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Crystal structure of (*S*)-5,7-diphenyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine

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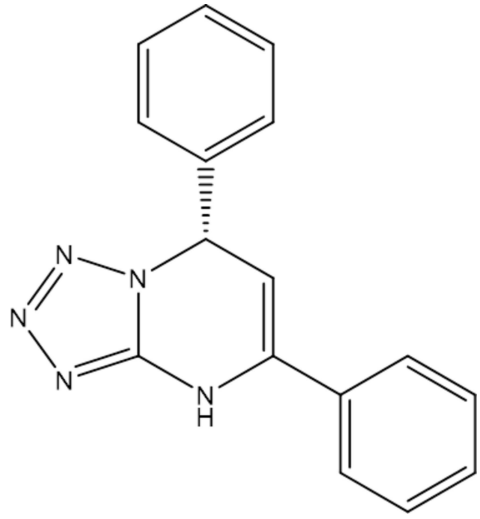
The title compound, $C_{16}H_{13}N_5$, was synthesized by coupling aminotetrazole with chalcone in the presence of an amine organocatalyst derived from chincona alkaloid. There are two molecules, *A* and *B*, in the asymmetric unit. In molecule *A*, the dihedral angles between the partly hydrogenated pyrimidine ring system (r.m.s. deviation = 0.056 Å) and the sp^2- and sp^3-bonded phenyl groups are 33.32 (11) and 86.53 (11)°, respectively. The equivalent data for molecule *B* are 0.049 Å, and 27.05 (10) and 85.27 (11)°, respectively. In the crystal, *A*+*B* dimers linked by pairs of N—H···N hydrogen bonds generate $R_2^2(8)$ loops. The dimers are linked by aromatic π–π stacking interactions [shortest centroid–centroid separation = 3.5367 (15) Å], which results in a three-dimensional network.

Keywords: crystal structure; tetrazolo[1,5-a]pyrimidine; π–π stacking; hydrogen bonding.

CCDC reference: 1048927

1. Related literature

For background to tetrazoles, see: Desenko *et al.* (2001); Ghorbani-Vaghei *et al.* (2013).



2. Experimental

2.1. Crystal data

$C_{16}H_{13}N_5$
M_r = 275.31
Monoclinic, $P2_1$
a = 8.7736 (2) Å
b = 8.8396 (2) Å
c = 17.6810 (4) Å
β = 98.8220 (9)°
V = 1355.03 (5) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 100 K
0.35 × 0.20 × 0.14 mm

2.2. Data collection

Bruker D8 APEX Cu diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.108, T_{max} = 0.818
21873 measured reflections
4926 independent reflections
4822 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.121
S = 1.08
4926 reflections
387 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Absolute structure: Flack *x* determined using 2194 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons & Flack, 2004)
Absolute structure parameter: 0.04 (13)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N5*A*	0.84 (4)	2.16 (4)	2.952 (3)	157 (3)
N1*A*—H1*AA*···N5	0.84 (4)	2.10 (4)	2.912 (3)	163 (4)

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7347).

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supporting information

Acta Cryst. (2015). E**71**, o220–o221 [doi:10.1107/S2056989015002996]

Crystal structure of (*S*)-5,7-diphenyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine

Ivy K. Price, Celine Rougeot and Jason E. Hein

S1. Experimental

(E)-Chalcone (0.4 g, 1.921 mmol) was dissolved in acetonitrile (9.6 ml) and heated to 80°C. 1H-tetrazol-5-amine (0.163 g, 1.921 mmol) and diphenyl hydrogen phosphate (0.096 g, 0.384 mmol) were then added as powders and stirred until the sample was homogenous. (R)-((1S,2R,4S,5R)-5-ethylquinuclidin-2-yl)(6-methoxyquinolin-4-yl)methanamine, (0.063 g, 0.192 mmol) was then added and the reaction stirred at 80°C for 24h. The same was cooled to room temp and allowed to stand uncapped to permit slow evaporation. Crystals initially formed were isolated and recrystallized from dichloro-methane as colourless blocks.

