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Dibenzyl({1-[(4-methyl-2-phenyl-4,5-dihydro-1,3-oxazol-4-yl)methyl]-1*H*-1,2,3-triazol-4-yl}methyl)-amine

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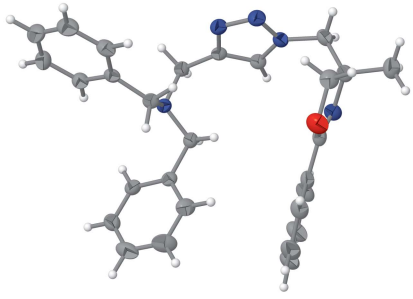
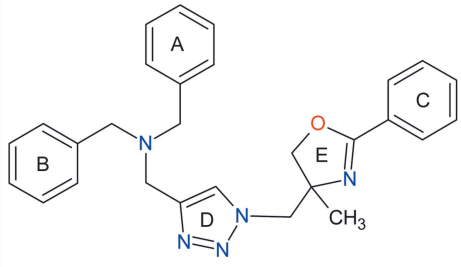
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{28}H_{29}N_5O$, the molecule adopts an approximate U-shape, a conformation imposed at least in part by an intramolecular π–π contact between the two five-membered rings, which display a centroid-to-centroid separation of 3.6522 (7) Å. The planes of these rings are inclined to one another by 66.12 (5)°. A weak intramolecular C—H···N hydrogen bond is also found. The planes of the phenyl rings of the amine unit are inclined at a dihedral angle of 81.10 (4)°, while that of the 4,5-dihydrooxazole ring makes an angle of 11.74 (8)° with its phenyl substituent. The crystal packing is stabilized by C—H···N hydrogen bonds that form chains parallel to the *b* axis. Several C—H···π(ring) contacts are also present.

3D view



Chemical scheme



Structure description

1,2,3-Triazoles are important heterocycles that display a large range of biological activities and are widely employed as pharmaceuticals and agrochemicals. Compounds containing the 1,2,3-triazole moiety are known to exhibit antibacterial (Głowacka, 2009; Aufort *et al.*, 2008; Demaray *et al.*, 2008), antifungal (Chan *et al.*, 2002; Jordan *et al.*, 2001), anticancer (Kamal *et al.*, 2008; Chen *et al.*, 2008) and antiviral activity (Zhou *et al.*, 2005; Lazrek *et al.*, 2001). Isoxazoles are components of a variety of complex biologically active structures and play roles as catalysts, ligands and intermediates in the synthesis of functional compounds (Miller *et al.*, 2009; Prasad *et al.*, 2007). Isoxazoles also appear in numerous medicinally active compounds and natural products of biological significance.

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

*Cg*3, *Cg*4 and *Cg*5 are the centroids of the C1–C6, C7–C12 and C13–C18 phenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19*A*···N2	0.97	2.58	3.2757 (16)	129
C23—H23···N2^{i}	0.93	2.45	3.3607 (16)	166
C27—H27*B*···N3	0.97	2.60	3.3456 (17)	134
C2—H2···*Cg*4^{ii}	0.93	2.63	3.56	154
C12—H12···*Cg*5	0.93	2.92	3.7081 (15)	143
C17—H17···*Cg*3^{iii}	0.93	2.84	3.7046 (16)	154
C24—H24*B*···*Cg*3^{i}	0.93	2.93	3.8795 (14)	165

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

The molecule of the title compound (Fig. 1) adopts an approximate U-shape, a conformation imposed at least in part by an intramolecular π–π contact between the two five-membered rings, *D* and *E* (see Scheme), with a centroid-to-centroid separation of 3.6522 (7) Å. These rings are inclined to one another by 66.12 (5)°. Phenyl rings *A* and *B* of the amine unit are inclined at a dihedral angle of 81.10 (4)°; they also make angles of 17.46 (5) and 86.69 (4)°, respectively, with the triazole ring (*D*). The 4,5-dihydrooxazole ring (*E*) makes a dihedral angle of 11.74 (8)° with its phenyl substituent (*C*). The crystal packing is stabilized by C—H···N hydrogen bonds, forming chains parallel to the *b* axis. Adjacent chains are linked by C—H···π(ring) hydrogen bonds (Table 1 and Fig. 2).

