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3-Methyl-5,6-diphenyl-1*H*-pyrazolo[1,2-*a*]cinnolin-1-one

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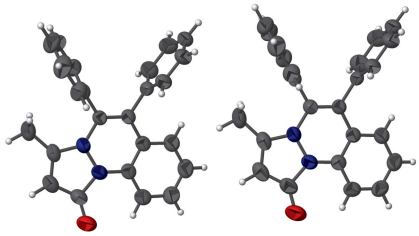
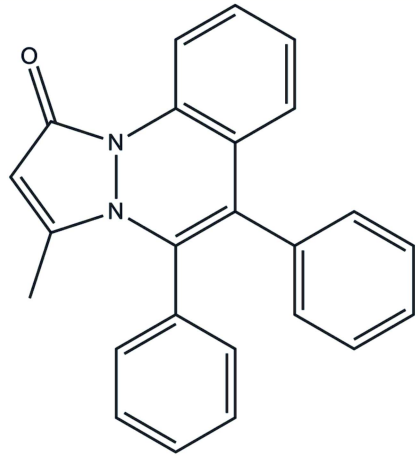
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{24}H_{18}N_2O$, comprises two crystallographically independent molecules (*A* and *B*), with slightly different conformations. In each molecule, there is an intramolecular C—H···O hydrogen bond forming an *S*(6) ring motif. The pyridazine rings of the pyrazolo[1,2-*a*]cinnoline units have screw-boat conformations. Their mean planes are inclined to the phenyl rings by 83.81 (8) and 74.19 (8)° in molecule *A*, and 89.72 (8) and 71.07 (8)° in molecule *B*. In the crystal, the *A* and *B* molecules are linked by a pair of C—H···O hydrogen bonds, forming an A–B dimer with an $R_2^2(14)$ ring motif. These dimers are linked by further C—H···O hydrogen bonds, forming ribbons propagating along the *b*-axis direction. The ribbons are linked by a number of C—H···π interactions, forming a three-dimensional structure.

3D view



Chemical scheme



Structure description

Pyrazole derivatives are reported to possess varied biological activities, such as anti-inflammatory (Windholz 2003), analgesic (Windholz 2003), hypoglycemic, sedative (Burger & Iorio, 1979), hypnotic (Burger & Iorio, 1980), antifungal and antibacterial (Kalluraya & Ramesh, 2001).

The asymmetric unit of the title compound, is composed of two crystallographically independent molecules (*A* and B*)*, with slightly different conformations (Fig. 1). Intramolecular C—H···O hydrogen bonds generate six-membered rings, producing *S*(6) ring motifs (Fig1, Table 1). The dihedral angles between the mean plane of the central pyridazine ring (which has a screw-boat conformation in both molecules) and the two outer phenyl rings are 83.81 (8) and 74.19 (8)° in molecule *A*, and 89.72 (8) and 71.07 (8)° in molecule *B*.

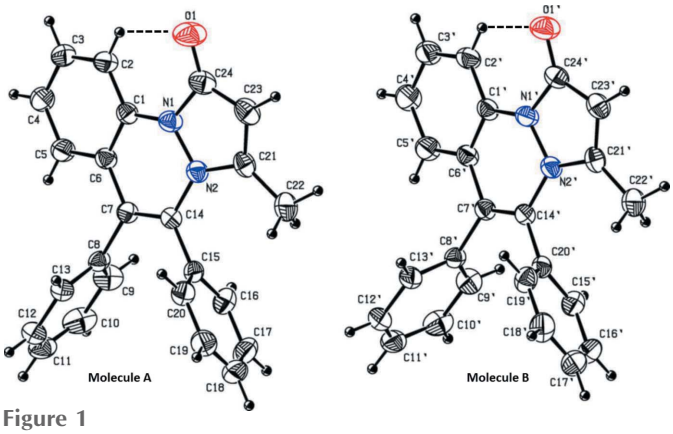


Figure 1
The molecular structure of the two independent molecules (*A* and *B*) of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular C—H···O hydrogen bonds are shown as dashed lines (see Table 1).

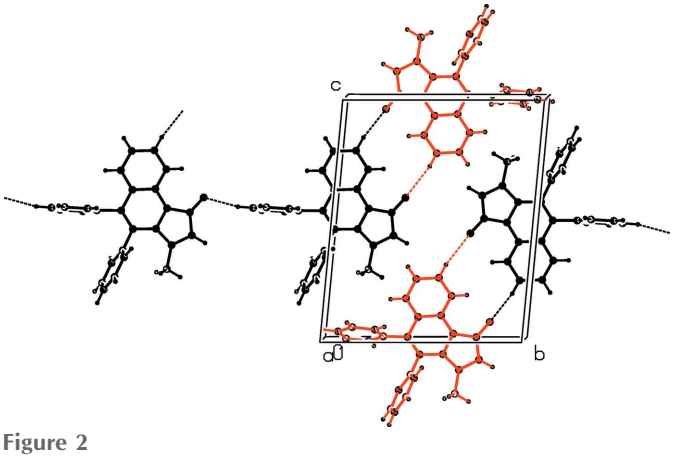


Figure 2
A view along the *a* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1; colour code: molecule *A* black, molecule *B* orange).

