IUCrData

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(*E*)-1-[5-Methyl-1-(*p*-tolyl)-1*H*-1,2,3-triazol-4-yl]-3-{3-[5-methyl-1-(*p*-tolyl)-1*H*-1,2,3-triazol-4-yl]-1-phenyl-1*H*-pyrazol-4-yl}prop-2-en-1-one

Mohammed Abu Bakr Abu El-Enin,[a] Bakr F. Abdel-Wahab,[b,c] Mohammed Baashen,[b] Hazem A. Ghabbour[a] and Gamal A. El-Hiti[d]*

[a]Department of Medicinal Chemistry, Faculty of Pharmacy, University of Mansoura, Mansoura 35516, Egypt, [b]Department of Chemistry, College of Science and Humanities, Shaqra University, Duwadimi, Saudi Arabia, [c]Applied Organic Chemistry Department, National Research Centre, Dokki, Giza, Egypt, and [d]Cornea Research Chair, Department of Optometry, College of Applied Medical Sciences, King Saud University, PO Box 10219, Riyadh 11433, Saudi Arabia. *Correspondence e-mail: gelhiti@ksu.edu.sa

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Keywords: crystal structure; pyrazole; triazole; C—H···π interactions.

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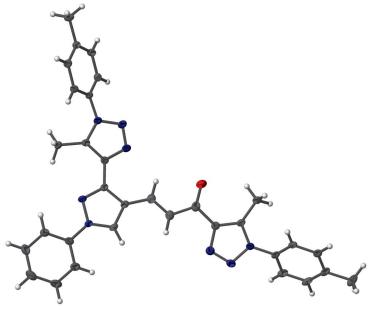
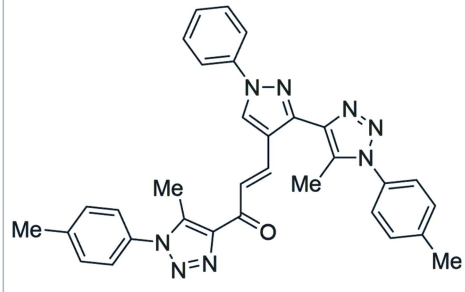
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{32}H_{28}N_8O$, the central pyrazole ring makes dihedral angles of 10.04 (14) and 11.37 (13)° with the two 1,2,3-triazole rings. In the molecule, there are weak intramolecular C—H···O and C—H···N contacts present that affect the molecular conformation. The configuration about the C=C bond is *E*. In the crystal, molecules are linked by C—H···π interactions, forming slabs parallel to the *ac* plane.

3D view



Chemical scheme



Structure description

Chalcones have a wide range of biological activities and have antiviral, antibacterial, antiprotozoal, insecticidal and immunosuppressive (Katsori & Hadjipavlou-Litina, 2011; Matos *et al.*, 2015; Repanas *et al.*, 2013) properties. 1,2,3-Triazoles are interesting heterocycles that have major applications in biotechnology and in particular in drug discovery (Totobenazara & Burke, 2015; Dheer *et al.*, 2017). Heterocycles containing a 1,2,3-triazole ring system have been used in the treatment of cancer cells (Yadav *et al.*, 2017). In addition, heterocycles having pyrazole moieties have antimicrobial, anticancer, anti-inflammatory, antidepressant, antioxidant and herbicidal properties (Ansari *et al.*, 2017). They also act as the core in many drugs such as Celebrex, Sildenafil and Difenamizole (Ansari *et al.*, 2017).

In the title compound (Fig. 1), the central pyrazole ring (N4/N5/C11–C13) makes dihedral angles of 10.04 (14) and 11.37 (13)° with the triazole rings C9/C10/N1–N3 and C23/C24/N6–N8, respectively. The *p*-tolyl rings (C1–C6 and C26—32) make nearly equal

