IUCrData

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7,9-Didodecyl-6-methyl-3*H*,7*H*,8*H*,9*H*,9a*H*-[1,2,4]triazolo[4,3-*b*][1,2,4]triazepin-8-one

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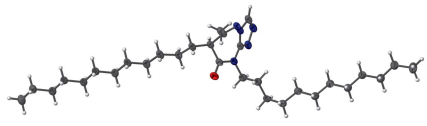
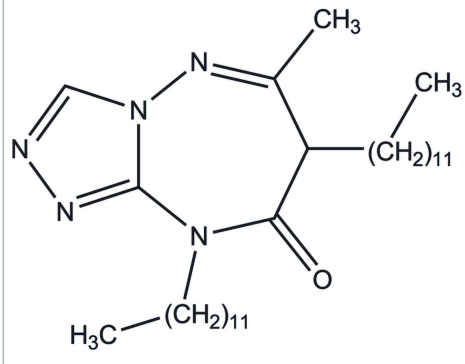
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{30}H_{55}N_5O$, forms a micellar structure in the crystal with the dodecyl chains intercalating and the bicyclic cores forming dimers across centres of symmetry, *via* weak C—H···N hydrogen bonds, and slipped π-stacking interactions between the five-membered rings.

3D view



Chemical scheme



Structure description

Triazolotriazepine derivatives have been used as potent inhibitors of bone resorption (Chikazu *et al.*, 2000). They also exhibit antifungal activity (Gupta *et al.*, 2011). In a continuation of our previous work on the preparation of new nitrogen-bridged heterocycles, we report herein the crystal structure of the title compound obtained by alkylation reaction under phase-transfer catalysis (Essassi *et al.*, 1977; Harmaoui *et al.*, 2015; El Bakri *et al.*, 2016*a*,*b*).

The title compound (Fig. 1) forms a micellar structure in the crystal, with the dodecyl chains intercalating (Fig. 2) and the bicyclic cores forming dimers across centres of symmetry, *via* C2—H2···N5($-x$, $-y$, $1-z$) hydrogen bonds, and slipped π-stacking interactions between the five-membered rings of the same two molecules (Table 1 and Fig. 3). The distance between the centroids of the two rings is 3.572 (1) Å, while the separation between the planes of the two rings is 3.062 (1) Å. A puckering analysis of the seven-membered ring yielded the parameters q_2 = 0.843 (1) Å, q_3 = 0.243 (1) Å, φ_2 = 30.07 (9)° and φ_3 = 121.0 (3)°. The total puckering amplitude is 0.888 (1) Å, and the ring is bowl-shaped.

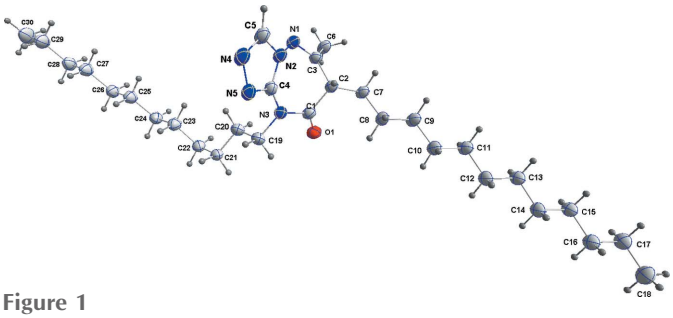


Figure 1
The title molecule with labelling scheme and 50% probability ellipsoids.

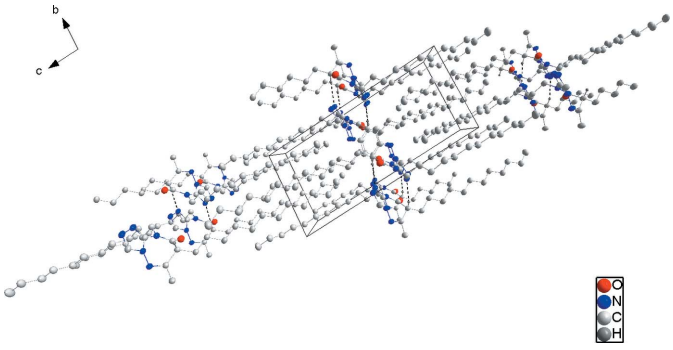


Figure 2
Packing viewed along the *a* axis with intermolecular C—H···N hydrogen bonds shown as dotted lines.