Synthesis and crystallization

A mixture of 0.65 mmol of 4-azidomethyl-4-methyl-2-phenyl-4,5-dihydrooxazole and 0.65 mmol of *N*,*N*-dibenzylprop-2-yn-1-amine in a minimum of toluene was heated under reflux with constant stirring for 72 h. After reaction, the solvent was evaporated under vacuum and the residue was extracted with ether. The organic layer was washed with water, dried with sodium sulfate (Na_2SO_4) and the solvent was removed. The product was purified by column chromatography on silica gel using ether–hexane (1:2 *v*/*v*) as eluant to afford the pure product. The purity of the compound was checked by determining its melting point (373–375 K). Suitable single crystals were obtained by recrystallization from chloroform ($CHCl_3$) (yield 84%). The structure of the product was also investigated by NMR spectroscopy (^{1}H and ^{13}C), MS data and elemental analysis. Analytical data: R_F = 0.51 (ether). Elemental analysis calculated for $C_{28}H_{29}N_5O$ (found): C 74.47 (74.87), H 6.47

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{29}N_5O$
M_r	451.56
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	9.8940 (3), 10.1125 (2), 24.8655 (7)
β (°)	95.096 (1)
V (Å^3)	2478.04 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.41 × 0.37 × 0.21
Data collection	
Diffractometer	Bruker APEXII CCD detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14425, 4561, 3913
R_{int}	0.022
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.036, 0.102, 1.06
No. of reflections	4561
No. of parameters	308
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.20

Computer programs: *APEX2* (Bruker, 2005), *SAINT* (Bruker, 2005), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

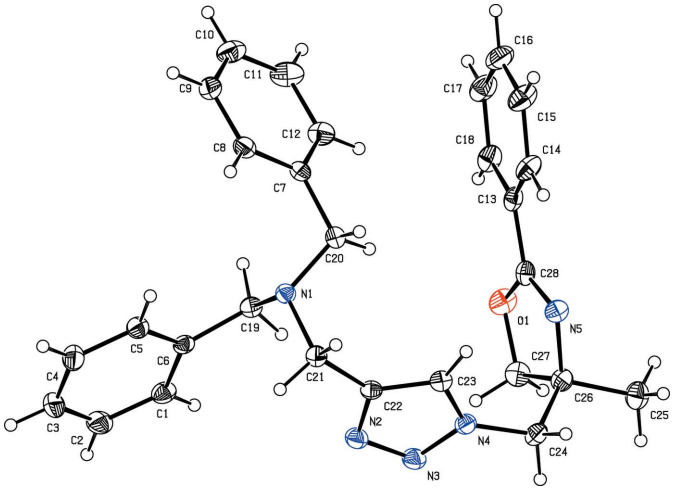


Figure 1
The structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

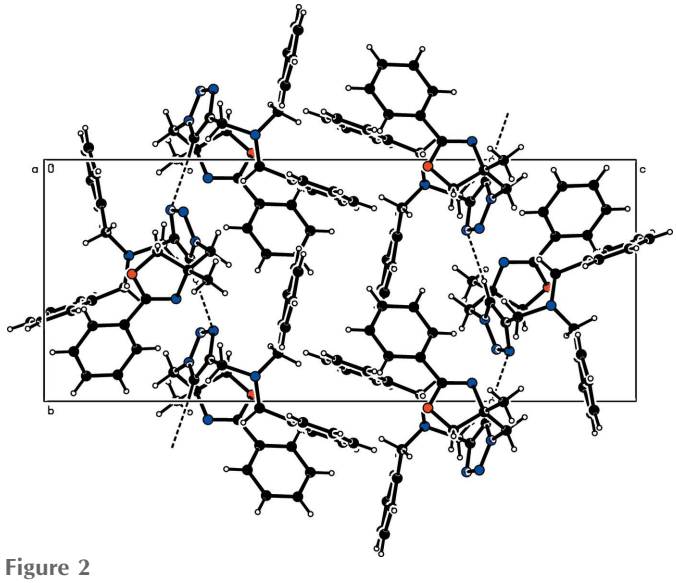


Figure 2
A view of the crystal packing along the *a* axis for the title compound. Hydrogen bonds are drawn as dashed lines.