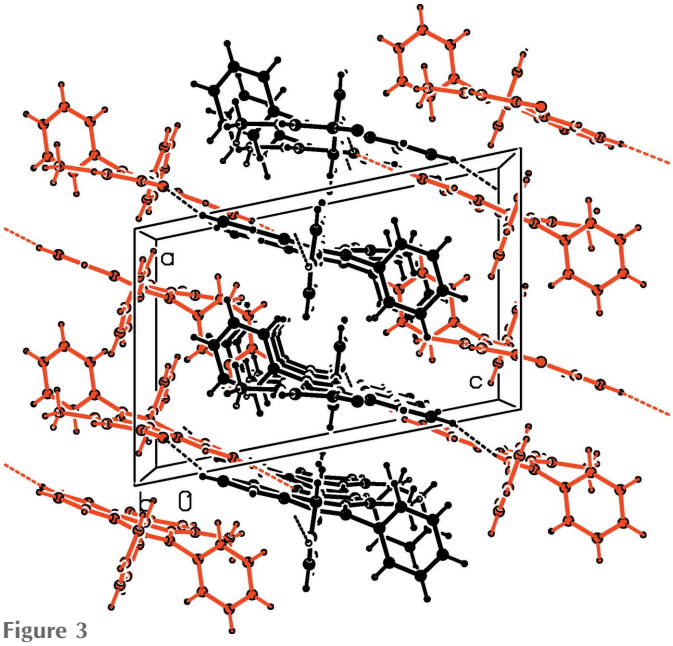


Figure 3
A view along the *b* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1; colour code: molecule *A* black, molecule *B* orange).

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

*Cg*1, *Cg*3, *Cg*4, *Cg*11 and *Cg*12 are the centroids of the N1/N2/C21–C24, C1–C6, C8–C13, C1′–C6′ and C8′–C13′ rings, respectively

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1	0.93	2.22	2.862 (2)	125
C2′—H2′···O1′	0.93	2.22	2.865 (2)	126
C3—H3···O1′^{i}	0.93	2.49	3.381 (2)	162
C3′—H3′···O1^{i}	0.93	2.54	3.456 (2)	170
C11—H11···O1^{ii}	0.93	2.49	3.274 (2)	142
C9—H9···*Cg*1^{iii}	0.93	2.92	3.796 (2)	158
C16—H16···*Cg*3^{iii}	0.93	3.00	3.822 (2)	149
C18—H18···*Cg*12^{iv}	0.93	2.95	3.869 (2)	169
C18′—H18′···*Cg*4^{iv}	0.93	2.98	3.867 (2)	161
C19—H19···*Cg*3^{v}	0.93	2.90	3.685 (2)	143
C19′—H19′···*Cg*11^{vi}	0.93	2.78	3.604 (2)	149

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{18}N_2O$
M_r	350.40
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, *b*, *c* (Å)	9.9251 (4), 12.2293 (4), 15.1738 (5)
α, β, γ (°)	84.318 (2), 78.538 (2), 89.880 (2)
V (Å^3)	1795.86 (11)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.20 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 20014)
T_{min}, T_{max}	0.984, 0.992
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26244, 7471, 5339
R_{int}	0.024
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.629
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.125, 1.01
No. of reflections	7471
No. of parameters	490
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.15

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

In the crystal, the *A* and *B* molecules are linked by a pair of C—H···O hydrogen bonds, forming an *A*–*B* dimer with an $R_2^2(14)$ ring motif (Fig. 2 and Table 1). These dimers are linked by further C—H···O hydrogen bonds, forming ribbons propagating along the *b*-axis direction (Fig. 3 and Table 1). The ribbons are linked by a number of C—H···π interactions, forming a three-dimensional structure (Table 1).

Synthesis and crystallization

To a dried 50 ml round-bottom flask, fitted with a reflux condenser, were added 5-methyl-2-phenyl-2,4-dihydro-3*H*-

pyrazol-3-one 1 (0.3 mmol), diphenyl acetylene (0.3 mmol), $[RuCl_2(p\text{-cymene})]_2$ (5 mol%), $Cu(OAc)_2$ (2 eq.) and $AgSbF_6$ (20 mol%) in toluene. The reaction mixture was refluxed for 16 h. After cooling to room temperature, the reaction mixture was diluted with CH_2Cl_2, filtered through Celite and the filtrate concentrated under reduced pressure. The crude product was purified through a silica gel column, using hexane and ethyl acetate as eluent, giving the title compound in 70% yield. Colourless block-like crystals were obtained by slow evaporation of a solution in ethanol.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170534 [https://doi.org/10.1107/S241431461700534X]