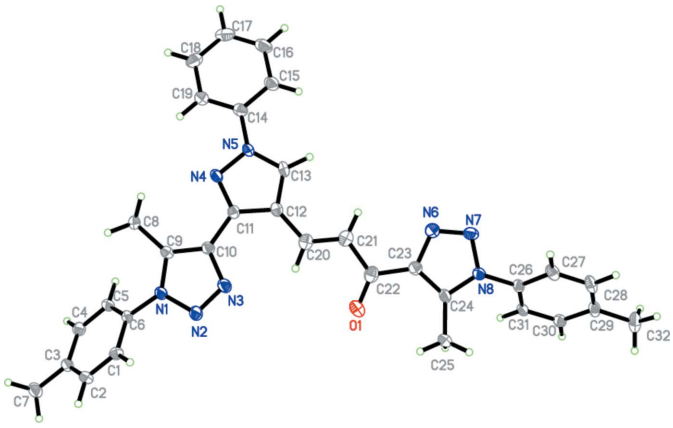


Figure 1
A view of the molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

dihedral angles, of 43.71 (13) and 48.35 (12)°, with the triazole rings to which they are attached, *viz*. C9/C10/N1–N3 and C23/C24/N6–N8, respectively. The phenyl ring (C14–C19) is inclined by 8.90 (13)° to the central pyrazole ring to which it is attached. There are some short C—H···N and C—H···O intramolecular contacts present (Table 1), and the configuration about the C20═C21 bond is *E*.

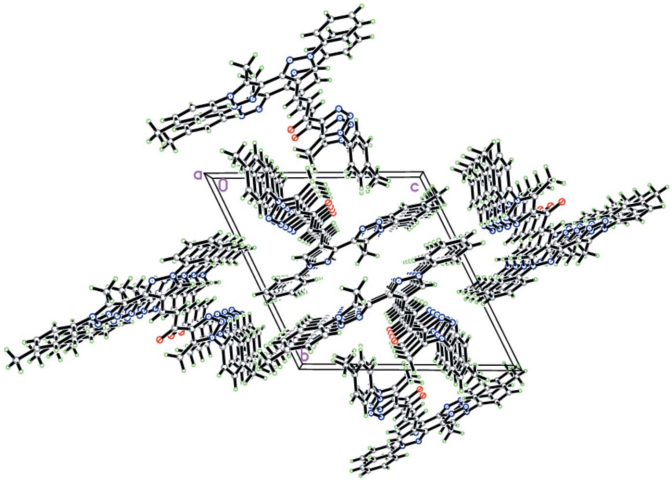


Figure 2
A view along the *a* axis of the crystal packing of the title compound.

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

*Cg*4, *Cg*5 and *Cg*6 are the centroids of rings C1–C6, C14–C19 and C26–C31, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···N4	0.98	2.57	3.141 (2)	118
C20—H20*A*···N3	0.95	2.43	3.049 (3)	122
C25—H25*A*···O1	0.98	2.51	3.112 (3)	119
C1—H1*A*···*Cg*5^{i}	0.95	2.86	3.613 (3)	137
C7—H7*A*···*Cg*6^{ii}	0.98	2.84	3.687 (2)	145
C18—H18*A*···*Cg*4^{iii}	0.95	2.76	3.503 (3)	136

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x-2, y, z+1$; (iii) $-x-1, -y+1, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{32}H_{28}N_8O$
M_r	540.62
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	6.6115 (4), 15.2036 (9), 15.3021 (8)
α, β, γ (°)	63.536 (2), 83.760 (2), 85.214 (2)
V (Å^3)	1367.75 (14)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.42 × 0.34 × 0.26
Data collection	
Diffractometer	Bruker APEXII D8 venture
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.878, 0.938
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26981, 6283, 4464
R_{int}	0.088
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.058, 0.154, 1.03
No. of reflections	6283
No. of parameters	374
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.67, −0.34

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

The crystal packing of the title compound is illustrated in Fig. 2. Molecules are linked only by C—H···π interactions, forming slabs parallel to the *ac* plane (Table 1 and Fig. 3).

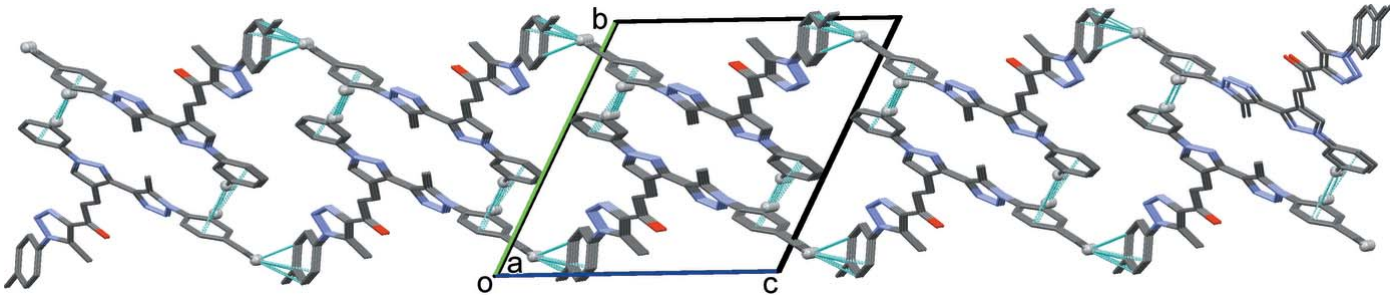


Figure 3
A view along the *a* axis of the crystal packing of the title compound, with the C—H···π interactions (Table 1) represented by dashed lines. Only H atoms H1*A*, H7*A* and H18*A* (grey balls) have been included.