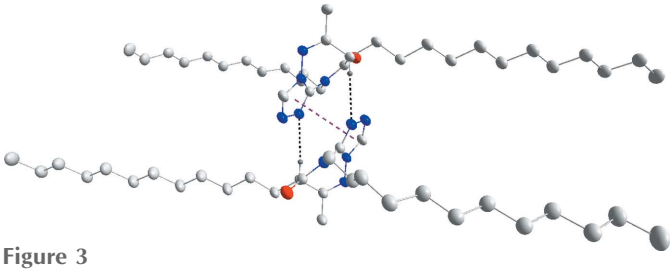


Figure 3
Detail of the pair-wise C—H···N hydrogen bonds and the π-stacking interaction between molecules related by the centre of symmetry at (0,0,1/2).

Synthesis and crystallization

To a solution of 6-methyl-7*H*-[1,2,4]triazolo[4,3-*b*][1,2,4]tria-][1,2,4]triazepin-8(9*H*)-one (0.2 g, 1.21 mmol) in *N*,*N*-dimethylformamide (10 ml), was added potassium carbonate (0.16 g, 1.21 mmol), dodecane bromide (0.35 ml, 1.21 mmol) and a catalytic amount of tetra *n*-butylammonium bromide. The reaction mixture was stirred for 12 h. The solution was then concentrated to dryness under reduced pressure, and the residue was extracted with dichloromethane. The precipitate formed under cooling was filtered and recrystallized from ethanol solution, to give crystals of the title compound with a yield of 60%.

Refinement

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N5^{i}	0.985 (16)	2.544 (16)	3.4749 (18)	157.5 (12)

Symmetry code: (i) $-x, -y, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{30}H_{55}N_5O$
M_r	501.79
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, b, c (Å)	8.8895 (7), 8.9652 (7), 19.6555 (15)
α, β, γ (°)	95.093 (3), 95.922 (3), 98.563 (3)
V (Å^3)	1532.1 (2)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.51
Crystal size (mm)	0.24 × 0.22 × 0.09
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.84, 0.95
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11896, 5705, 4818
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.135, 1.06
No. of reflections	5705
No. of parameters	545
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.24

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161587 [https://doi.org/10.1107/S241431461601587X]