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Crystal data

$C_{24}H_{18}N_2O$
M_r = 350.40
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.9251 (4) Å
b = 12.2293 (4) Å
c = 15.1738 (5) Å
α = 84.318 (2)°
β = 78.538 (2)°
γ = 89.880 (2)°
V = 1795.86 (11) Å^3
Z = 4
$F(000)$ = 736
D_x = 1.296 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7471 reflections
θ = 1.4–26.6°
μ = 0.08 mm^{-1}
T = 293 K
Block, colourless
0.20 × 0.15 × 0.10 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 20014)
T_{min} = 0.984, T_{max} = 0.992
26244 measured reflections
7471 independent reflections
5339 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 26.6°, θ_{min} = 1.4°
h = −12→12
k = −15→13
l = −17→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.01
7471 reflections
490 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.4013P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0046 (7)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.15479 (14)	0.09128 (12)	0.61216 (10)	0.0482 (3)
C1′	0.13725 (15)	0.56650 (12)	0.09148 (10)	0.0498 (4)
C2′	0.06903 (17)	0.60730 (14)	0.16999 (11)	0.0618 (4)
H2′	0.0647	0.6827	0.1736	0.074*
C2	0.09775 (17)	0.13502 (14)	0.69203 (11)	0.0594 (4)
H2	0.0962	0.2107	0.6943	0.071*
C3′	0.00711 (18)	0.53485 (15)	0.24336 (12)	0.0698 (5)
H3′	−0.0384	0.5621	0.2961	0.084*
C3	0.04332 (18)	0.06529 (15)	0.76824 (11)	0.0652 (4)
H3	0.0041	0.0945	0.8215	0.078*
C4′	0.01280 (19)	0.42348 (16)	0.23837 (12)	0.0728 (5)
H4′	−0.0289	0.3754	0.2875	0.087*
C4	0.04671 (18)	−0.04632 (15)	0.76597 (11)	0.0687 (5)
H4	0.0095	−0.0925	0.8175	0.082*
C5	0.10524 (18)	−0.09005 (14)	0.68738 (11)	0.0627 (4)
H5	0.1081	−0.1660	0.6866	0.075*
C5′	0.08075 (17)	0.38318 (14)	0.16001 (11)	0.0641 (4)
H5′	0.0834	0.3076	0.1569	0.077*
C6	0.16065 (15)	−0.02226 (12)	0.60856 (10)	0.0485 (3)
C6′	0.14578 (15)	0.45328 (12)	0.08511 (10)	0.0499 (4)
C7	0.22899 (14)	−0.06595 (11)	0.52486 (9)	0.0462 (3)
C7′	0.22902 (15)	0.41255 (11)	0.00459 (10)	0.0466 (3)
C8′	0.25727 (15)	0.29247 (11)	0.00764 (9)	0.0463 (3)
C8	0.25278 (16)	−0.18661 (11)	0.52569 (9)	0.0483 (3)
C9′	0.16563 (18)	0.21977 (14)	−0.01398 (12)	0.0646 (4)
H9′	0.0895	0.2464	−0.0358	0.078*
C9	0.14860 (19)	−0.25754 (14)	0.51906 (13)	0.0714 (5)
H9	0.0644	−0.2297	0.5104	0.086*
C10	0.1679 (2)	−0.37019 (16)	0.52519 (14)	0.0842 (6)
H10	0.0965	−0.4173	0.5209	0.101*
C10′	0.1860 (2)	0.10750 (15)	−0.00343 (13)	0.0736 (5)
H10′	0.1235	0.0593	−0.0181	0.088*
C11	0.2905 (3)	−0.41224 (14)	0.53747 (12)	0.0785 (6)
H11	0.3024	−0.4879	0.5426	0.094*
C11′	0.2976 (2)	0.06734 (14)	0.02845 (11)	0.0698 (5)

H11′	0.3102	−0.0081	0.0366	0.084*
C12′	0.3904 (2)	0.13831 (13)	0.04833 (12)	0.0689 (5)
H12′	0.4671	0.1111	0.0692	0.083*
C12	0.3954 (2)	−0.34339 (14)	0.54221 (12)	0.0751 (5)
H12	0.4798	−0.3721	0.5496	0.090*
C13′	0.37103 (18)	0.25057 (12)	0.03771 (11)	0.0573 (4)
H13′	0.4354	0.2982	0.0510	0.069*
C13	0.37763 (19)	−0.23078 (13)	0.53616 (11)	0.0600 (4)
H13	0.4504	−0.1844	0.5392	0.072*
C14′	0.28439 (14)	0.48240 (11)	−0.06700 (9)	0.0458 (3)
C14	0.27179 (14)	0.00173 (11)	0.44925 (9)	0.0450 (3)
C15	0.34601 (15)	−0.03659 (11)	0.36324 (9)	0.0454 (3)
C15′	0.37988 (15)	0.44902 (11)	−0.14754 (9)	0.0471 (3)
C16′	0.33317 (18)	0.39598 (13)	−0.21222 (11)	0.0612 (4)
H16′	0.2401	0.3787	−0.2048	0.073*
C16	0.27580 (18)	−0.08795 (14)	0.30889 (11)	0.0611 (4)
H16	0.1811	−0.0985	0.3260	0.073*
C17′	0.4235 (2)	0.36848 (16)	−0.28764 (12)	0.0784 (6)
H17′	0.3913	0.3340	−0.3315	0.094*
C17	0.3451 (2)	−0.12393 (15)	0.22904 (12)	0.0777 (6)
H17	0.2969	−0.1579	0.1923	0.093*
C18	0.4851 (2)	−0.10957 (16)	0.20403 (12)	0.0797 (6)
H18	0.5318	−0.1337	0.1502	0.096*
C18′	0.5605 (2)	0.39185 (18)	−0.29805 (13)	0.0832 (6)
H18′	0.6216	0.3729	−0.3489	0.100*
C19′	0.60834 (19)	0.44324 (18)	−0.23369 (13)	0.0783 (6)
H19′	0.7017	0.4591	−0.2411	0.094*
C19	0.5559 (2)	−0.05984 (16)	0.25822 (12)	0.0739 (5)
H19	0.6508	−0.0505	0.2412	0.089*
C20	0.48752 (16)	−0.02358 (14)	0.33765 (11)	0.0586 (4)
H20	0.5364	0.0098	0.3743	0.070*
C20′	0.51909 (17)	0.47125 (14)	−0.15853 (11)	0.0613 (4)
H20′	0.5522	0.5053	−0.1148	0.074*
C21′	0.28812 (17)	0.68383 (13)	−0.12931 (11)	0.0566 (4)
C21	0.26618 (16)	0.20089 (13)	0.38316 (11)	0.0574 (4)
C22′	0.3399 (2)	0.67642 (15)	−0.22668 (12)	0.0765 (5)
H22A	0.3379	0.7477	−0.2592	0.115*
H22B	0.2829	0.6260	−0.2482	0.115*
H22C	0.4327	0.6508	−0.2360	0.115*
C22	0.2999 (2)	0.18924 (15)	0.28496 (12)	0.0785 (6)
H22D	0.3919	0.1631	0.2691	0.118*
H22E	0.2928	0.2593	0.2517	0.118*
H22F	0.2367	0.1378	0.2705	0.118*
C23′	0.25706 (18)	0.77768 (13)	−0.08866 (12)	0.0623 (4)
H23′	0.2702	0.8484	−0.1180	0.075*
C23	0.24147 (19)	0.29558 (14)	0.42277 (13)	0.0684 (5)
H23	0.2488	0.3654	0.3915	0.082*
C24	0.20346 (18)	0.27457 (13)	0.51675 (13)	0.0644 (4)