Synthesis and crystallization

The title compound was synthesized from the reaction of an equimolar mixture of 1-(5-methyl-1-(*p*-tolyl)-1*H*-1,2,3-triazol-4-yl)ethanone and 3-(5-methyl-1-(*p*-tolyl)-1*H*-1,2,3-triazol-4-yl)-1-phenyl-1*H*-pyrazole-4-carbaldehyde in alcoholic sodium hydroxide at room temperature for 4 h. The mixture was then filtered, washed with cold water, and dried. It was recrystallized from dimethylformamide to give yellow block-like crystals of the title compound in 72% yield.

Refinement

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

Funding information

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full crystallographic data

IUCrData (2017). **2**, x171729 [https://doi.org/10.1107/S2414314617017291]

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Crystal data

$C_{32}H_{28}N_8O$
M_r = 540.62
Triclinic, $P\overline{1}$
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b = 15.2036 (9) Å
c = 15.3021 (8) Å
α = 63.536 (2)°
β = 83.760 (2)°
γ = 85.214 (2)°
V = 1367.75 (14) Å^3
Z = 2
$F(000)$ = 568
D_x = 1.313 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9973 reflections
θ = 2.5–30.5°
μ = 0.08 mm^{-1}
T = 100 K
Block, yellow
0.42 × 0.34 × 0.26 mm

Data collection

Bruker APEXII D8 venture diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.878, T_{max} = 0.938
26981 measured reflections
6283 independent reflections
4464 reflections with $I > 2\sigma(I)$
R_{int} = 0.088
θ_{max} = 27.5°, θ_{min} = 2.5°
h = −8→8
k = −19→19
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.154
S = 1.03
6283 reflections
374 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.7631P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.7951 (2)	0.17053 (13)	0.50320 (11)	0.0370 (4)
N1	−0.0630 (2)	0.28980 (13)	0.68222 (11)	0.0200 (4)
N2	0.1336 (2)	0.25485 (14)	0.68809 (12)	0.0263 (4)
N3	0.2198 (2)	0.29057 (14)	0.59887 (12)	0.0252 (4)
N4	−0.0032 (2)	0.45359 (12)	0.36951 (11)	0.0193 (4)
N5	0.0870 (2)	0.47640 (12)	0.27774 (11)	0.0183 (4)
N6	1.0191 (3)	0.27777 (13)	0.25446 (12)	0.0222 (4)
N7	1.1863 (3)	0.25088 (13)	0.21820 (12)	0.0228 (4)
N8	1.2726 (2)	0.17300 (13)	0.29442 (11)	0.0194 (4)
C1	−0.1322 (3)	0.23458 (15)	0.85782 (14)	0.0208 (4)
H1A	−0.0037	0.2567	0.8603	0.025*
C2	−0.2567 (3)	0.18693 (16)	0.94265 (14)	0.0232 (4)
H2A	−0.2114	0.1757	1.0037	0.028*
C3	−0.4471 (3)	0.15496 (15)	0.94053 (14)	0.0213 (4)
C4	−0.5095 (3)	0.17178 (15)	0.85029 (14)	0.0218 (4)
H4A	−0.6390	0.1508	0.8474	0.026*
C5	−0.3870 (3)	0.21844 (15)	0.76466 (14)	0.0212 (4)
H5A	−0.4314	0.2291	0.7036	0.025*
C6	−0.1987 (3)	0.24947 (15)	0.76896 (13)	0.0185 (4)
C7	−0.5837 (3)	0.10487 (17)	1.03297 (15)	0.0270 (5)
H7A	−0.5004	0.0711	1.0888	0.040*
H7B	−0.6642	0.0569	1.0269	0.040*
H7C	−0.6753	0.1541	1.0433	0.040*
C8	−0.2994 (3)	0.40571 (15)	0.55863 (14)	0.0213 (4)
H8A	−0.2758	0.4652	0.4972	0.032*
H8B	−0.3588	0.4241	0.6100	0.032*
H8C	−0.3932	0.3644	0.5495	0.032*
C9	−0.1023 (3)	0.35002 (15)	0.58793 (13)	0.0180 (4)
C10	0.0801 (3)	0.34833 (15)	0.53545 (13)	0.0184 (4)
C11	0.1313 (3)	0.39191 (14)	0.42960 (13)	0.0171 (4)
C12	0.3092 (3)	0.37502 (14)	0.37716 (14)	0.0185 (4)
C13	0.2718 (3)	0.43107 (15)	0.28052 (14)	0.0202 (4)
H13A	0.3609	0.4368	0.2253	0.024*
C14	−0.0290 (3)	0.53202 (15)	0.19575 (14)	0.0212 (4)
C15	0.0583 (3)	0.55568 (16)	0.10112 (14)	0.0274 (5)
H15A	0.1957	0.5363	0.0909	0.033*
C16	−0.0578 (4)	0.60778 (17)	0.02237 (15)	0.0324 (5)
H16A	0.0009	0.6246	−0.0423	0.039*
C17	−0.2587 (4)	0.63555 (17)	0.03701 (16)	0.0337 (5)