(6.18), N 15.51% (15.11%). MS (EI): *m*/*z* (relative intensity %) 451 (100%) $[M]^+$. Spectroscopic data: ^{1}H (300.13 MHz, $CDCl_3$): δ 1.42 (3H, CH_3, *s*), 3.37–3.47 (4H, dibenzyl, *AB*, *J* = 13.47 Hz), 3.66–3.73 [2H, $CH_2N(Bn)_2$, *AB*, *J* = 14.64 Hz], 4.06–4.52 (2H, 4,5-dihydrooxazole, *AB*, *J* = 8.92 Hz), 4.45–4.53 (2H, CH_2-triazole, *AB*, *J* = 14.10 Hz), 7.18–7.91 ($15H_{arom}$), 7.61 ($1H^5_{1,2,3\text{-triazole}}$, *s*). ^{13}C (75.47 MHz; $CDCl_3$): δ 25.11 (1C, CH_3), 47.61 [1C, $CH_2N(Bn)_2$], 57.40 (1C, 4,5-dihydrooxazole), 57.30 (2C, dibenzyl), 70.67 (1C, CH_2-triazole), 74.67 [1C, CH_2(4,5-dihydrooxazole)], 131.94 and 150.32 (2C, C^4 and C^5 of 1,2,3-triazole), 124.61–139.50 ($18C_{arom}$), 164.56 (1C, C═N of 4,5-dihydrooxazole).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. One reflection (*i.e.* 002) was found to be affected by the beam stop and was omitted from the final refinement cycles.

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full crystallographic data

IUCrData (2017). **2**, x170860 [https://doi.org/10.1107/S2414314617008604]

Dibenzyl({1-[(4-methyl-2-phenyl-4,5-dihydro-1,3-oxazol-4-yl)methyl]-1*H*-1,2,3-triazol-4-yl}methyl)amine

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Dibenzyl({1-[(4-methyl-2-phenyl-4,5-dihydro-1,3-oxazol-4-yl)methyl]-1*H*-1,2,3-triazol-4-yl}methyl)amine

Crystal data

$C_{28}H_{29}N_5O$
M_r = 451.56
Monoclinic, $P2_1/c$
a = 9.8940 (3) Å
b = 10.1125 (2) Å
c = 24.8655 (7) Å
β = 95.096 (1)°
V = 2478.04 (11) Å^3
Z = 4
$F(000)$ = 960
D_x = 1.210 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 412 reflections
θ = 1.9–26.4°
μ = 0.08 mm^{-1}
T = 296 K
Prism, colourless
0.41 × 0.37 × 0.21 mm