C24′	0.20272 (17)	0.75271 (12)	0.00338 (12)	0.0570 (4)
N1′	0.20321 (13)	0.63712 (10)	0.01742 (9)	0.0528 (3)
N1	0.20948 (13)	0.15955 (10)	0.53328 (9)	0.0533 (3)
N2	0.24796 (13)	0.11533 (9)	0.44992 (8)	0.0507 (3)
N2′	0.25753 (13)	0.59608 (9)	−0.06569 (8)	0.0515 (3)
O1	0.16919 (17)	0.33509 (10)	0.57734 (10)	0.0944 (5)
O1′	0.15812 (14)	0.81121 (9)	0.06473 (9)	0.0781 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0416 (8)	0.0506 (8)	0.0524 (9)	0.0037 (6)	−0.0093 (6)	−0.0049 (7)
C1′	0.0439 (8)	0.0501 (8)	0.0539 (9)	0.0086 (6)	−0.0078 (7)	−0.0020 (7)
C2′	0.0593 (10)	0.0597 (10)	0.0626 (10)	0.0165 (8)	−0.0026 (8)	−0.0075 (8)
C2	0.0602 (10)	0.0574 (9)	0.0614 (10)	0.0112 (8)	−0.0100 (8)	−0.0145 (8)
C3′	0.0644 (11)	0.0756 (12)	0.0605 (10)	0.0169 (9)	0.0063 (8)	−0.0024 (9)
C3	0.0647 (11)	0.0761 (12)	0.0531 (10)	0.0166 (9)	−0.0047 (8)	−0.0135 (8)
C4′	0.0691 (12)	0.0745 (12)	0.0607 (11)	0.0063 (9)	0.0129 (9)	0.0093 (9)
C4	0.0726 (12)	0.0734 (12)	0.0505 (9)	0.0114 (9)	0.0058 (8)	0.0027 (8)
C5	0.0715 (11)	0.0561 (9)	0.0531 (9)	0.0072 (8)	0.0024 (8)	−0.0002 (7)
C5′	0.0628 (10)	0.0613 (10)	0.0594 (10)	0.0054 (8)	0.0053 (8)	0.0019 (8)
C6	0.0452 (8)	0.0482 (8)	0.0500 (8)	0.0040 (6)	−0.0052 (6)	−0.0036 (6)
C6′	0.0454 (8)	0.0482 (8)	0.0541 (9)	0.0066 (6)	−0.0064 (7)	−0.0026 (7)
C7	0.0458 (8)	0.0440 (8)	0.0465 (8)	−0.0002 (6)	−0.0049 (6)	−0.0025 (6)
C7′	0.0471 (8)	0.0428 (7)	0.0484 (8)	0.0020 (6)	−0.0075 (6)	−0.0014 (6)
C8′	0.0520 (8)	0.0429 (7)	0.0402 (7)	−0.0017 (6)	−0.0013 (6)	−0.0022 (6)
C8	0.0597 (9)	0.0431 (8)	0.0376 (7)	−0.0032 (7)	0.0004 (6)	−0.0022 (6)
C9′	0.0611 (10)	0.0590 (10)	0.0739 (11)	−0.0073 (8)	−0.0144 (8)	−0.0048 (8)
C9	0.0637 (11)	0.0624 (11)	0.0825 (13)	−0.0136 (9)	0.0004 (9)	−0.0097 (9)
C10	0.0969 (16)	0.0608 (12)	0.0820 (13)	−0.0337 (11)	0.0169 (12)	−0.0143 (10)
C10′	0.0861 (14)	0.0561 (10)	0.0740 (12)	−0.0243 (10)	−0.0017 (10)	−0.0122 (9)
C11	0.1251 (19)	0.0445 (9)	0.0549 (10)	−0.0006 (11)	0.0083 (11)	−0.0053 (8)
C11′	0.1054 (15)	0.0416 (9)	0.0559 (10)	0.0016 (9)	−0.0014 (10)	−0.0024 (7)
C12′	0.0926 (13)	0.0501 (9)	0.0675 (11)	0.0167 (9)	−0.0236 (10)	−0.0081 (8)
C12	0.1071 (15)	0.0523 (10)	0.0682 (11)	0.0205 (10)	−0.0210 (10)	−0.0112 (8)
C13′	0.0688 (10)	0.0462 (8)	0.0607 (10)	0.0050 (7)	−0.0203 (8)	−0.0093 (7)
C13	0.0759 (11)	0.0492 (9)	0.0579 (10)	0.0065 (8)	−0.0181 (8)	−0.0101 (7)
C14′	0.0462 (8)	0.0428 (7)	0.0483 (8)	0.0037 (6)	−0.0097 (6)	−0.0030 (6)
C14	0.0425 (8)	0.0428 (7)	0.0493 (8)	0.0000 (6)	−0.0089 (6)	−0.0037 (6)
C15	0.0501 (8)	0.0428 (7)	0.0417 (7)	−0.0005 (6)	−0.0080 (6)	0.0011 (6)
C15′	0.0512 (9)	0.0449 (8)	0.0432 (8)	0.0018 (6)	−0.0082 (6)	0.0025 (6)
C16′	0.0658 (10)	0.0636 (10)	0.0555 (10)	−0.0019 (8)	−0.0153 (8)	−0.0055 (8)
C16	0.0643 (10)	0.0670 (10)	0.0528 (9)	−0.0109 (8)	−0.0150 (8)	−0.0027 (8)
C17′	0.1082 (17)	0.0792 (13)	0.0503 (10)	0.0105 (11)	−0.0180 (10)	−0.0149 (9)
C17	0.1137 (18)	0.0716 (12)	0.0523 (10)	−0.0074 (11)	−0.0253 (11)	−0.0102 (9)
C18	0.1079 (17)	0.0764 (13)	0.0472 (10)	0.0192 (12)	0.0021 (10)	−0.0057 (9)
C18′	0.0907 (16)	0.0978 (15)	0.0504 (11)	0.0261 (12)	0.0074 (10)	0.0000 (10)
C19′	0.0547 (10)	0.1083 (15)	0.0637 (12)	0.0098 (10)	−0.0003 (9)	0.0070 (11)