H17A	−0.3380	0.6704	−0.0173	0.040*
C18	−0.3436 (4)	0.61221 (16)	0.13137 (16)	0.0302 (5)
H18A	−0.4809	0.6318	0.1416	0.036*
C19	−0.2287 (3)	0.56036 (16)	0.21084 (15)	0.0251 (5)
H19A	−0.2871	0.5444	0.2754	0.030*
C20	0.4818 (3)	0.30783 (16)	0.41561 (15)	0.0232 (4)
H20A	0.4693	0.2635	0.4833	0.028*
C21	0.6557 (3)	0.30219 (16)	0.36538 (16)	0.0247 (5)
H21A	0.6782	0.3466	0.2981	0.030*
C22	0.8134 (3)	0.22675 (16)	0.41472 (16)	0.0257 (5)
C23	0.9948 (3)	0.21833 (15)	0.35317 (14)	0.0202 (4)
C24	1.1576 (3)	0.15204 (16)	0.37967 (14)	0.0209 (4)
C25	1.2209 (3)	0.07752 (18)	0.47675 (14)	0.0307 (5)
H25A	1.1465	0.0911	0.5287	0.046*
H25B	1.3675	0.0807	0.4792	0.046*
H25C	1.1903	0.0117	0.4862	0.046*
C26	1.4548 (3)	0.12449 (16)	0.27571 (13)	0.0200 (4)
C27	1.6177 (3)	0.18001 (17)	0.21906 (14)	0.0251 (5)
H27A	1.6094	0.2497	0.1930	0.030*
C28	1.7930 (3)	0.13189 (18)	0.20111 (15)	0.0262 (5)
H28A	1.9051	0.1695	0.1622	0.031*
C29	1.8091 (3)	0.03052 (17)	0.23828 (15)	0.0248 (5)
C30	1.6415 (3)	−0.02356 (17)	0.29395 (14)	0.0227 (4)
H30A	1.6491	−0.0932	0.3194	0.027*
C31	1.4648 (3)	0.02278 (16)	0.31252 (13)	0.0210 (4)
H31A	1.3513	−0.0146	0.3501	0.025*
C32	2.0027 (3)	−0.0207 (2)	0.22046 (18)	0.0357 (6)
H32A	2.0394	−0.0753	0.2823	0.054*
H32B	2.1124	0.0260	0.1939	0.054*
H32C	1.9823	−0.0461	0.1735	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0352 (9)	0.0439 (10)	0.0236 (8)	0.0030 (8)	0.0066 (7)	−0.0101 (8)
N1	0.0153 (8)	0.0290 (10)	0.0153 (8)	−0.0012 (7)	−0.0011 (6)	−0.0094 (7)
N2	0.0127 (8)	0.0428 (12)	0.0196 (9)	−0.0008 (8)	−0.0003 (7)	−0.0107 (8)
N3	0.0170 (8)	0.0373 (11)	0.0177 (8)	−0.0020 (8)	0.0005 (7)	−0.0091 (8)
N4	0.0200 (8)	0.0232 (9)	0.0144 (8)	−0.0016 (7)	0.0015 (6)	−0.0084 (7)
N5	0.0195 (8)	0.0209 (9)	0.0145 (8)	−0.0003 (7)	0.0021 (6)	−0.0086 (7)
N6	0.0216 (9)	0.0243 (10)	0.0222 (9)	−0.0028 (7)	−0.0028 (7)	−0.0111 (8)
N7	0.0251 (9)	0.0242 (10)	0.0168 (8)	−0.0018 (7)	−0.0035 (7)	−0.0066 (7)
N8	0.0182 (8)	0.0252 (9)	0.0145 (8)	−0.0006 (7)	−0.0014 (6)	−0.0086 (7)
C1	0.0192 (10)	0.0243 (11)	0.0197 (10)	0.0007 (8)	−0.0045 (8)	−0.0101 (9)
C2	0.0272 (11)	0.0273 (12)	0.0151 (9)	0.0016 (9)	−0.0033 (8)	−0.0094 (9)
C3	0.0231 (10)	0.0215 (11)	0.0171 (9)	0.0019 (8)	0.0013 (8)	−0.0078 (8)
C4	0.0179 (10)	0.0253 (11)	0.0209 (10)	−0.0023 (8)	−0.0002 (8)	−0.0092 (9)
C5	0.0203 (10)	0.0282 (12)	0.0154 (9)	0.0014 (9)	−0.0028 (8)	−0.0099 (9)