Data collection

Bruker APEXII CCD detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
14425 measured reflections
4561 independent reflections
3913 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.5°, θ_{min} = 2.1°
h = −11→11
k = −12→11
l = −30→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 1.06
4561 reflections
308 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 0.5133P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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}
N1	−0.19432 (10)	0.39663 (9)	0.14326 (4)	0.0260 (2)
N5	0.32594 (11)	0.57568 (10)	0.22306 (4)	0.0319 (3)
N4	0.18147 (11)	0.33879 (10)	0.25538 (4)	0.0292 (2)
N2	0.03788 (11)	0.20795 (10)	0.21388 (4)	0.0336 (3)
N3	0.16377 (11)	0.21560 (10)	0.23540 (5)	0.0355 (3)
O1	0.38824 (10)	0.47298 (10)	0.14862 (4)	0.0412 (2)
C19	−0.14782 (13)	0.30100 (12)	0.10479 (5)	0.0281 (3)
H19A	−0.0572	0.2717	0.1175	0.034*
H19B	−0.1423	0.3445	0.0703	0.034*
C7	−0.18132 (13)	0.58240 (11)	0.08073 (5)	0.0290 (3)
C6	−0.23884 (13)	0.18192 (11)	0.09664 (4)	0.0264 (3)
C28	0.32787 (12)	0.57631 (12)	0.17225 (5)	0.0288 (3)
C5	−0.37929 (13)	0.19406 (12)	0.09226 (5)	0.0310 (3)
H5	−0.4187	0.2758	0.0980	0.037*
C26	0.39945 (13)	0.45638 (13)	0.24346 (5)	0.0310 (3)
C22	−0.02513 (12)	0.32656 (11)	0.21996 (4)	0.0259 (3)
C21	−0.17030 (12)	0.34983 (12)	0.19938 (5)	0.0276 (3)
H21A	−0.2198	0.2678	0.2026	0.033*
H21B	−0.2084	0.4142	0.2227	0.033*
C23	0.06687 (12)	0.41007 (12)	0.24656 (5)	0.0283 (3)
H23	0.0531	0.4974	0.2564	0.034*
C20	−0.13622 (14)	0.52809 (12)	0.13586 (5)	0.0323 (3)
H20A	−0.0380	0.5224	0.1401	0.039*
H20B	−0.1646	0.5876	0.1633	0.039*
C13	0.27476 (12)	0.68248 (13)	0.13586 (5)	0.0303 (3)
C8	−0.31850 (14)	0.58700 (12)	0.06262 (5)	0.0347 (3)
H8	−0.3829	0.5599	0.0854	0.042*
C24	0.31270 (13)	0.37969 (14)	0.28102 (5)	0.0341 (3)
H24A	0.3623	0.3018	0.2942	0.041*
H24B	0.2983	0.4347	0.3120	0.041*
C4	−0.46108 (15)	0.08543 (14)	0.07939 (5)	0.0394 (3)
H4	−0.5550	0.0947	0.0766	0.047*
C18	0.30205 (14)	0.68722 (15)	0.08200 (5)	0.0391 (3)
H18	0.3503	0.6191	0.0674	0.047*
C1	−0.18359 (15)	0.05817 (13)	0.08830 (5)	0.0352 (3)
H1	−0.0898	0.0480	0.0916	0.042*
C14	0.19990 (14)	0.78383 (15)	0.15650 (5)	0.0393 (3)
H14	0.1791	0.7802	0.1922	0.047*
C27	0.42583 (14)	0.38068 (14)	0.19164 (5)	0.0371 (3)
H27A	0.5207	0.3561	0.1919	0.045*
H27B	0.3707	0.3014	0.1878	0.045*
C10	−0.26549 (17)	0.67233 (14)	−0.02277 (6)	0.0452 (4)
H10	−0.2932	0.7012	−0.0575	0.054*
C11	−0.12981 (17)	0.67023 (16)	−0.00493 (6)	0.0489 (4)
H11	−0.0659	0.6992	−0.0276	0.059*