S1.1. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

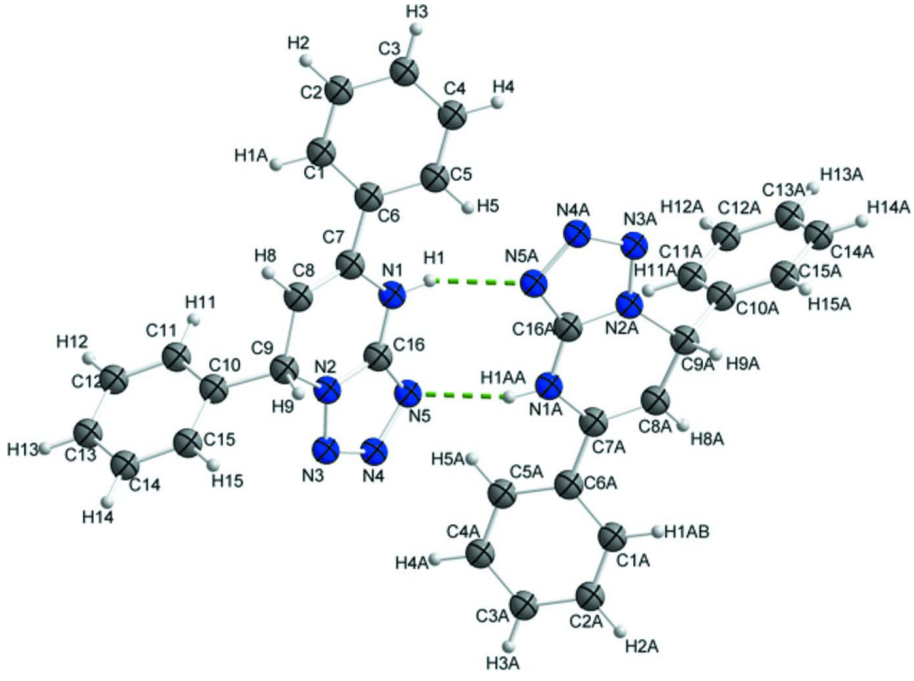

Figure 1

Asymmetric unit of (*S*)-5,7-diphenyl-4,7-dihydrotetrazol[1,5-a]pyrimidine, in ellipsoid thermal representation (50% of probability). The two molecule of the asymmetric unit are linked by hydrogen bonds (dashed green lines).

(*S*)-5,7-Diphenyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine

Crystal data

$C_{16}H_{13}N_5$
$M_r = 275.31$
Monoclinic, $P2_1$
$a = 8.7736$ (2) Å
$b = 8.8396$ (2) Å
$c = 17.6810$ (4) Å
$\beta = 98.8220$ (9)°
$V = 1355.03$ (5) Å^3
$Z = 4$
$F(000) = 576$
$D_x = 1.350$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 9874 reflections
$\theta = 2.5$–68.2°
$\mu = 0.68$ mm^{-1}
$T = 100$ K
Block, clear colorless
0.35 × 0.20 × 0.14 mm

Data collection

Bruker D8 APEX Cu diffractometer
Radiation source: Micro Focus Rotating Anode, Bruker FR-591
Multilayer Mirrors monochromator
Detector resolution: 8.0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
$T_{min} = 0.108$, $T_{max} = 0.818$
21873 measured reflections
4926 independent reflections
4822 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 68.2°$, $\theta_{min} = 2.5°$
$h = -10\rightarrow10$
$k = -10\rightarrow10$
$l = -21\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.121$
$S = 1.08$
4926 reflections
387 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.099P)^2 + 0.0265P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Absolute structure: Flack *x* determined using 2194 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons & Flack, 2004)
Absolute structure parameter: 0.04 (13)

Special details

Experimental. Absorption correction: SADABS-2012/1 (Bruker, 2013) was used for absorption correction. wR2(int) was 0.0856 before and 0.0465 after correction. The Ratio of minimum to maximum transmission is 0.1320. The $\lambda/2$ correction factor is 0.0015.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.1241 (2)	0.7357 (3)	0.20818 (12)	0.0437 (4)
H1	0.128 (4)	0.690 (4)	0.250 (2)	0.054 (9)*
N2	0.1544 (2)	0.7090 (2)	0.07940 (12)	0.0433 (4)