C19	0.0629 (11)	0.0847 (13)	0.0644 (11)	0.0144 (10)	0.0055 (9)	0.0026 (10)
C20	0.0508 (9)	0.0670 (10)	0.0561 (9)	0.0002 (8)	−0.0075 (7)	−0.0042 (8)
C20′	0.0540 (10)	0.0767 (11)	0.0519 (9)	−0.0005 (8)	−0.0096 (7)	−0.0019 (8)
C21′	0.0596 (10)	0.0503 (9)	0.0579 (9)	−0.0009 (7)	−0.0142 (7)	0.0097 (7)
C21	0.0536 (9)	0.0503 (9)	0.0644 (10)	−0.0013 (7)	−0.0104 (7)	0.0097 (7)
C22′	0.0976 (15)	0.0638 (11)	0.0606 (11)	0.0032 (10)	−0.0077 (10)	0.0136 (8)
C22	0.1015 (15)	0.0645 (11)	0.0625 (11)	0.0042 (10)	−0.0113 (10)	0.0177 (9)
C23′	0.0667 (11)	0.0463 (9)	0.0728 (11)	−0.0015 (7)	−0.0160 (9)	0.0036 (8)
C23	0.0709 (11)	0.0463 (9)	0.0822 (13)	−0.0048 (8)	−0.0094 (9)	0.0093 (8)
C24	0.0689 (11)	0.0429 (9)	0.0784 (12)	−0.0070 (8)	−0.0073 (9)	−0.0056 (8)
C24′	0.0586 (10)	0.0428 (8)	0.0698 (11)	0.0020 (7)	−0.0128 (8)	−0.0061 (7)
N1′	0.0562 (8)	0.0447 (7)	0.0556 (8)	0.0068 (6)	−0.0059 (6)	−0.0071 (6)
N1	0.0580 (8)	0.0427 (7)	0.0574 (8)	−0.0003 (6)	−0.0065 (6)	−0.0071 (6)
N2	0.0557 (8)	0.0441 (7)	0.0497 (7)	0.0024 (5)	−0.0062 (6)	−0.0004 (5)
N2′	0.0579 (8)	0.0435 (7)	0.0497 (7)	0.0058 (6)	−0.0057 (6)	0.0013 (5)
O1	0.1340 (13)	0.0476 (7)	0.0939 (10)	−0.0064 (7)	0.0012 (9)	−0.0177 (7)
O1′	0.0954 (10)	0.0518 (7)	0.0843 (9)	0.0024 (6)	−0.0063 (7)	−0.0170 (6)

Geometric parameters (Å, º)