C12	−0.08751 (15)	0.62532 (14)	0.04651 (6)	0.0391 (3)
H12	0.0045	0.6240	0.0581	0.047*
C3	−0.40408 (17)	−0.03654 (14)	0.07068 (6)	0.0441 (4)
H3	−0.4593	−0.1091	0.0618	0.053*
C9	−0.36000 (16)	0.63142 (13)	0.01117 (6)	0.0401 (3)
H9	−0.4519	0.6337	−0.0005	0.048*
C2	−0.26504 (17)	−0.05000 (13)	0.07525 (6)	0.0435 (4)
H2	−0.2261	−0.1319	0.0695	0.052*
C16	0.18507 (16)	0.89492 (17)	0.07129 (6)	0.0497 (4)
H16	0.1560	0.9664	0.0497	0.060*
C25	0.52999 (14)	0.49757 (16)	0.27626 (6)	0.0442 (4)
H25A	0.5862	0.5460	0.2536	0.066*
H25B	0.5776	0.4202	0.2900	0.066*
H25C	0.5085	0.5524	0.3058	0.066*
C15	0.15607 (16)	0.88998 (17)	0.12459 (6)	0.0498 (4)
H15	0.1072	0.9580	0.1390	0.060*
C17	0.25715 (15)	0.79375 (17)	0.05018 (6)	0.0477 (4)
H17	0.2759	0.7969	0.0142	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0284 (6)	0.0251 (5)	0.0246 (5)	−0.0006 (4)	0.0026 (4)	0.0001 (4)
N5	0.0338 (6)	0.0354 (6)	0.0268 (5)	0.0033 (5)	0.0058 (4)	−0.0002 (4)
N4	0.0279 (6)	0.0306 (5)	0.0288 (5)	0.0009 (4)	0.0011 (4)	0.0029 (4)
N2	0.0316 (6)	0.0275 (5)	0.0414 (6)	0.0008 (5)	0.0013 (5)	0.0038 (5)
N3	0.0338 (7)	0.0281 (6)	0.0440 (6)	0.0033 (5)	0.0004 (5)	0.0045 (5)
O1	0.0493 (6)	0.0448 (6)	0.0301 (5)	0.0107 (5)	0.0075 (4)	−0.0069 (4)
C19	0.0292 (7)	0.0306 (6)	0.0251 (6)	0.0014 (5)	0.0060 (5)	0.0013 (5)
C7	0.0336 (7)	0.0210 (6)	0.0323 (6)	−0.0003 (5)	0.0018 (5)	−0.0002 (5)
C6	0.0332 (7)	0.0272 (6)	0.0186 (5)	0.0020 (5)	0.0020 (5)	0.0015 (4)
C28	0.0216 (6)	0.0369 (7)	0.0282 (6)	−0.0032 (5)	0.0046 (5)	−0.0057 (5)
C5	0.0335 (7)	0.0292 (6)	0.0304 (6)	0.0030 (5)	0.0029 (5)	−0.0015 (5)
C26	0.0272 (7)	0.0341 (7)	0.0319 (6)	0.0027 (5)	0.0028 (5)	−0.0006 (5)
C22	0.0280 (7)	0.0266 (6)	0.0239 (6)	0.0004 (5)	0.0058 (5)	0.0038 (5)
C21	0.0272 (7)	0.0304 (6)	0.0259 (6)	−0.0012 (5)	0.0055 (5)	0.0002 (5)
C23	0.0294 (7)	0.0292 (6)	0.0267 (6)	0.0029 (5)	0.0053 (5)	0.0002 (5)
C20	0.0331 (7)	0.0288 (6)	0.0339 (6)	−0.0043 (5)	−0.0024 (5)	0.0004 (5)
C13	0.0228 (7)	0.0418 (7)	0.0260 (6)	−0.0048 (5)	0.0008 (5)	−0.0020 (5)
C8	0.0337 (8)	0.0295 (6)	0.0406 (7)	−0.0034 (5)	0.0021 (6)	0.0046 (5)
C24	0.0300 (7)	0.0418 (7)	0.0297 (6)	0.0017 (6)	−0.0020 (5)	0.0040 (5)
C4	0.0354 (8)	0.0418 (8)	0.0402 (7)	−0.0044 (6)	−0.0016 (6)	−0.0025 (6)
C18	0.0337 (8)	0.0544 (9)	0.0298 (7)	−0.0021 (6)	0.0059 (6)	−0.0015 (6)
C1	0.0382 (8)	0.0335 (7)	0.0332 (7)	0.0102 (6)	0.0001 (6)	0.0001 (5)
C14	0.0388 (8)	0.0524 (8)	0.0259 (6)	0.0086 (7)	−0.0005 (6)	−0.0014 (6)
C27	0.0356 (8)	0.0375 (7)	0.0390 (7)	0.0046 (6)	0.0073 (6)	−0.0026 (6)
C10	0.0648 (11)	0.0400 (8)	0.0302 (7)	0.0137 (7)	0.0013 (7)	0.0018 (6)
C11	0.0555 (10)	0.0525 (9)	0.0420 (8)	0.0123 (8)	0.0221 (7)	0.0104 (7)