N3	0.2314 (2)	0.6164 (3)	0.03696 (12)	0.0467 (5)
N4	0.3068 (3)	0.5225 (3)	0.08421 (12)	0.0476 (5)
N5	0.2824 (2)	0.5492 (3)	0.15778 (12)	0.0458 (5)
C1	−0.0730 (3)	1.0885 (3)	0.24985 (15)	0.0468 (5)
H1A	−0.0506	1.1491	0.2085	0.056*
C2	−0.1410 (3)	1.1537 (3)	0.30742 (15)	0.0499 (6)
H2	−0.1652	1.2585	0.3052	0.060*
C3	−0.1741 (3)	1.0677 (4)	0.36812 (15)	0.0508 (6)
H3	−0.2212	1.1131	0.4074	0.061*
C4	−0.1382 (3)	0.9151 (4)	0.37142 (15)	0.0530 (6)
H4	−0.1598	0.8557	0.4133	0.064*
C5	−0.0705 (3)	0.8486 (3)	0.31339 (15)	0.0489 (6)
H5	−0.0469	0.7436	0.3157	0.059*
C6	−0.0369 (3)	0.9346 (3)	0.25178 (14)	0.0432 (5)
C7	0.0289 (3)	0.8631 (3)	0.18799 (14)	0.0424 (5)
C8	−0.0012 (3)	0.9102 (3)	0.11511 (14)	0.0431 (5)
H8	−0.0540	1.0037	0.1054	0.052*
C9	0.0427 (3)	0.8252 (3)	0.04719 (13)	0.0423 (5)
H9	−0.0515	0.7721	0.0211	0.051*
C10	0.1090 (3)	0.9162 (3)	−0.01272 (14)	0.0416 (5)
C11	0.2279 (3)	1.0198 (3)	0.00668 (13)	0.0438 (5)
H11	0.2646	1.0408	0.0590	0.053*
C12	0.2929 (3)	1.0926 (3)	−0.05011 (15)	0.0472 (5)
H12	0.3754	1.1619	−0.0367	0.057*
C13	0.2374 (3)	1.0641 (3)	−0.12674 (15)	0.0476 (5)
H13	0.2808	1.1151	−0.1656	0.057*
C14	0.1189 (3)	0.9613 (3)	−0.14640 (14)	0.0465 (5)
H14	0.0813	0.9415	−0.1988	0.056*
C15	0.0552 (3)	0.8874 (3)	−0.08959 (14)	0.0436 (5)
H15	−0.0258	0.8165	−0.1032	0.052*
C16	0.1852 (3)	0.6651 (3)	0.15244 (13)	0.0418 (5)
N1A	0.2796 (3)	0.3097 (3)	0.27062 (12)	0.0457 (5)
H1AA	0.287 (4)	0.364 (5)	0.232 (2)	0.054 (9)*
N2A	0.1962 (2)	0.2931 (3)	0.39031 (12)	0.0440 (5)
N3A	0.1134 (3)	0.3784 (3)	0.43317 (12)	0.0479 (5)
N4A	0.0776 (3)	0.5003 (3)	0.39495 (12)	0.0477 (5)
N5A	0.1334 (2)	0.4997 (3)	0.32690 (11)	0.0448 (5)
C1A	0.4542 (3)	−0.0403 (3)	0.21227 (15)	0.0455 (5)
H1AB	0.4120	−0.1095	0.2446	0.055*
C2A	0.5287 (3)	−0.0939 (3)	0.15462 (15)	0.0480 (5)
H2A	0.5370	−0.1999	0.1474	0.058*
C3A	0.5921 (3)	0.0054 (3)	0.10666 (14)	0.0463 (5)
H3A	0.6431	−0.0322	0.0669	0.056*
C4A	0.5795 (3)	0.1605 (3)	0.11792 (14)	0.0465 (5)
H4A	0.6229	0.2292	0.0858	0.056*
C5A	0.5040 (3)	0.2156 (3)	0.17564 (14)	0.0441 (5)
H5A	0.4956	0.3217	0.1826	0.053*
C6A	0.4401 (3)	0.1156 (3)	0.22367 (13)	0.0436 (5)