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Crystal data

$C_{30}H_{55}N_5O$
M_r = 501.79
Triclinic, $P\overline{1}$
a = 8.8895 (7) Å
b = 8.9652 (7) Å
c = 19.6555 (15) Å
α = 95.093 (3)°
β = 95.922 (3)°
γ = 98.563 (3)°
V = 1532.1 (2) Å^3
Z = 2
$F(000)$ = 556
D_x = 1.088 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9089 reflections
θ = 5.0–72.6°
μ = 0.51 mm^{-1}
T = 150 K
Plate, colourless
0.24 × 0.22 × 0.09 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; Bruker, 2016)
T_{min} = 0.84, T_{max} = 0.95
11896 measured reflections
5705 independent reflections
4818 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 72.6°, θ_{min} = 5.0°
h = −9→10
k = −11→10
l = −21→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
S = 1.06
5705 reflections
545 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
$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.2812P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.45566 (11)	0.27197 (11)	0.49999 (5)	0.0424 (3)
N1	0.02842 (13)	0.34896 (12)	0.41655 (6)	0.0341 (3)
N2	−0.01039 (13)	0.19478 (12)	0.42508 (6)	0.0339 (3)
N3	0.24079 (13)	0.12205 (12)	0.44702 (6)	0.0341 (3)
N4	−0.14934 (14)	−0.03199 (13)	0.40412 (6)	0.0416 (3)
N5	0.00352 (14)	−0.04911 (13)	0.42035 (6)	0.0379 (3)
C1	0.31635 (15)	0.24759 (15)	0.48942 (7)	0.0332 (3)
C2	0.21506 (15)	0.35300 (14)	0.51936 (7)	0.0318 (3)
H2	0.1329 (18)	0.2876 (18)	0.5376 (8)	0.034 (4)*
C3	0.13968 (15)	0.42197 (14)	0.45922 (7)	0.0323 (3)
C4	0.08281 (15)	0.08795 (14)	0.43266 (7)	0.0327 (3)
C5	−0.15362 (17)	0.11278 (16)	0.40653 (8)	0.0397 (3)
H5	−0.244 (2)	0.1628 (19)	0.3975 (8)	0.043 (4)*
C6	0.19538 (19)	0.58068 (16)	0.44484 (8)	0.0398 (3)
H6A	0.134 (2)	0.609 (2)	0.4066 (10)	0.056 (5)*
H6B	0.190 (2)	0.652 (2)	0.4837 (10)	0.052 (5)*
H6C	0.303 (2)	0.592 (2)	0.4360 (10)	0.058 (5)*
C7	0.30173 (16)	0.47174 (15)	0.57624 (7)	0.0349 (3)
H7A	0.387 (2)	0.537 (2)	0.5580 (9)	0.044 (4)*
H7B	0.2302 (18)	0.5415 (18)	0.5891 (8)	0.035 (4)*
C8	0.35884 (18)	0.40684 (15)	0.64135 (7)	0.0367 (3)
H8A	0.276 (2)	0.334 (2)	0.6556 (9)	0.048 (5)*
H8B	0.436 (2)	0.341 (2)	0.6285 (9)	0.048 (5)*
C9	0.42445 (19)	0.53097 (16)	0.69965 (8)	0.0417 (4)
H9A	0.506 (2)	0.608 (2)	0.6840 (10)	0.057 (5)*
H9B	0.341 (2)	0.589 (2)	0.7127 (10)	0.057 (5)*
C10	0.49422 (19)	0.47228 (16)	0.76379 (8)	0.0405 (3)
H10A	0.422 (2)	0.392 (2)	0.7769 (10)	0.054 (5)*
H10B	0.579 (2)	0.421 (2)	0.7539 (10)	0.054 (5)*
C11	0.55100 (18)	0.59269 (16)	0.82448 (8)	0.0411 (3)
H11A	0.627 (2)	0.678 (2)	0.8093 (9)	0.052 (5)*
H11B	0.458 (2)	0.638 (2)	0.8377 (10)	0.054 (5)*
C12	0.62686 (19)	0.52907 (17)	0.88617 (8)	0.0410 (3)
H12A	0.559 (2)	0.441 (2)	0.8985 (9)	0.046 (5)*
H12B	0.715 (2)	0.482 (2)	0.8725 (10)	0.055 (5)*
C13	0.67791 (18)	0.64442 (17)	0.94923 (8)	0.0395 (3)
H13A	0.748 (2)	0.736 (2)	0.9361 (9)	0.047 (5)*
H13B	0.585 (2)	0.686 (2)	0.9639 (9)	0.051 (5)*
C14	0.75696 (19)	0.57803 (17)	1.00942 (8)	0.0405 (3)
H14A	0.687 (2)	0.490 (2)	1.0206 (9)	0.049 (5)*
H14B	0.848 (2)	0.536 (2)	0.9943 (9)	0.049 (5)*
C15	0.80604 (18)	0.69082 (17)	1.07346 (8)	0.0393 (3)
H15A	0.717 (2)	0.731 (2)	1.0884 (9)	0.043 (4)*
H15B	0.8740 (19)	0.782 (2)	1.0627 (8)	0.041 (4)*
C16	0.88550 (19)	0.62427 (18)	1.13337 (8)	0.0416 (3)