C1—C2	1.389 (2)	C13—H13	0.9300
C1—C6	1.396 (2)	C14′—N2′	1.4164 (17)
C1—N1	1.4036 (19)	C14′—C15′	1.4817 (19)
C1′—C2′	1.386 (2)	C14—N2	1.4094 (17)
C1′—N1′	1.3982 (19)	C14—C15	1.4844 (19)
C1′—C6′	1.399 (2)	C15—C16	1.376 (2)
C2′—C3′	1.392 (2)	C15—C20	1.386 (2)
C2′—H2′	0.9300	C15′—C16′	1.381 (2)
C2—C3	1.384 (2)	C15′—C20′	1.383 (2)
C2—H2	0.9300	C16′—C17′	1.376 (2)
C3′—C4′	1.372 (2)	C16′—H16′	0.9300
C3′—H3′	0.9300	C16—C17	1.381 (2)
C3—C4	1.369 (2)	C16—H16	0.9300
C3—H3	0.9300	C17′—C18′	1.365 (3)
C4′—C5′	1.381 (2)	C17′—H17′	0.9300
C4′—H4′	0.9300	C17—C18	1.373 (3)
C4—C5	1.377 (2)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.367 (3)
C5—C6	1.402 (2)	C18—H18	0.9300
C5—H5	0.9300	C18′—C19′	1.371 (3)
C5′—C6′	1.400 (2)	C18′—H18′	0.9300
C5′—H5′	0.9300	C19′—C20′	1.370 (2)
C6—C7	1.4660 (19)	C19′—H19′	0.9300
C6′—C7′	1.463 (2)	C19—C20	1.374 (2)
C7—C14	1.3422 (19)	C19—H19	0.9300
C7—C8	1.4931 (19)	C20—H20	0.9300
C7′—C14′	1.3388 (19)	C20′—H20′	0.9300
C7′—C8′	1.4924 (19)	C21′—C23′	1.362 (2)

C8′—C13′	1.379 (2)	C21′—N2′	1.3621 (18)
C8′—C9′	1.380 (2)	C21′—C22′	1.476 (2)
C8—C9	1.376 (2)	C21—C23	1.357 (2)
C8—C13	1.382 (2)	C21—N2	1.3682 (18)
C9′—C10′	1.386 (2)	C21—C22	1.482 (2)
C9′—H9′	0.9300	C22′—H22A	0.9600
C9—C10	1.387 (3)	C22′—H22B	0.9600
C9—H9	0.9300	C22′—H22C	0.9600
C10—C11	1.359 (3)	C22—H22D	0.9600
C10—H10	0.9300	C22—H22E	0.9600
C10′—C11′	1.365 (3)	C22—H22F	0.9600
C10′—H10′	0.9300	C23′—C24′	1.397 (2)
C11—C12	1.358 (3)	C23′—H23′	0.9300
C11—H11	0.9300	C23—C24	1.399 (3)
C11′—C12′	1.363 (3)	C23—H23	0.9300
C11′—H11′	0.9300	C24—O1	1.232 (2)
C12′—C13′	1.384 (2)	C24—N1	1.4074 (19)
C12′—H12′	0.9300	C24′—O1′	1.2415 (19)
C12—C13	1.384 (2)	C24′—N1′	1.4087 (19)
C12—H12	0.9300	N1′—N2′	1.4095 (17)
C13′—H13′	0.9300	N1—N2	1.4075 (17)

C2—C1—C6	120.69 (14)	C7—C14—N2	119.67 (13)
C2—C1—N1	121.18 (13)	C7—C14—C15	123.21 (13)
C6—C1—N1	118.12 (13)	N2—C14—C15	117.11 (12)
C2′—C1′—N1′	121.02 (14)	C16—C15—C20	119.05 (14)
C2′—C1′—C6′	120.91 (14)	C16—C15—C14	120.50 (14)
N1′—C1′—C6′	118.03 (13)	C20—C15—C14	120.42 (13)
C1′—C2′—C3′	119.71 (16)	C16′—C15′—C20′	118.99 (15)
C1′—C2′—H2′	120.1	C16′—C15′—C14′	121.52 (14)
C3′—C2′—H2′	120.1	C20′—C15′—C14′	119.49 (13)
C3—C2—C1	119.63 (15)	C17′—C16′—C15′	120.37 (17)
C3—C2—H2	120.2	C17′—C16′—H16′	119.8
C1—C2—H2	120.2	C15′—C16′—H16′	119.8
C4′—C3′—C2′	120.44 (16)	C15—C16—C17	120.42 (17)
C4′—C3′—H3′	119.8	C15—C16—H16	119.8
C2′—C3′—H3′	119.8	C17—C16—H16	119.8
C4—C3—C2	120.64 (15)	C18′—C17′—C16′	120.01 (18)
C4—C3—H3	119.7	C18′—C17′—H17′	120.0
C2—C3—H3	119.7	C16′—C17′—H17′	120.0
C3′—C4′—C5′	119.67 (16)	C18—C17—C16	119.95 (17)
C3′—C4′—H4′	120.2	C18—C17—H17	120.0
C5′—C4′—H4′	120.2	C16—C17—H17	120.0
C3—C4—C5	119.92 (16)	C19—C18—C17	119.99 (17)
C3—C4—H4	120.0	C19—C18—H18	120.0
C5—C4—H4	120.0	C17—C18—H18	120.0
C4—C5—C6	121.22 (15)	C17′—C18′—C19′	120.12 (17)
C4—C5—H5	119.4	C17′—C18′—H18′	119.9