C7A	0.3557 (3)	0.1710 (3)	0.28455 (13)	0.0433 (5)
C8A	0.3471 (3)	0.0932 (3)	0.34915 (14)	0.0449 (5)
H8A	0.4061	0.0030	0.3576	0.054*
C9A	0.2507 (3)	0.1381 (3)	0.40930 (13)	0.0443 (5)
H9A	0.1593	0.0693	0.4054	0.053*
C10A	0.3383 (3)	0.1305 (3)	0.49058 (13)	0.0446 (5)
C11A	0.4812 (3)	0.1996 (3)	0.50895 (15)	0.0494 (6)
H11A	0.5249	0.2526	0.4708	0.059*
C12A	0.5608 (3)	0.1912 (3)	0.58352 (17)	0.0545 (6)
H12A	0.6589	0.2379	0.5961	0.065*
C13A	0.4957 (3)	0.1140 (4)	0.63933 (15)	0.0555 (6)
H13A	0.5492	0.1086	0.6902	0.067*
C14A	0.3542 (3)	0.0456 (4)	0.62091 (16)	0.0557 (6)
H14A	0.3104	−0.0069	0.6592	0.067*
C15A	0.2745 (3)	0.0526 (3)	0.54644 (15)	0.0505 (6)
H15A	0.1771	0.0044	0.5340	0.061*
C16A	0.2063 (3)	0.3686 (3)	0.32569 (13)	0.0423 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0488 (10)	0.0444 (11)	0.0386 (10)	0.0017 (9)	0.0090 (8)	0.0034 (9)
N2	0.0474 (10)	0.0416 (10)	0.0422 (9)	0.0005 (8)	0.0110 (8)	0.0017 (8)
N3	0.0517 (10)	0.0450 (11)	0.0454 (10)	0.0021 (9)	0.0143 (8)	0.0024 (9)
N4	0.0543 (11)	0.0452 (11)	0.0461 (10)	0.0046 (9)	0.0169 (9)	0.0037 (9)
N5	0.0493 (10)	0.0453 (11)	0.0442 (10)	0.0046 (9)	0.0119 (8)	0.0039 (9)
C1	0.0497 (12)	0.0459 (14)	0.0443 (12)	0.0005 (10)	0.0059 (10)	0.0010 (9)
C2	0.0516 (12)	0.0467 (14)	0.0510 (12)	0.0061 (11)	0.0065 (10)	−0.0033 (11)
C3	0.0506 (12)	0.0575 (15)	0.0458 (12)	0.0035 (11)	0.0125 (9)	−0.0067 (11)
C4	0.0601 (14)	0.0559 (15)	0.0450 (12)	0.0009 (12)	0.0146 (11)	0.0026 (11)
C5	0.0540 (13)	0.0473 (14)	0.0460 (12)	0.0029 (11)	0.0101 (10)	0.0013 (10)
C6	0.0420 (11)	0.0447 (13)	0.0424 (11)	−0.0005 (10)	0.0049 (9)	−0.0017 (9)
C7	0.0407 (10)	0.0424 (12)	0.0446 (11)	−0.0009 (10)	0.0084 (9)	−0.0004 (9)
C8	0.0432 (10)	0.0421 (12)	0.0448 (12)	0.0010 (10)	0.0092 (9)	0.0013 (9)
C9	0.0423 (11)	0.0438 (12)	0.0407 (11)	0.0003 (9)	0.0062 (9)	0.0000 (9)
C10	0.0423 (11)	0.0408 (12)	0.0423 (11)	0.0044 (9)	0.0084 (9)	0.0018 (9)
C11	0.0450 (11)	0.0454 (13)	0.0406 (11)	0.0026 (10)	0.0049 (9)	−0.0001 (9)
C12	0.0465 (11)	0.0457 (13)	0.0499 (13)	−0.0021 (10)	0.0086 (9)	0.0016 (10)
C13	0.0505 (12)	0.0488 (13)	0.0451 (12)	0.0025 (11)	0.0127 (9)	0.0067 (10)
C14	0.0523 (12)	0.0476 (13)	0.0394 (11)	0.0048 (11)	0.0064 (9)	0.0008 (10)
C15	0.0456 (11)	0.0406 (11)	0.0445 (12)	0.0021 (10)	0.0068 (9)	−0.0007 (9)
C16	0.0439 (11)	0.0405 (12)	0.0415 (11)	−0.0031 (9)	0.0081 (9)	0.0016 (9)
N1A	0.0532 (11)	0.0447 (11)	0.0408 (10)	0.0035 (9)	0.0128 (8)	0.0032 (9)
N2A	0.0453 (10)	0.0466 (12)	0.0406 (10)	0.0033 (9)	0.0083 (8)	0.0014 (8)
N3A	0.0518 (11)	0.0496 (11)	0.0437 (10)	0.0050 (9)	0.0114 (8)	0.0004 (9)
N4A	0.0513 (10)	0.0500 (12)	0.0428 (10)	0.0055 (9)	0.0102 (8)	0.0018 (9)
N5A	0.0471 (10)	0.0465 (11)	0.0414 (10)	0.0034 (9)	0.0090 (8)	0.0018 (8)
C1A	0.0479 (12)	0.0451 (12)	0.0440 (11)	0.0001 (10)	0.0087 (9)	0.0042 (10)

