3—C4	−0.7 (2)	C10—C9—C14—C13	−0.5 (2)
C2—C3—C4—C5	1.5 (2)	C7—C9—C14—C13	178.27 (15)
C3—C4—C5—C6	0.1 (2)	C12—C13—C14—C9	0.1 (3)
C7—N1—C6—C1	−0.69 (19)	C8—N2—C15—C16	103.20 (13)
C7—N1—C6—C5	−178.96 (12)	C1—N2—C15—C16	−75.10 (14)
N2—C1—C6—N1	4.56 (18)	N4—N5—C16—C17	−0.90 (13)
C2—C1—C6—N1	−174.98 (12)	C18—N5—C16—C17	174.34 (12)
N2—C1—C6—C5	−177.20 (11)	N4—N5—C16—C15	176.59 (11)
C2—C1—C6—C5	3.26 (18)	C18—N5—C16—C15	−8.2 (2)
C4—C5—C6—N1	175.80 (12)	N2—C15—C16—N5	−76.76 (15)
C4—C5—C6—C1	−2.51 (19)	N2—C15—C16—C17	99.98 (15)
C6—N1—C7—C8	−3.34 (18)	N4—N3—C17—C16	−0.61 (14)
C6—N1—C7—C9	177.67 (11)	N5—C16—C17—N3	0.91 (13)
C1—N2—C8—O1	179.23 (11)	C15—C16—C17—N3	−176.34 (12)

C15—N2—C8—O1	0.97 (17)	N4—N5—C18—C19	−92.47 (13)
C1—N2—C8—C7	0.80 (17)	C16—N5—C18—C19	92.57 (15)
C15—N2—C8—C7	−177.45 (10)	C20—O3—C19—O2	−1.8 (2)
N1—C7—C8—O1	−175.08 (12)	C20—O3—C19—C18	178.01 (12)
C9—C7—C8—O1	3.85 (19)	N5—C18—C19—O2	−4.81 (19)
N1—C7—C8—N2	3.29 (18)	N5—C18—C19—O3	175.42 (10)
C9—C7—C8—N2	−177.78 (11)	C19—O3—C20—C21	−174.39 (14)

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the triazole ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···N4^{i}	0.973 (16)	2.462 (16)	3.2183 (17)	134.3 (12)
C12—H12···N3^{ii}	0.988 (19)	2.572 (19)	3.4094 (18)	142.5 (15)
C15—H15*A*···*Cg*1^{iii}	0.997 (16)	2.657 (15)	3.3580 (14)	127.5 (10)
C15—H15*B*···O2^{iv}	0.986 (15)	2.464 (15)	3.2459 (16)	135.9 (11)

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1/2; (ii) −*x*+1/2, −*y*+1, *z*+1/2; (iii) *x*−1/2, *y*, −*z*−1/2; (iv) *x*+1/2, *y*, −*z*+1/2.