C6	0.0155 (9)	0.0230 (11)	0.0149 (9)	0.0000 (8)	0.0015 (7)	−0.0072 (8)
C7	0.0285 (11)	0.0286 (12)	0.0202 (10)	−0.0033 (9)	0.0052 (9)	−0.0086 (9)
C8	0.0180 (10)	0.0235 (11)	0.0197 (10)	0.0020 (8)	0.0015 (8)	−0.0084 (9)
C9	0.0193 (10)	0.0201 (10)	0.0149 (9)	−0.0030 (8)	−0.0009 (7)	−0.0077 (8)
C10	0.0172 (9)	0.0224 (11)	0.0163 (9)	−0.0013 (8)	−0.0029 (7)	−0.0087 (8)
C11	0.0151 (9)	0.0192 (10)	0.0182 (9)	−0.0031 (8)	0.0002 (7)	−0.0092 (8)
C12	0.0181 (9)	0.0192 (10)	0.0198 (9)	−0.0041 (8)	0.0019 (8)	−0.0104 (8)
C13	0.0192 (10)	0.0234 (11)	0.0195 (9)	−0.0040 (8)	0.0054 (8)	−0.0119 (9)
C14	0.0285 (11)	0.0175 (10)	0.0174 (9)	−0.0016 (8)	−0.0015 (8)	−0.0077 (8)
C15	0.0359 (12)	0.0258 (12)	0.0193 (10)	0.0022 (10)	0.0010 (9)	−0.0103 (9)
C16	0.0511 (15)	0.0272 (12)	0.0170 (10)	0.0008 (11)	−0.0013 (10)	−0.0088 (9)
C17	0.0475 (15)	0.0253 (12)	0.0248 (11)	0.0042 (11)	−0.0124 (10)	−0.0067 (10)
C18	0.0304 (12)	0.0232 (12)	0.0322 (12)	0.0040 (10)	−0.0068 (10)	−0.0077 (10)
C19	0.0270 (11)	0.0241 (11)	0.0208 (10)	−0.0006 (9)	0.0008 (8)	−0.0076 (9)
C20	0.0211 (10)	0.0237 (11)	0.0280 (11)	−0.0021 (9)	−0.0023 (8)	−0.0138 (9)
C21	0.0232 (11)	0.0243 (11)	0.0289 (11)	−0.0012 (9)	−0.0027 (9)	−0.0137 (9)
C22	0.0217 (10)	0.0278 (12)	0.0315 (12)	−0.0014 (9)	−0.0025 (9)	−0.0162 (10)
C23	0.0190 (10)	0.0234 (11)	0.0198 (10)	−0.0027 (8)	−0.0020 (8)	−0.0106 (9)
C24	0.0184 (10)	0.0292 (11)	0.0165 (9)	−0.0015 (8)	0.0010 (8)	−0.0117 (9)
C25	0.0281 (12)	0.0427 (14)	0.0167 (10)	0.0069 (10)	0.0000 (9)	−0.0107 (10)
C26	0.0161 (9)	0.0336 (12)	0.0140 (9)	−0.0005 (8)	−0.0001 (7)	−0.0141 (9)
C27	0.0264 (11)	0.0322 (12)	0.0207 (10)	−0.0082 (9)	0.0027 (8)	−0.0150 (9)
C28	0.0212 (10)	0.0419 (14)	0.0236 (10)	−0.0117 (10)	0.0070 (8)	−0.0217 (10)
C29	0.0177 (10)	0.0427 (14)	0.0218 (10)	−0.0031 (9)	0.0011 (8)	−0.0215 (10)
C30	0.0205 (10)	0.0312 (12)	0.0176 (9)	−0.0008 (9)	−0.0017 (8)	−0.0116 (9)
C31	0.0167 (10)	0.0307 (12)	0.0142 (9)	−0.0037 (9)	0.0005 (7)	−0.0085 (9)
C32	0.0200 (11)	0.0532 (16)	0.0441 (14)	−0.0046 (11)	0.0062 (10)	−0.0320 (13)