C2A	0.0483 (12)	0.0465 (13)	0.0491 (12)	0.0060 (11)	0.0068 (10)	−0.0004 (10)
C3A	0.0410 (11)	0.0537 (14)	0.0448 (12)	0.0037 (10)	0.0086 (9)	−0.0024 (10)
C4A	0.0425 (11)	0.0522 (14)	0.0448 (11)	−0.0022 (10)	0.0066 (9)	0.0007 (11)
C5A	0.0442 (11)	0.0431 (13)	0.0449 (11)	−0.0010 (9)	0.0062 (9)	−0.0001 (10)
C6A	0.0417 (10)	0.0476 (12)	0.0407 (11)	0.0013 (10)	0.0041 (9)	0.0009 (10)
C7A	0.0435 (11)	0.0433 (12)	0.0429 (11)	−0.0009 (10)	0.0058 (9)	−0.0017 (9)
C8A	0.0494 (11)	0.0435 (13)	0.0422 (12)	0.0031 (10)	0.0086 (9)	−0.0002 (9)
C9A	0.0468 (11)	0.0441 (13)	0.0426 (11)	0.0010 (10)	0.0089 (9)	0.0013 (10)
C10A	0.0488 (11)	0.0433 (12)	0.0426 (12)	0.0062 (10)	0.0099 (9)	0.0009 (10)
C11A	0.0539 (13)	0.0469 (13)	0.0482 (13)	0.0008 (11)	0.0110 (10)	0.0030 (10)
C12A	0.0533 (13)	0.0503 (14)	0.0578 (14)	0.0013 (12)	0.0018 (11)	−0.0025 (12)
C13A	0.0658 (15)	0.0560 (15)	0.0433 (12)	0.0136 (13)	0.0033 (11)	−0.0002 (11)
C14A	0.0652 (15)	0.0591 (15)	0.0444 (12)	0.0069 (14)	0.0132 (11)	0.0086 (12)
C15A	0.0514 (12)	0.0529 (14)	0.0484 (13)	0.0023 (12)	0.0114 (10)	0.0032 (11)
C16A	0.0421 (11)	0.0437 (13)	0.0409 (11)	−0.0006 (10)	0.0055 (9)	0.0002 (10)

Geometric parameters (Å, º)