H16A	0.977 (2)	0.585 (2)	1.1186 (10)	0.053 (5)*
H16B	0.820 (2)	0.538 (2)	1.1450 (10)	0.052 (5)*
C17	0.93187 (19)	0.73634 (18)	1.19785 (8)	0.0432 (4)
H17A	0.840 (2)	0.776 (2)	1.2122 (10)	0.054 (5)*
H17B	0.999 (2)	0.826 (2)	1.1865 (9)	0.047 (5)*
C18	1.0118 (2)	0.6687 (2)	1.25739 (9)	0.0542 (4)
H18A	0.946 (2)	0.580 (3)	1.2698 (11)	0.063 (6)*
H18B	1.110 (3)	0.631 (3)	1.2441 (11)	0.069 (6)*
H18C	1.038 (3)	0.739 (3)	1.2985 (12)	0.078 (7)*
C19	0.33053 (18)	0.01086 (16)	0.41839 (7)	0.0377 (3)
H19A	0.269 (2)	−0.090 (2)	0.4172 (9)	0.047 (5)*
H19B	0.423 (2)	0.018 (2)	0.4497 (10)	0.053 (5)*
C20	0.36916 (18)	0.04379 (16)	0.34731 (8)	0.0389 (3)
H20A	0.425 (2)	0.147 (2)	0.3486 (10)	0.058 (5)*
H20B	0.275 (2)	0.044 (2)	0.3159 (9)	0.051 (5)*
C21	0.46416 (16)	−0.06797 (16)	0.31747 (7)	0.0365 (3)
H21A	0.4037 (18)	−0.1743 (19)	0.3148 (8)	0.036 (4)*
H21B	0.558 (2)	−0.0686 (19)	0.3493 (9)	0.042 (4)*
C22	0.50409 (17)	−0.03997 (17)	0.24531 (8)	0.0392 (3)
H22A	0.584 (2)	−0.106 (2)	0.2336 (9)	0.051 (5)*
H22B	0.550 (2)	0.066 (2)	0.2436 (9)	0.045 (4)*
C23	0.36489 (17)	−0.07753 (18)	0.19116 (8)	0.0398 (3)
H23A	0.313 (2)	−0.182 (2)	0.1939 (9)	0.046 (5)*
H23B	0.291 (2)	−0.007 (2)	0.2020 (9)	0.052 (5)*
C24	0.39822 (17)	−0.06601 (17)	0.11712 (8)	0.0392 (3)
H24A	0.475 (2)	−0.136 (2)	0.1071 (9)	0.052 (5)*
H24B	0.444 (2)	0.039 (2)	0.1127 (9)	0.044 (4)*
C25	0.25471 (17)	−0.11520 (18)	0.06640 (8)	0.0396 (3)
H25A	0.209 (2)	−0.218 (2)	0.0731 (9)	0.046 (5)*
H25B	0.179 (2)	−0.048 (2)	0.0759 (10)	0.056 (5)*
C26	0.27837 (18)	−0.10872 (18)	−0.00890 (8)	0.0401 (3)
H26A	0.354 (2)	−0.178 (2)	−0.0212 (10)	0.060 (5)*
H26B	0.323 (2)	−0.002 (2)	−0.0143 (9)	0.047 (5)*
C27	0.13099 (18)	−0.16044 (19)	−0.05681 (8)	0.0410 (3)
H27A	0.086 (2)	−0.264 (2)	−0.0495 (9)	0.051 (5)*
H27B	0.056 (2)	−0.093 (2)	−0.0457 (10)	0.059 (5)*
C28	0.14696 (19)	−0.15499 (19)	−0.13293 (8)	0.0441 (4)
H28A	0.222 (2)	−0.224 (2)	−0.1459 (10)	0.057 (5)*
H28B	0.194 (2)	−0.049 (2)	−0.1405 (10)	0.056 (5)*
C29	−0.0032 (2)	−0.2072 (2)	−0.17858 (8)	0.0499 (4)
H29A	−0.049 (2)	−0.312 (3)	−0.1713 (11)	0.069 (6)*
H29B	−0.078 (3)	−0.138 (3)	−0.1629 (12)	0.079 (7)*
C30	0.0099 (3)	−0.1989 (3)	−0.25445 (10)	0.0656 (5)
H30A	0.082 (3)	−0.266 (3)	−0.2704 (13)	0.089 (8)*
H30B	0.049 (3)	−0.092 (3)	−0.2641 (14)	0.095 (8)*
H30C	−0.093 (3)	−0.240 (3)	−0.2837 (13)	0.084 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0316 (6)	0.0416 (6)	0.0510 (6)	0.0038 (4)	−0.0038 (4)	0.0024 (4)