C6—C5—H5	119.4	C19′—C18′—H18′	119.9
C4′—C5′—C6′	121.63 (16)	C20′—C19′—C18′	120.29 (18)
C4′—C5′—H5′	119.2	C20′—C19′—H19′	119.9
C6′—C5′—H5′	119.2	C18′—C19′—H19′	119.9
C1—C6—C5	117.89 (14)	C18—C19—C20	120.38 (18)
C1—C6—C7	119.40 (13)	C18—C19—H19	119.8
C5—C6—C7	122.66 (13)	C20—C19—H19	119.8
C1′—C6′—C5′	117.62 (14)	C19—C20—C15	120.20 (16)
C1′—C6′—C7′	119.61 (13)	C19—C20—H20	119.9
C5′—C6′—C7′	122.62 (13)	C15—C20—H20	119.9
C14—C7—C6	120.49 (13)	C19′—C20′—C15′	120.20 (16)
C14—C7—C8	120.62 (13)	C19′—C20′—H20′	119.9
C6—C7—C8	118.88 (12)	C15′—C20′—H20′	119.9
C14′—C7′—C6′	120.53 (13)	C23′—C21′—N2′	108.69 (14)
C14′—C7′—C8′	121.55 (13)	C23′—C21′—C22′	126.36 (15)
C6′—C7′—C8′	117.81 (12)	N2′—C21′—C22′	124.89 (15)
C13′—C8′—C9′	118.28 (14)	C23—C21—N2	108.06 (15)
C13′—C8′—C7′	120.80 (13)	C23—C21—C22	126.95 (15)
C9′—C8′—C7′	120.79 (14)	N2—C21—C22	124.91 (15)
C9—C8—C13	118.08 (15)	C21′—C22′—H22A	109.5
C9—C8—C7	120.53 (15)	C21′—C22′—H22B	109.5
C13—C8—C7	121.36 (14)	H22A—C22′—H22B	109.5
C8′—C9′—C10′	120.64 (17)	C21′—C22′—H22C	109.5
C8′—C9′—H9′	119.7	H22A—C22′—H22C	109.5
C10′—C9′—H9′	119.7	H22B—C22′—H22C	109.5
C8—C9—C10	120.65 (19)	C21—C22—H22D	109.5
C8—C9—H9	119.7	C21—C22—H22E	109.5
C10—C9—H9	119.7	H22D—C22—H22E	109.5
C11—C10—C9	120.41 (18)	C21—C22—H22F	109.5
C11—C10—H10	119.8	H22D—C22—H22F	109.5
C9—C10—H10	119.8	H22E—C22—H22F	109.5
C11′—C10′—C9′	120.26 (17)	C21′—C23′—C24′	110.44 (14)
C11′—C10′—H10′	119.9	C21′—C23′—H23′	124.8
C9′—C10′—H10′	119.9	C24′—C23′—H23′	124.8
C12—C11—C10	119.77 (17)	C21—C23—C24	111.16 (15)
C12—C11—H11	120.1	C21—C23—H23	124.4
C10—C11—H11	120.1	C24—C23—H23	124.4
C12′—C11′—C10′	119.70 (16)	O1—C24—C23	132.52 (16)
C12′—C11′—H11′	120.1	O1—C24—N1	123.03 (16)
C10′—C11′—H11′	120.1	C23—C24—N1	104.44 (14)
C11′—C12′—C13′	120.41 (17)	O1′—C24′—C23′	132.34 (15)
C11′—C12′—H12′	119.8	O1′—C24′—N1′	122.78 (15)
C13′—C12′—H12′	119.8	C23′—C24′—N1′	104.86 (14)
C11—C12—C13	120.43 (19)	C1′—N1′—C24′	129.65 (13)
C11—C12—H12	119.8	C1′—N1′—N2′	120.51 (11)
C13—C12—H12	119.8	C24′—N1′—N2′	108.48 (12)
C8′—C13′—C12′	120.68 (16)	C1—N1—N2	120.48 (11)
C8′—C13′—H13′	119.7	C1—N1—C24	129.01 (13)