N1—H1	0.84 (4)	N1A—H1AA	0.84 (4)
N1—C7	1.414 (3)	N1A—C7A	1.399 (4)
N1—C16	1.346 (3)	N1A—C16A	1.351 (3)
N2—N3	1.357 (3)	N2A—N3A	1.356 (3)
N2—C9	1.473 (3)	N2A—C9A	1.473 (3)
N2—C16	1.336 (3)	N2A—C16A	1.338 (3)
N3—N4	1.287 (3)	N3A—N4A	1.285 (3)
N4—N5	1.371 (3)	N4A—N5A	1.367 (3)
N5—C16	1.326 (3)	N5A—C16A	1.326 (4)
C1—H1A	0.9500	C1A—H1AB	0.9500
C1—C2	1.382 (4)	C1A—C2A	1.377 (4)
C1—C6	1.396 (4)	C1A—C6A	1.401 (4)
C2—H2	0.9500	C2A—H2A	0.9500
C2—C3	1.382 (4)	C2A—C3A	1.394 (4)
C3—H3	0.9500	C3A—H3A	0.9500
C3—C4	1.385 (4)	C3A—C4A	1.392 (4)
C4—H4	0.9500	C4A—H4A	0.9500
C4—C5	1.392 (4)	C4A—C5A	1.387 (4)
C5—H5	0.9500	C5A—H5A	0.9500
C5—C6	1.396 (4)	C5A—C6A	1.401 (3)
C6—C7	1.485 (3)	C6A—C7A	1.480 (3)
C7—C8	1.341 (4)	C7A—C8A	1.345 (4)
C8—H8	0.9500	C8A—H8A	0.9500
C8—C9	1.516 (3)	C8A—C9A	1.510 (3)
C9—H9	1.0000	C9A—H9A	1.0000
C9—C10	1.515 (3)	C9A—C10A	1.524 (3)
C10—C11	1.391 (4)	C10A—C11A	1.388 (4)
C10—C15	1.392 (3)	C10A—C15A	1.390 (3)
C11—H11	0.9500	C11A—H11A	0.9500
C11—C12	1.387 (3)	C11A—C12A	1.396 (4)

C12—H12	0.9500	C12A—H12A	0.9500
C12—C13	1.391 (4)	C12A—C13A	1.392 (4)
C13—H13	0.9500	C13A—H13A	0.9500
C13—C14	1.384 (4)	C13A—C14A	1.374 (5)
C14—H14	0.9500	C14A—H14A	0.9500
C14—C15	1.386 (4)	C14A—C15A	1.394 (4)
C15—H15	0.9500	C15A—H15A	0.9500

C7—N1—H1	123 (2)	C7A—N1A—H1AA	123 (3)
C16—N1—H1	117 (3)	C16A—N1A—H1AA	118 (3)
C16—N1—C7	118.1 (2)	C16A—N1A—C7A	118.5 (2)
N3—N2—C9	124.36 (19)	N3A—N2A—C9A	124.9 (2)
C16—N2—N3	108.4 (2)	C16A—N2A—N3A	108.1 (2)
C16—N2—C9	126.9 (2)	C16A—N2A—C9A	126.6 (2)
N4—N3—N2	106.25 (19)	N4A—N3A—N2A	106.32 (19)
N3—N4—N5	111.4 (2)	N3A—N4A—N5A	111.6 (2)
C16—N5—N4	104.9 (2)	C16A—N5A—N4A	104.9 (2)
C2—C1—H1A	119.7	C2A—C1A—H1AB	119.7
C2—C1—C6	120.7 (2)	C2A—C1A—C6A	120.5 (2)
C6—C1—H1A	119.7	C6A—C1A—H1AB	119.7
C1—C2—H2	119.7	C1A—C2A—H2A	119.6
C3—C2—C1	120.6 (2)	C1A—C2A—C3A	120.8 (2)
C3—C2—H2	119.7	C3A—C2A—H2A	119.6
C2—C3—H3	120.2	C2A—C3A—H3A	120.5
C2—C3—C4	119.7 (2)	C4A—C3A—C2A	119.0 (2)
C4—C3—H3	120.2	C4A—C3A—H3A	120.5
C3—C4—H4	120.0	C3A—C4A—H4A	119.7
C3—C4—C5	120.0 (3)	C5A—C4A—C3A	120.6 (2)
C5—C4—H4	120.0	C5A—C4A—H4A	119.7
C4—C5—H5	119.7	C4A—C5A—H5A	119.9
C4—C5—C6	120.7 (3)	C4A—C5A—C6A	120.3 (2)
C6—C5—H5	119.7	C6A—C5A—H5A	119.8
C1—C6—C5	118.4 (2)	C1A—C6A—C5A	118.8 (2)
C1—C6—C7	120.6 (2)	C1A—C6A—C7A	119.7 (2)
C5—C6—C7	120.9 (2)	C5A—C6A—C7A	121.5 (2)
N1—C7—C6	115.5 (2)	N1A—C7A—C6A	116.1 (2)
C8—C7—N1	120.8 (2)	C8A—C7A—N1A	120.7 (2)
C8—C7—C6	123.7 (2)	C8A—C7A—C6A	123.2 (2)
C7—C8—H8	117.6	C7A—C8A—H8A	117.5
C7—C8—C9	124.8 (2)	C7A—C8A—C9A	125.0 (2)
C9—C8—H8	117.6	C9A—C8A—H8A	117.5
N2—C9—C8	105.94 (18)	N2A—C9A—C8A	106.3 (2)
N2—C9—H9	107.8	N2A—C9A—H9A	108.7
N2—C9—C10	109.68 (18)	N2A—C9A—C10A	110.8 (2)
C8—C9—H9	107.8	C8A—C9A—H9A	108.7
C10—C9—C8	117.5 (2)	C8A—C9A—C10A	113.40 (19)
C10—C9—H9	107.8	C10A—C9A—H9A	108.7
C11—C10—C9	122.1 (2)	C11A—C10A—C9A	120.5 (2)