N1	0.0359 (6)	0.0248 (5)	0.0383 (6)	0.0008 (4)	−0.0058 (5)	0.0038 (4)
N2	0.0337 (6)	0.0255 (5)	0.0378 (6)	−0.0013 (4)	−0.0073 (4)	0.0020 (4)
N3	0.0341 (6)	0.0303 (6)	0.0358 (6)	0.0047 (4)	−0.0026 (4)	0.0007 (4)
N4	0.0411 (7)	0.0325 (6)	0.0447 (7)	−0.0037 (5)	−0.0089 (5)	0.0001 (5)
N5	0.0415 (7)	0.0293 (6)	0.0384 (6)	−0.0008 (5)	−0.0042 (5)	0.0004 (5)
C1	0.0317 (7)	0.0296 (6)	0.0361 (7)	0.0024 (5)	−0.0039 (5)	0.0052 (5)
C2	0.0310 (7)	0.0257 (6)	0.0358 (7)	0.0012 (5)	−0.0047 (5)	0.0031 (5)
C3	0.0309 (7)	0.0272 (6)	0.0365 (7)	0.0033 (5)	−0.0040 (5)	0.0022 (5)
C4	0.0352 (7)	0.0289 (6)	0.0310 (6)	0.0016 (5)	−0.0025 (5)	0.0009 (5)
C5	0.0367 (8)	0.0321 (7)	0.0438 (8)	−0.0030 (5)	−0.0099 (6)	0.0002 (6)
C6	0.0403 (9)	0.0300 (7)	0.0447 (8)	−0.0009 (6)	−0.0085 (6)	0.0067 (6)
C7	0.0339 (7)	0.0267 (6)	0.0398 (7)	0.0014 (5)	−0.0088 (6)	0.0008 (5)
C8	0.0414 (8)	0.0270 (6)	0.0380 (7)	0.0026 (6)	−0.0065 (6)	0.0003 (5)
C9	0.0442 (9)	0.0296 (7)	0.0452 (8)	0.0026 (6)	−0.0137 (6)	−0.0017 (6)
C10	0.0449 (9)	0.0309 (7)	0.0413 (8)	0.0043 (6)	−0.0075 (6)	−0.0022 (6)
C11	0.0402 (8)	0.0346 (7)	0.0436 (8)	0.0054 (6)	−0.0103 (6)	−0.0037 (6)
C12	0.0442 (9)	0.0352 (7)	0.0402 (8)	0.0069 (6)	−0.0051 (6)	−0.0037 (6)
C13	0.0372 (8)	0.0363 (7)	0.0414 (8)	0.0064 (6)	−0.0055 (6)	−0.0042 (6)
C14	0.0414 (8)	0.0378 (8)	0.0396 (8)	0.0069 (6)	−0.0025 (6)	−0.0030 (6)
C15	0.0365 (8)	0.0382 (8)	0.0407 (8)	0.0061 (6)	−0.0021 (6)	−0.0026 (6)
C16	0.0416 (9)	0.0399 (8)	0.0411 (8)	0.0057 (6)	−0.0009 (6)	0.0001 (6)
C17	0.0407 (9)	0.0443 (8)	0.0406 (8)	0.0019 (6)	−0.0021 (6)	−0.0013 (6)
C18	0.0572 (11)	0.0587 (11)	0.0419 (9)	0.0027 (9)	−0.0048 (8)	0.0031 (8)
C19	0.0408 (8)	0.0325 (7)	0.0399 (7)	0.0119 (6)	−0.0018 (6)	0.0022 (5)
C20	0.0435 (8)	0.0336 (7)	0.0406 (7)	0.0131 (6)	0.0006 (6)	0.0035 (6)
C21	0.0329 (7)	0.0327 (7)	0.0425 (7)	0.0094 (5)	−0.0052 (6)	−0.0005 (5)
C22	0.0326 (8)	0.0391 (8)	0.0447 (8)	0.0076 (6)	0.0014 (6)	−0.0013 (6)
C23	0.0331 (8)	0.0450 (8)	0.0411 (8)	0.0079 (6)	0.0030 (6)	0.0031 (6)
C24	0.0365 (8)	0.0395 (8)	0.0414 (8)	0.0073 (6)	0.0048 (6)	0.0007 (6)
C25	0.0377 (8)	0.0432 (8)	0.0389 (7)	0.0095 (6)	0.0052 (6)	0.0035 (6)
C26	0.0403 (8)	0.0414 (8)	0.0392 (8)	0.0092 (6)	0.0056 (6)	0.0027 (6)
C27	0.0402 (8)	0.0449 (8)	0.0389 (8)	0.0110 (6)	0.0045 (6)	0.0028 (6)
C28	0.0501 (9)	0.0434 (8)	0.0395 (8)	0.0113 (7)	0.0051 (6)	0.0024 (6)
C29	0.0544 (10)	0.0536 (10)	0.0419 (8)	0.0169 (8)	−0.0010 (7)	−0.0005 (7)
C30	0.0879 (16)	0.0689 (13)	0.0408 (9)	0.0264 (12)	−0.0031 (9)	−0.0010 (8)