C12	0.0330 (8)	0.0393 (7)	0.0458 (8)	0.0049 (6)	0.0086 (6)	0.0061 (6)
C3	0.0579 (10)	0.0327 (7)	0.0400 (7)	−0.0094 (7)	−0.0052 (7)	−0.0052 (6)
C9	0.0419 (8)	0.0323 (7)	0.0439 (8)	0.0012 (6)	−0.0090 (6)	0.0012 (6)
C2	0.0631 (11)	0.0261 (7)	0.0404 (7)	0.0076 (7)	−0.0010 (7)	−0.0045 (6)
C16	0.0428 (9)	0.0608 (10)	0.0436 (8)	0.0033 (8)	−0.0069 (7)	0.0163 (7)
C25	0.0336 (8)	0.0508 (8)	0.0477 (8)	−0.0038 (7)	0.0003 (6)	−0.0022 (7)
C15	0.0480 (9)	0.0576 (10)	0.0421 (8)	0.0170 (8)	−0.0054 (7)	0.0014 (7)
C17	0.0420 (9)	0.0715 (11)	0.0298 (7)	−0.0055 (8)	0.0038 (6)	0.0112 (7)

Geometric parameters (Å, º)

N1—C19	1.4630 (15)	C13—C18	1.3905 (17)
N1—C20	1.4665 (15)	C8—C9	1.3834 (19)
N1—C21	1.4727 (15)	C8—H8	0.9300
N5—C28	1.2651 (15)	C24—H24A	0.9700
N5—C26	1.4752 (16)	C24—H24B	0.9700
N4—C23	1.3451 (16)	C4—C3	1.381 (2)
N4—N3	1.3467 (15)	C4—H4	0.9300
N4—C24	1.4547 (17)	C18—C17	1.386 (2)
N2—N3	1.3135 (16)	C18—H18	0.9300
N2—C22	1.3664 (16)	C1—C2	1.380 (2)
O1—C28	1.3625 (15)	C1—H1	0.9300
O1—C27	1.4432 (16)	C14—C15	1.382 (2)
C19—C6	1.5065 (17)	C14—H14	0.9300
C19—H19A	0.9700	C27—H27A	0.9700
C19—H19B	0.9700	C27—H27B	0.9700
C7—C12	1.3837 (18)	C10—C11	1.376 (2)
C7—C8	1.3923 (19)	C10—C9	1.378 (2)
C7—C20	1.5069 (17)	C10—H10	0.9300
C6—C1	1.3886 (17)	C11—C12	1.386 (2)
C6—C5	1.3896 (18)	C11—H11	0.9300
C28—C13	1.4708 (18)	C12—H12	0.9300
C5—C4	1.3849 (19)	C3—C2	1.377 (2)
C5—H5	0.9300	C3—H3	0.9300
C26—C25	1.5231 (19)	C9—H9	0.9300
C26—C24	1.5339 (17)	C2—H2	0.9300
C26—C27	1.5409 (17)	C16—C17	1.378 (2)
C22—C23	1.3683 (17)	C16—C15	1.382 (2)
C22—C21	1.4998 (17)	C16—H16	0.9300
C21—H21A	0.9700	C25—H25A	0.9600
C21—H21B	0.9700	C25—H25B	0.9600
C23—H23	0.9300	C25—H25C	0.9600
C20—H20A	0.9700	C15—H15	0.9300
C20—H20B	0.9700	C17—H17	0.9300
C13—C14	1.3891 (19)		
C19—N1—C20	111.57 (9)	N4—C24—C26	113.76 (10)
C19—N1—C21	111.94 (9)	N4—C24—H24A	108.8