C11—C10—C15	119.4 (2)	C11A—C10A—C15A	120.0 (2)
C15—C10—C9	118.4 (2)	C15A—C10A—C9A	119.5 (2)
C10—C11—H11	119.9	C10A—C11A—H11A	120.0
C12—C11—C10	120.2 (2)	C10A—C11A—C12A	120.1 (2)
C12—C11—H11	119.9	C12A—C11A—H11A	120.0
C11—C12—H12	120.0	C11A—C12A—H12A	120.2
C11—C12—C13	120.0 (2)	C13A—C12A—C11A	119.7 (3)
C13—C12—H12	120.0	C13A—C12A—H12A	120.2
C12—C13—H13	120.0	C12A—C13A—H13A	120.0
C14—C13—C12	120.1 (2)	C14A—C13A—C12A	120.1 (2)
C14—C13—H13	120.0	C14A—C13A—H13A	120.0
C13—C14—H14	120.1	C13A—C14A—H14A	119.7
C13—C14—C15	119.9 (2)	C13A—C14A—C15A	120.6 (3)
C15—C14—H14	120.1	C15A—C14A—H14A	119.7
C10—C15—H15	119.8	C10A—C15A—C14A	119.6 (2)
C14—C15—C10	120.5 (2)	C10A—C15A—H15A	120.2
C14—C15—H15	119.8	C14A—C15A—H15A	120.2
N2—C16—N1	121.9 (2)	N2A—C16A—N1A	121.6 (2)
N5—C16—N1	129.1 (2)	N5A—C16A—N1A	129.3 (2)
N5—C16—N2	109.0 (2)	N5A—C16A—N2A	109.1 (2)
N1—C7—C8—C9	8.3 (4)	N1A—C7A—C8A—C9A	4.0 (4)
N2—N3—N4—N5	0.1 (3)	N2A—N3A—N4A—N5A	0.3 (3)
N2—C9—C10—C11	−72.2 (3)	N2A—C9A—C10A—C11A	−69.2 (3)
N2—C9—C10—C15	103.6 (2)	N2A—C9A—C10A—C15A	111.3 (3)
N3—N2—C9—C8	−174.5 (2)	N3A—N2A—C9A—C8A	−175.8 (2)
N3—N2—C9—C10	−46.7 (3)	N3A—N2A—C9A—C10A	−52.2 (3)
N3—N2—C16—N1	−179.7 (2)	N3A—N2A—C16A—N1A	−178.4 (2)
N3—N2—C16—N5	1.4 (3)	N3A—N2A—C16A—N5A	0.6 (3)
N3—N4—N5—C16	0.7 (3)	N3A—N4A—N5A—C16A	0.0 (3)
N4—N5—C16—N1	179.9 (2)	N4A—N5A—C16A—N1A	178.5 (2)
N4—N5—C16—N2	−1.3 (3)	N4A—N5A—C16A—N2A	−0.4 (3)
C1—C2—C3—C4	0.3 (4)	C1A—C2A—C3A—C4A	0.2 (4)
C1—C6—C7—N1	151.9 (2)	C1A—C6A—C7A—N1A	−149.0 (2)
C1—C6—C7—C8	−30.0 (4)	C1A—C6A—C7A—C8A	29.2 (4)
C2—C1—C6—C5	−0.3 (4)	C2A—C1A—C6A—C5A	−0.4 (4)
C2—C1—C6—C7	176.9 (2)	C2A—C1A—C6A—C7A	178.3 (2)
C2—C3—C4—C5	−0.6 (4)	C2A—C3A—C4A—C5A	−0.5 (4)
C3—C4—C5—C6	0.5 (4)	C3A—C4A—C5A—C6A	0.3 (4)
C4—C5—C6—C1	−0.1 (4)	C4A—C5A—C6A—C1A	0.1 (4)
C4—C5—C6—C7	−177.2 (2)	C4A—C5A—C6A—C7A	−178.5 (2)
C5—C6—C7—N1	−31.0 (3)	C5A—C6A—C7A—N1A	29.6 (3)
C5—C6—C7—C8	147.1 (3)	C5A—C6A—C7A—C8A	−152.2 (2)
C6—C1—C2—C3	0.2 (4)	C6A—C1A—C2A—C3A	0.2 (4)
C6—C7—C8—C9	−169.7 (2)	C6A—C7A—C8A—C9A	−174.1 (2)
C7—N1—C16—N2	−2.1 (3)	C7A—N1A—C16A—N2A	−4.6 (3)
C7—N1—C16—N5	176.6 (2)	C7A—N1A—C16A—N5A	176.6 (2)
C7—C8—C9—N2	−14.0 (3)	C7A—C8A—C9A—N2A	−10.7 (3)