Geometric parameters (Å, º)

O1—C1	1.2177 (17)	C15—H15B	0.993 (18)
N1—C3	1.2840 (17)	C16—C17	1.526 (2)
N1—N2	1.4031 (15)	C16—H16A	0.99 (2)
N2—C4	1.3646 (17)	C16—H16B	0.96 (2)
N2—C5	1.3684 (17)	C17—C18	1.525 (2)
N3—C1	1.3804 (16)	C17—H17A	0.99 (2)

N3—C4	1.3858 (18)	C17—H17B	0.981 (19)
N3—C19	1.4753 (18)	C18—H18A	0.98 (2)
N4—C5	1.3009 (19)	C18—H18B	1.03 (2)
N4—N5	1.3976 (18)	C18—H18C	0.97 (2)
N5—C4	1.3112 (17)	C19—C20	1.516 (2)
C1—C2	1.5212 (19)	C19—H19A	0.982 (19)
C2—C3	1.5226 (17)	C19—H19B	0.968 (19)
C2—C7	1.5309 (17)	C20—C21	1.5202 (19)
C2—H2	0.985 (16)	C20—H20A	0.98 (2)
C3—C6	1.4967 (18)	C20—H20B	0.989 (19)
C5—H5	0.985 (17)	C21—C22	1.530 (2)
C6—H6A	0.96 (2)	C21—H21A	1.016 (16)
C6—H6B	0.96 (2)	C21—H21B	0.990 (17)
C6—H6C	0.98 (2)	C22—C23	1.522 (2)
C7—C8	1.5232 (19)	C22—H22A	1.021 (19)
C7—H7A	1.003 (18)	C22—H22B	0.982 (18)
C7—H7B	0.991 (17)	C23—C24	1.524 (2)
C8—C9	1.5278 (18)	C23—H23A	0.989 (19)
C8—H8A	0.986 (19)	C23—H23B	1.01 (2)
C8—H8B	1.008 (18)	C24—C25	1.519 (2)
C9—C10	1.518 (2)	C24—H24A	1.020 (19)
C9—H9A	1.02 (2)	C24—H24B	0.988 (18)
C9—H9B	1.01 (2)	C25—C26	1.521 (2)
C10—C11	1.5257 (19)	C25—H25A	0.978 (19)
C10—H10A	0.96 (2)	C25—H25B	0.99 (2)
C10—H10B	0.96 (2)	C26—C27	1.518 (2)
C11—C12	1.523 (2)	C26—H26A	1.01 (2)
C11—H11A	1.03 (2)	C26—H26B	1.002 (19)
C11—H11B	1.02 (2)	C27—C28	1.522 (2)
C12—C13	1.5259 (19)	C27—H27A	0.988 (19)
C12—H12A	0.987 (19)	C27—H27B	0.99 (2)
C12—H12B	0.99 (2)	C28—C29	1.516 (2)
C13—C14	1.525 (2)	C28—H28A	1.01 (2)
C13—H13A	1.025 (19)	C28—H28B	1.01 (2)
C13—H13B	1.02 (2)	C29—C30	1.515 (3)
C14—C15	1.5254 (19)	C29—H29A	1.00 (2)
C14—H14A	0.99 (2)	C29—H29B	1.03 (2)
C14—H14B	1.01 (2)	C30—H30A	1.00 (3)
C15—C16	1.523 (2)	C30—H30B	1.01 (3)
C15—H15A	0.980 (19)	C30—H30C	1.03 (3)

C3—N1—N2	115.03 (11)	C17—C16—H16A	109.8 (11)
C4—N2—C5	104.47 (11)	C15—C16—H16B	109.9 (11)
C4—N2—N1	129.11 (11)	C17—C16—H16B	108.4 (11)
C5—N2—N1	123.86 (11)	H16A—C16—H16B	105.7 (16)
C1—N3—C4	123.85 (12)	C18—C17—C16	113.25 (14)
C1—N3—C19	119.05 (11)	C18—C17—H17A	110.1 (11)
C4—N3—C19	116.98 (11)	C16—C17—H17A	109.5 (11)