Geometric parameters (Å, º)

O1—C22	1.236 (3)	C12—C20	1.451 (3)
N1—N2	1.359 (2)	C13—H13A	0.9500
N1—C9	1.361 (2)	C14—C19	1.382 (3)
N1—C6	1.432 (2)	C14—C15	1.396 (3)
N2—N3	1.306 (2)	C15—C16	1.385 (3)
N3—C10	1.366 (3)	C15—H15A	0.9500
N4—C11	1.336 (3)	C16—C17	1.385 (3)
N4—N5	1.366 (2)	C16—H16A	0.9500
N5—C13	1.347 (3)	C17—C18	1.388 (3)
N5—C14	1.426 (3)	C17—H17A	0.9500
N6—N7	1.300 (2)	C18—C19	1.387 (3)
N6—C23	1.371 (3)	C18—H18A	0.9500
N7—N8	1.374 (2)	C19—H19A	0.9500
N8—C24	1.355 (2)	C20—C21	1.331 (3)
N8—C26	1.429 (3)	C20—H20A	0.9500
C1—C2	1.384 (3)	C21—C22	1.474 (3)
C1—C6	1.390 (3)	C21—H21A	0.9500
C1—H1A	0.9500	C22—C23	1.476 (3)

C2—C3	1.396 (3)	C23—C24	1.374 (3)
C2—H2A	0.9500	C24—C25	1.491 (3)
C3—C4	1.391 (3)	C25—H25A	0.9800
C3—C7	1.508 (3)	C25—H25B	0.9800
C4—C5	1.383 (3)	C25—H25C	0.9800
C4—H4A	0.9500	C26—C27	1.386 (3)
C5—C6	1.386 (3)	C26—C31	1.388 (3)
C5—H5A	0.9500	C27—C28	1.387 (3)
C7—H7A	0.9800	C27—H27A	0.9500
C7—H7B	0.9800	C28—C29	1.384 (3)
C7—H7C	0.9800	C28—H28A	0.9500
C8—C9	1.490 (3)	C29—C30	1.397 (3)
C8—H8A	0.9800	C29—C32	1.505 (3)
C8—H8B	0.9800	C30—C31	1.382 (3)
C8—H8C	0.9800	C30—H30A	0.9500
C9—C10	1.379 (3)	C31—H31A	0.9500
C10—C11	1.462 (3)	C32—H32A	0.9800
C11—C12	1.422 (3)	C32—H32B	0.9800
C12—C13	1.377 (3)	C32—H32C	0.9800

N2—N1—C9	111.26 (15)	C15—C14—N5	119.88 (18)
N2—N1—C6	117.81 (16)	C16—C15—C14	119.2 (2)
C9—N1—C6	130.29 (16)	C16—C15—H15A	120.4
N3—N2—N1	107.08 (16)	C14—C15—H15A	120.4
N2—N3—C10	109.07 (16)	C15—C16—C17	120.6 (2)
C11—N4—N5	104.41 (15)	C15—C16—H16A	119.7
C13—N5—N4	111.86 (15)	C17—C16—H16A	119.7
C13—N5—C14	129.12 (16)	C16—C17—C18	119.7 (2)
N4—N5—C14	118.53 (15)	C16—C17—H17A	120.1
N7—N6—C23	109.15 (17)	C18—C17—H17A	120.1
N6—N7—N8	107.08 (15)	C19—C18—C17	120.2 (2)
C24—N8—N7	110.62 (16)	C19—C18—H18A	119.9
C24—N8—C26	129.57 (17)	C17—C18—H18A	119.9
N7—N8—C26	119.76 (15)	C14—C19—C18	119.74 (19)
C2—C1—C6	118.81 (18)	C14—C19—H19A	120.1
C2—C1—H1A	120.6	C18—C19—H19A	120.1
C6—C1—H1A	120.6	C21—C20—C12	126.4 (2)
C1—C2—C3	121.52 (18)	C21—C20—H20A	116.8
C1—C2—H2A	119.2	C12—C20—H20A	116.8
C3—C2—H2A	119.2	C20—C21—C22	119.7 (2)
C4—C3—C2	118.15 (18)	C20—C21—H21A	120.2
C4—C3—C7	120.57 (18)	C22—C21—H21A	120.2
C2—C3—C7	121.27 (18)	O1—C22—C21	122.4 (2)
C5—C4—C3	121.35 (18)	O1—C22—C23	120.5 (2)
C5—C4—H4A	119.3	C21—C22—C23	117.07 (18)
C3—C4—H4A	119.3	N6—C23—C24	108.92 (17)
C4—C5—C6	119.24 (18)	N6—C23—C22	122.34 (19)
C4—C5—H5A	120.4	C24—C23—C22	128.70 (18)