C7—C8—C9—C10	−137.0 (3)	C7A—C8A—C9A—C10A	−132.7 (3)
C8—C9—C10—C11	48.8 (3)	C8A—C9A—C10A—C11A	50.3 (3)
C8—C9—C10—C15	−135.3 (2)	C8A—C9A—C10A—C15A	−129.2 (2)
C9—N2—N3—N4	−174.4 (2)	C9A—N2A—N3A—N4A	−174.9 (2)
C9—N2—C16—N1	−6.4 (4)	C9A—N2A—C16A—N1A	−4.2 (4)
C9—N2—C16—N5	174.7 (2)	C9A—N2A—C16A—N5A	174.8 (2)
C9—C10—C11—C12	175.2 (2)	C9A—C10A—C11A—C12A	−179.6 (2)
C9—C10—C15—C14	−176.1 (2)	C9A—C10A—C15A—C14A	−179.9 (3)
C10—C11—C12—C13	1.2 (4)	C10A—C11A—C12A—C13A	−0.3 (4)
C11—C10—C15—C14	−0.2 (4)	C11A—C10A—C15A—C14A	0.6 (4)
C11—C12—C13—C14	−1.0 (4)	C11A—C12A—C13A—C14A	0.4 (4)
C12—C13—C14—C15	0.3 (4)	C12A—C13A—C14A—C15A	0.0 (5)
C13—C14—C15—C10	0.3 (4)	C13A—C14A—C15A—C10A	−0.5 (4)
C15—C10—C11—C12	−0.6 (3)	C15A—C10A—C11A—C12A	−0.2 (4)
C16—N1—C7—C6	179.1 (2)	C16A—N1A—C7A—C6A	−177.2 (2)
C16—N1—C7—C8	1.0 (3)	C16A—N1A—C7A—C8A	4.5 (3)
C16—N2—N3—N4	−0.9 (3)	C16A—N2A—N3A—N4A	−0.5 (3)
C16—N2—C9—C8	13.2 (3)	C16A—N2A—C9A—C8A	10.9 (3)
C16—N2—C9—C10	141.0 (2)	C16A—N2A—C9A—C10A	134.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N5*A*	0.84 (4)	2.16 (4)	2.952 (3)	157 (3)
N1*A*—H1*AA*···N5	0.84 (4)	2.10 (4)	2.912 (3)	163 (4)