C5—N4—N5	107.30 (11)	C18—C17—H17B	109.8 (10)
C4—N5—N4	106.66 (11)	C16—C17—H17B	109.1 (10)
O1—C1—N3	120.92 (13)	H17A—C17—H17B	104.8 (15)
O1—C1—C2	123.27 (12)	C17—C18—H18A	110.8 (12)
N3—C1—C2	115.79 (11)	C17—C18—H18B	111.2 (12)
C1—C2—C3	106.74 (11)	H18A—C18—H18B	106.4 (17)
C1—C2—C7	113.06 (11)	C17—C18—H18C	112.9 (14)
C3—C2—C7	113.32 (10)	H18A—C18—H18C	106.9 (19)
C1—C2—H2	106.2 (9)	H18B—C18—H18C	108.4 (18)
C3—C2—H2	106.8 (9)	N3—C19—C20	111.16 (11)
C7—C2—H2	110.2 (9)	N3—C19—H19A	107.4 (10)
N1—C3—C6	115.35 (12)	C20—C19—H19A	111.3 (10)
N1—C3—C2	123.32 (11)	N3—C19—H19B	107.0 (11)
C6—C3—C2	121.31 (11)	C20—C19—H19B	110.3 (11)
N5—C4—N2	110.79 (12)	H19A—C19—H19B	109.4 (15)
N5—C4—N3	125.37 (12)	C19—C20—C21	111.94 (12)
N2—C4—N3	123.71 (11)	C19—C20—H20A	110.7 (11)
N4—C5—N2	110.77 (13)	C21—C20—H20A	109.0 (11)
N4—C5—H5	127.7 (10)	C19—C20—H20B	110.6 (11)
N2—C5—H5	121.5 (10)	C21—C20—H20B	110.3 (11)
C3—C6—H6A	111.4 (11)	H20A—C20—H20B	103.9 (15)
C3—C6—H6B	110.8 (11)	C20—C21—C22	113.66 (12)
H6A—C6—H6B	106.8 (16)	C20—C21—H21A	108.5 (9)
C3—C6—H6C	110.5 (11)	C22—C21—H21A	108.0 (9)
H6A—C6—H6C	109.9 (16)	C20—C21—H21B	110.2 (10)
H6B—C6—H6C	107.3 (16)	C22—C21—H21B	110.8 (10)
C8—C7—C2	114.45 (11)	H21A—C21—H21B	105.3 (13)
C8—C7—H7A	111.5 (10)	C23—C22—C21	112.44 (12)
C2—C7—H7A	110.5 (10)	C23—C22—H22A	109.6 (10)
C8—C7—H7B	107.4 (9)	C21—C22—H22A	107.8 (10)
C2—C7—H7B	107.5 (9)	C23—C22—H22B	108.1 (10)
H7A—C7—H7B	105.0 (13)	C21—C22—H22B	111.3 (10)
C7—C8—C9	112.14 (11)	H22A—C22—H22B	107.5 (14)
C7—C8—H8A	110.3 (10)	C22—C23—C24	115.38 (13)
C9—C8—H8A	111.2 (11)	C22—C23—H23A	109.4 (10)
C7—C8—H8B	107.1 (10)	C24—C23—H23A	107.6 (10)
C9—C8—H8B	112.5 (10)	C22—C23—H23B	108.3 (11)
H8A—C8—H8B	103.2 (14)	C24—C23—H23B	108.4 (11)
C10—C9—C8	114.01 (12)	H23A—C23—H23B	107.6 (14)
C10—C9—H9A	107.9 (11)	C25—C24—C23	111.74 (12)
C8—C9—H9A	110.8 (11)	C25—C24—H24A	108.6 (10)
C10—C9—H9B	108.4 (11)	C23—C24—H24A	107.7 (10)
C8—C9—H9B	109.4 (11)	C25—C24—H24B	111.0 (10)
H9A—C9—H9B	106.1 (16)	C23—C24—H24B	108.8 (10)
C9—C10—C11	115.08 (12)	H24A—C24—H24B	109.0 (14)
C9—C10—H10A	109.2 (11)	C24—C25—C26	115.11 (13)
C11—C10—H10A	110.7 (12)	C24—C25—H25A	109.3 (10)
C9—C10—H10B	110.8 (11)	C26—C25—H25A	109.2 (10)