C6—C5—H5A	120.4	N8—C24—C23	104.22 (17)
C5—C6—C1	120.92 (17)	N8—C24—C25	123.29 (18)
C5—C6—N1	119.71 (17)	C23—C24—C25	132.29 (18)
C1—C6—N1	119.15 (17)	C24—C25—H25A	109.5
C3—C7—H7A	109.5	C24—C25—H25B	109.5
C3—C7—H7B	109.5	H25A—C25—H25B	109.5
H7A—C7—H7B	109.5	C24—C25—H25C	109.5
C3—C7—H7C	109.5	H25A—C25—H25C	109.5
H7A—C7—H7C	109.5	H25B—C25—H25C	109.5
H7B—C7—H7C	109.5	C27—C26—C31	120.89 (19)
C9—C8—H8A	109.5	C27—C26—N8	119.39 (19)
C9—C8—H8B	109.5	C31—C26—N8	119.71 (17)
H8A—C8—H8B	109.5	C26—C27—C28	118.7 (2)
C9—C8—H8C	109.5	C26—C27—H27A	120.7
H8A—C8—H8C	109.5	C28—C27—H27A	120.7
H8B—C8—H8C	109.5	C29—C28—C27	121.79 (19)
N1—C9—C10	103.47 (17)	C29—C28—H28A	119.1
N1—C9—C8	123.94 (17)	C27—C28—H28A	119.1
C10—C9—C8	132.48 (17)	C28—C29—C30	118.32 (19)
N3—C10—C9	109.10 (16)	C28—C29—C32	121.08 (19)
N3—C10—C11	120.75 (17)	C30—C29—C32	120.6 (2)
C9—C10—C11	130.02 (18)	C31—C30—C29	121.0 (2)
N4—C11—C12	111.88 (16)	C31—C30—H30A	119.5
N4—C11—C10	119.48 (17)	C29—C30—H30A	119.5
C12—C11—C10	128.59 (18)	C30—C31—C26	119.34 (18)
C13—C12—C11	103.66 (17)	C30—C31—H31A	120.3
C13—C12—C20	127.75 (18)	C26—C31—H31A	120.3
C11—C12—C20	128.38 (18)	C29—C32—H32A	109.5
N5—C13—C12	108.19 (16)	C29—C32—H32B	109.5
N5—C13—H13A	125.9	H32A—C32—H32B	109.5
C12—C13—H13A	125.9	C29—C32—H32C	109.5
C19—C14—C15	120.50 (19)	H32A—C32—H32C	109.5
C19—C14—N5	119.61 (17)	H32B—C32—H32C	109.5

C9—N1—N2—N3	−1.0 (2)	C13—N5—C14—C19	170.5 (2)
C6—N1—N2—N3	170.78 (17)	N4—N5—C14—C19	−0.7 (3)
N1—N2—N3—C10	0.0 (2)	C13—N5—C14—C15	−8.2 (3)
C11—N4—N5—C13	−0.4 (2)	N4—N5—C14—C15	−179.39 (18)
C11—N4—N5—C14	172.27 (16)	C19—C14—C15—C16	−0.1 (3)
C23—N6—N7—N8	−0.2 (2)	N5—C14—C15—C16	178.52 (19)
N6—N7—N8—C24	−0.7 (2)	C14—C15—C16—C17	−0.5 (3)
N6—N7—N8—C26	176.95 (16)	C15—C16—C17—C18	0.9 (3)
C6—C1—C2—C3	−0.8 (3)	C16—C17—C18—C19	−0.7 (3)
C1—C2—C3—C4	0.3 (3)	C15—C14—C19—C18	0.4 (3)
C1—C2—C3—C7	−178.8 (2)	N5—C14—C19—C18	−178.29 (19)
C2—C3—C4—C5	0.3 (3)	C17—C18—C19—C14	0.1 (3)
C7—C3—C4—C5	179.4 (2)	C13—C12—C20—C21	14.5 (3)
C3—C4—C5—C6	−0.3 (3)	C11—C12—C20—C21	−171.7 (2)