C20—N1—C21	112.22 (9)	C26—C24—H24A	108.8
C28—N5—C26	107.27 (10)	N4—C24—H24B	108.8
C23—N4—N3	110.82 (10)	C26—C24—H24B	108.8
C23—N4—C24	128.73 (11)	H24A—C24—H24B	107.7
N3—N4—C24	120.42 (10)	C3—C4—C5	120.41 (14)
N3—N2—C22	109.19 (10)	C3—C4—H4	119.8
N2—N3—N4	106.99 (10)	C5—C4—H4	119.8
C28—O1—C27	105.69 (9)	C17—C18—C13	119.78 (14)
N1—C19—C6	113.41 (10)	C17—C18—H18	120.1
N1—C19—H19A	108.9	C13—C18—H18	120.1
C6—C19—H19A	108.9	C2—C1—C6	121.33 (13)
N1—C19—H19B	108.9	C2—C1—H1	119.3
C6—C19—H19B	108.9	C6—C1—H1	119.3
H19A—C19—H19B	107.7	C15—C14—C13	120.77 (13)
C12—C7—C8	118.59 (12)	C15—C14—H14	119.6
C12—C7—C20	120.87 (12)	C13—C14—H14	119.6
C8—C7—C20	120.52 (11)	O1—C27—C26	104.29 (10)
C1—C6—C5	118.17 (12)	O1—C27—H27A	110.9
C1—C6—C19	120.12 (11)	C26—C27—H27A	110.9
C5—C6—C19	121.44 (11)	O1—C27—H27B	110.9
N5—C28—O1	118.22 (12)	C26—C27—H27B	110.9
N5—C28—C13	125.58 (11)	H27A—C27—H27B	108.9
O1—C28—C13	116.16 (10)	C11—C10—C9	119.57 (13)
C4—C5—C6	120.51 (12)	C11—C10—H10	120.2
C4—C5—H5	119.7	C9—C10—H10	120.2
C6—C5—H5	119.7	C10—C11—C12	120.56 (14)
N5—C26—C25	109.22 (11)	C10—C11—H11	119.7
N5—C26—C24	109.72 (10)	C12—C11—H11	119.7
C25—C26—C24	107.82 (11)	C7—C12—C11	120.41 (14)
N5—C26—C27	103.51 (10)	C7—C12—H12	119.8
C25—C26—C27	112.65 (11)	C11—C12—H12	119.8
C24—C26—C27	113.80 (11)	C2—C3—C4	119.62 (13)
N2—C22—C23	107.75 (11)	C2—C3—H3	120.2
N2—C22—C21	122.17 (11)	C4—C3—H3	120.2
C23—C22—C21	130.08 (11)	C10—C9—C8	120.15 (14)
N1—C21—C22	116.28 (9)	C10—C9—H9	119.9
N1—C21—H21A	108.2	C8—C9—H9	119.9
C22—C21—H21A	108.2	C3—C2—C1	119.95 (13)
N1—C21—H21B	108.2	C3—C2—H2	120.0
C22—C21—H21B	108.2	C1—C2—H2	120.0
H21A—C21—H21B	107.4	C17—C16—C15	119.83 (14)
N4—C23—C22	105.25 (11)	C17—C16—H16	120.1
N4—C23—H23	127.4	C15—C16—H16	120.1
C22—C23—H23	127.4	C26—C25—H25A	109.5
N1—C20—C7	110.91 (10)	C26—C25—H25B	109.5
N1—C20—H20A	109.5	H25A—C25—H25B	109.5
C7—C20—H20A	109.5	C26—C25—H25C	109.5
N1—C20—H20B	109.5	H25A—C25—H25C	109.5

C7—C20—H20B	109.5	H25B—C25—H25C	109.5
H20A—C20—H20B	108.0	C16—C15—C14	119.84 (15)
C14—C13—C18	119.08 (13)	C16—C15—H15	120.1
C14—C13—C28	118.97 (11)	C14—C15—H15	120.1
C18—C13—C28	121.90 (12)	C16—C17—C18	120.68 (13)
C9—C8—C7	120.71 (13)	C16—C17—H17	119.7
C9—C8—H8	119.6	C18—C17—H17	119.7
C7—C8—H8	119.6		

Hydrogen-bond geometry (Å, º)

Cg3, Cg4 and Cg5 are the centroids of the C1-C6, C7-C12 and C13-C18 phenyl rings respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19*A*···N2	0.97	2.58	3.2757 (16)	129
C23—H23···N2^{i}	0.93	2.45	3.3607 (16)	166
C27—H27*B*···N3	0.97	2.60	3.3456 (17)	134
C2—H2···*Cg*4^{ii}	0.93	2.63	3.56	154
C12—H12···*Cg*5	0.93	2.92	3.7081 (15)	143
C17—H17···*Cg*3^{iii}	0.93	2.84	3.7046 (16)	154
C24—H24*B*···*Cg*3^{i}	0.93	2.93	3.8795 (14)	165

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