C11—C10—H10B	107.8 (12)	C24—C25—H25B	109.2 (11)
H10A—C10—H10B	102.6 (16)	C26—C25—H25B	106.4 (11)
C12—C11—C10	112.89 (12)	H25A—C25—H25B	107.4 (15)
C12—C11—H11A	109.5 (10)	C27—C26—C25	112.44 (13)
C10—C11—H11A	109.6 (10)	C27—C26—H26A	107.9 (11)
C12—C11—H11B	110.0 (11)	C25—C26—H26A	109.1 (11)
C10—C11—H11B	107.1 (11)	C27—C26—H26B	111.3 (10)
H11A—C11—H11B	107.7 (15)	C25—C26—H26B	107.3 (10)
C11—C12—C13	114.47 (12)	H26A—C26—H26B	108.7 (15)
C11—C12—H12A	110.3 (10)	C26—C27—C28	114.92 (13)
C13—C12—H12A	110.1 (10)	C26—C27—H27A	110.5 (10)
C11—C12—H12B	109.4 (11)	C28—C27—H27A	108.8 (11)
C13—C12—H12B	110.2 (11)	C26—C27—H27B	108.8 (11)
H12A—C12—H12B	101.7 (15)	C28—C27—H27B	106.4 (11)
C14—C13—C12	113.11 (12)	H27A—C27—H27B	107.2 (15)
C14—C13—H13A	110.3 (10)	C29—C28—C27	112.92 (14)
C12—C13—H13A	109.7 (10)	C29—C28—H28A	108.3 (11)
C14—C13—H13B	109.5 (10)	C27—C28—H28A	108.1 (11)
C12—C13—H13B	108.6 (11)	C29—C28—H28B	111.5 (11)
H13A—C13—H13B	105.3 (15)	C27—C28—H28B	108.9 (11)
C13—C14—C15	113.90 (13)	H28A—C28—H28B	106.8 (15)
C13—C14—H14A	108.4 (11)	C30—C29—C28	113.61 (17)
C15—C14—H14A	109.7 (11)	C30—C29—H29A	109.4 (12)
C13—C14—H14B	109.1 (10)	C28—C29—H29A	111.7 (12)
C15—C14—H14B	110.1 (11)	C30—C29—H29B	109.6 (13)
H14A—C14—H14B	105.3 (15)	C28—C29—H29B	106.6 (13)
C16—C15—C14	113.75 (13)	H29A—C29—H29B	105.6 (18)
C16—C15—H15A	108.9 (10)	C29—C30—H30A	110.3 (14)
C14—C15—H15A	109.7 (10)	C29—C30—H30B	111.4 (15)
C16—C15—H15B	109.2 (10)	H30A—C30—H30B	108 (2)
C14—C15—H15B	110.7 (10)	C29—C30—H30C	111.0 (14)
H15A—C15—H15B	104.1 (14)	H30A—C30—H30C	105 (2)
C15—C16—C17	113.71 (13)	H30B—C30—H30C	111 (2)
C15—C16—H16A	109.0 (11)		

C3—N1—N2—C4	−48.18 (19)	N5—N4—C5—N2	−1.22 (17)
C3—N1—N2—C5	152.86 (14)	C4—N2—C5—N4	1.05 (16)
C5—N4—N5—C4	0.89 (16)	N1—N2—C5—N4	164.34 (12)
C4—N3—C1—O1	−179.78 (12)	C1—C2—C7—C8	−66.68 (17)
C19—N3—C1—O1	4.44 (19)	C3—C2—C7—C8	171.69 (12)
C4—N3—C1—C2	−1.58 (19)	C2—C7—C8—C9	−172.05 (13)
C19—N3—C1—C2	−177.36 (11)	C7—C8—C9—C10	−175.44 (14)
O1—C1—C2—C3	112.27 (14)	C8—C9—C10—C11	−176.11 (14)
N3—C1—C2—C3	−65.88 (14)	C9—C10—C11—C12	−177.18 (14)
O1—C1—C2—C7	−12.99 (19)	C10—C11—C12—C13	−177.03 (14)
N3—C1—C2—C7	168.86 (11)	C11—C12—C13—C14	−178.55 (14)
N2—N1—C3—C6	172.28 (12)	C12—C13—C14—C15	−178.85 (14)
N2—N1—C3—C2	−5.9 (2)	C13—C14—C15—C16	−179.78 (14)

C1—C2—C3—N1	75.46 (16)	C14—C15—C16—C17	−178.91 (14)
C7—C2—C3—N1	−159.43 (14)	C15—C16—C17—C18	−179.79 (14)
C1—C2—C3—C6	−102.59 (15)	C1—N3—C19—C20	−94.60 (15)
C7—C2—C3—C6	22.51 (19)	C4—N3—C19—C20	89.34 (15)
N4—N5—C4—N2	−0.24 (15)	N3—C19—C20—C21	178.96 (11)
N4—N5—C4—N3	−176.25 (12)	C19—C20—C21—C22	179.29 (12)
C5—N2—C4—N5	−0.46 (16)	C20—C21—C22—C23	−69.87 (16)
N1—N2—C4—N5	−162.53 (12)	C21—C22—C23—C24	−174.73 (12)
C5—N2—C4—N3	175.63 (13)	C22—C23—C24—C25	176.29 (13)
N1—N2—C4—N3	13.6 (2)	C23—C24—C25—C26	−179.37 (13)
C1—N3—C4—N5	−148.14 (14)	C24—C25—C26—C27	179.54 (13)
C19—N3—C4—N5	27.72 (19)	C25—C26—C27—C28	179.41 (13)
C1—N3—C4—N2	36.3 (2)	C26—C27—C28—C29	−179.83 (13)
C19—N3—C4—N2	−147.79 (13)	C27—C28—C29—C30	178.61 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N5^{i}	0.985 (16)	2.544 (16)	3.4749 (18)	157.5 (12)

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