C4—C5—C6—C1	−0.2 (3)	C12—C20—C21—C22	−177.51 (18)
C4—C5—C6—N1	174.40 (19)	C20—C21—C22—O1	−3.5 (3)
C2—C1—C6—C5	0.8 (3)	C20—C21—C22—C23	174.59 (18)
C2—C1—C6—N1	−173.85 (19)	N7—N6—C23—C24	1.0 (2)
N2—N1—C6—C5	−131.5 (2)	N7—N6—C23—C22	−176.70 (17)
C9—N1—C6—C5	38.4 (3)	O1—C22—C23—N6	178.60 (19)
N2—N1—C6—C1	43.2 (3)	C21—C22—C23—N6	0.5 (3)
C9—N1—C6—C1	−146.9 (2)	O1—C22—C23—C24	1.4 (3)
N2—N1—C9—C10	1.5 (2)	C21—C22—C23—C24	−176.76 (19)
C6—N1—C9—C10	−168.92 (19)	N7—N8—C24—C23	1.3 (2)
N2—N1—C9—C8	−175.12 (18)	C26—N8—C24—C23	−176.08 (18)
C6—N1—C9—C8	14.5 (3)	N7—N8—C24—C25	−174.10 (19)
N2—N3—C10—C9	1.0 (2)	C26—N8—C24—C25	8.6 (3)
N2—N3—C10—C11	−175.34 (17)	N6—C23—C24—N8	−1.4 (2)
N1—C9—C10—N3	−1.5 (2)	C22—C23—C24—N8	176.15 (19)
C8—C9—C10—N3	174.7 (2)	N6—C23—C24—C25	173.4 (2)
N1—C9—C10—C11	174.38 (19)	C22—C23—C24—C25	−9.1 (4)
C8—C9—C10—C11	−9.4 (4)	C24—N8—C26—C27	−134.0 (2)
N5—N4—C11—C12	0.4 (2)	N7—N8—C26—C27	48.9 (2)
N5—N4—C11—C10	−177.21 (16)	C24—N8—C26—C31	47.5 (3)
N3—C10—C11—N4	−175.34 (18)	N7—N8—C26—C31	−129.68 (19)
C9—C10—C11—N4	9.2 (3)	C31—C26—C27—C28	−1.1 (3)
N3—C10—C11—C12	7.5 (3)	N8—C26—C27—C28	−179.64 (17)
C9—C10—C11—C12	−167.9 (2)	C26—C27—C28—C29	−0.1 (3)
N4—C11—C12—C13	−0.2 (2)	C27—C28—C29—C30	1.0 (3)
C10—C11—C12—C13	177.11 (19)	C27—C28—C29—C32	−178.24 (19)
N4—C11—C12—C20	−175.15 (18)	C28—C29—C30—C31	−0.8 (3)
C10—C11—C12—C20	2.2 (3)	C32—C29—C30—C31	178.52 (18)
N4—N5—C13—C12	0.3 (2)	C29—C30—C31—C26	−0.4 (3)
C14—N5—C13—C12	−171.41 (18)	C27—C26—C31—C30	1.4 (3)
C11—C12—C13—N5	−0.1 (2)	N8—C26—C31—C30	179.90 (16)
C20—C12—C13—N5	174.93 (18)		

Hydrogen-bond geometry (Å, º)

Cg4, Cg5 and Cg6 are the centroids of rings C1–C6, C14–C19 and C26–C31, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···N4	0.98	2.57	3.141 (2)	118
C20—H20*A*···N3	0.95	2.43	3.049 (3)	122
C25—H25*A*···O1	0.98	2.51	3.112 (3)	119
C1—H1*A*···*Cg*5^{i}	0.95	2.86	3.613 (3)	137
C7—H7*A*···*Cg*6^{ii}	0.98	2.84	3.687 (2)	145
C18—H18*A*···*Cg*4^{iii}	0.95	2.76	3.503 (3)	136

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