C12′—C13′—H13′	119.7	N2—N1—C24	108.60 (12)
C8—C13—C12	120.63 (17)	C21—N2—N1	107.72 (12)
C8—C13—H13	119.7	C21—N2—C14	132.80 (13)
C12—C13—H13	119.7	N1—N2—C14	119.19 (11)
C7′—C14′—N2′	119.45 (13)	C21′—N2′—N1′	107.52 (12)
C7′—C14′—C15′	123.80 (13)	C21′—N2′—C14′	132.91 (13)
N2′—C14′—C15′	116.67 (12)	N1′—N2′—C14′	119.08 (11)
N1′—C1′—C2′—C3′	−178.48 (15)	N2′—C14′—C15′—C16′	−106.61 (16)
C6′—C1′—C2′—C3′	−0.5 (2)	C7′—C14′—C15′—C20′	−103.33 (18)
C6—C1—C2—C3	−1.5 (2)	N2′—C14′—C15′—C20′	73.41 (18)
N1—C1—C2—C3	179.25 (14)	C20′—C15′—C16′—C17′	−1.8 (2)
C1′—C2′—C3′—C4′	−0.2 (3)	C14′—C15′—C16′—C17′	178.25 (15)
C1—C2—C3—C4	0.8 (3)	C20—C15—C16—C17	−1.3 (2)
C2′—C3′—C4′—C5′	0.1 (3)	C14—C15—C16—C17	−179.75 (14)
C2—C3—C4—C5	0.3 (3)	C15′—C16′—C17′—C18′	1.2 (3)
C3—C4—C5—C6	−0.7 (3)	C15—C16—C17—C18	0.7 (3)
C3′—C4′—C5′—C6′	0.6 (3)	C16—C17—C18—C19	0.1 (3)
C2—C1—C6—C5	1.1 (2)	C16′—C17′—C18′—C19′	−0.3 (3)
N1—C1—C6—C5	−179.67 (14)	C17′—C18′—C19′—C20′	0.1 (3)
C2—C1—C6—C7	−176.28 (13)	C17—C18—C19—C20	−0.3 (3)
N1—C1—C6—C7	3.0 (2)	C18—C19—C20—C15	−0.4 (3)
C4—C5—C6—C1	0.1 (2)	C16—C15—C20—C19	1.2 (2)
C4—C5—C6—C7	177.30 (15)	C14—C15—C20—C19	179.58 (14)
C2′—C1′—C6′—C5′	1.2 (2)	C18′—C19′—C20′—C15′	−0.7 (3)
N1′—C1′—C6′—C5′	179.27 (14)	C16′—C15′—C20′—C19′	1.6 (2)
C2′—C1′—C6′—C7′	−174.41 (14)	C14′—C15′—C20′—C19′	−178.47 (15)
N1′—C1′—C6′—C7′	3.6 (2)	N2′—C21′—C23′—C24′	−0.97 (19)
C4′—C5′—C6′—C1′	−1.3 (2)	C22′—C21′—C23′—C24′	176.27 (16)
C4′—C5′—C6′—C7′	174.20 (16)	N2—C21—C23—C24	−1.2 (2)
C1—C6—C7—C14	−7.5 (2)	C22—C21—C23—C24	175.78 (17)
C5—C6—C7—C14	175.24 (15)	C21—C23—C24—O1	−177.8 (2)
C1—C6—C7—C8	171.18 (13)	C21—C23—C24—N1	1.4 (2)
C5—C6—C7—C8	−6.0 (2)	C21′—C23′—C24′—O1′	−177.99 (18)
C1′—C6′—C7′—C14′	−7.5 (2)	C21′—C23′—C24′—N1′	0.52 (19)
C5′—C6′—C7′—C14′	177.10 (15)	C2′—C1′—N1′—C24′	−7.1 (2)
C1′—C6′—C7′—C8′	168.57 (13)	C6′—C1′—N1′—C24′	174.87 (14)
C5′—C6′—C7′—C8′	−6.9 (2)	C2′—C1′—N1′—N2′	−172.14 (13)
C14′—C7′—C8′—C13′	86.48 (19)	C6′—C1′—N1′—N2′	9.8 (2)
C6′—C7′—C8′—C13′	−89.52 (18)	O1′—C24′—N1′—C1′	12.4 (3)
C14′—C7′—C8′—C9′	−97.74 (18)	C23′—C24′—N1′—C1′	−166.32 (15)
C6′—C7′—C8′—C9′	86.27 (18)	O1′—C24′—N1′—N2′	178.79 (15)
C14—C7—C8—C9	−100.48 (18)	C23′—C24′—N1′—N2′	0.10 (16)
C6—C7—C8—C9	80.80 (18)	C2—C1—N1—N2	−170.43 (13)
C14—C7—C8—C13	81.75 (19)	C6—C1—N1—N2	10.3 (2)
C6—C7—C8—C13	−96.97 (17)	C2—C1—N1—C24	−8.1 (2)
C13′—C8′—C9′—C10′	1.6 (2)	C6—C1—N1—C24	172.68 (15)
C7′—C8′—C9′—C10′	−174.26 (15)	O1—C24—N1—C1	14.2 (3)

C13—C8—C9—C10	1.7 (2)	C23—C24—N1—C1	−165.04 (15)
C7—C8—C9—C10	−176.15 (15)	O1—C24—N1—N2	178.26 (17)
C8—C9—C10—C11	−0.3 (3)	C23—C24—N1—N2	−1.02 (17)
C8′—C9′—C10′—C11′	−0.1 (3)	C23—C21—N2—N1	0.54 (17)
C9—C10—C11—C12	−1.1 (3)	C22—C21—N2—N1	−176.55 (16)
C9′—C10′—C11′—C12′	−1.2 (3)	C23—C21—N2—C14	−173.02 (15)
C10′—C11′—C12′—C13′	1.0 (3)	C22—C21—N2—C14	9.9 (3)
C10—C11—C12—C13	1.1 (3)	C1—N1—N2—C21	165.95 (13)
C9′—C8′—C13′—C12′	−1.8 (2)	C24—N1—N2—C21	0.32 (16)
C7′—C8′—C13′—C12′	174.04 (14)	C1—N1—N2—C14	−19.45 (19)
C11′—C12′—C13′—C8′	0.6 (3)	C24—N1—N2—C14	174.92 (13)
C9—C8—C13—C12	−1.7 (2)	C7—C14—N2—C21	−172.29 (15)
C7—C8—C13—C12	176.11 (14)	C15—C14—N2—C21	8.5 (2)
C11—C12—C13—C8	0.3 (3)	C7—C14—N2—N1	14.7 (2)
C6′—C7′—C14′—N2′	−2.4 (2)	C15—C14—N2—N1	−164.52 (12)
C8′—C7′—C14′—N2′	−178.27 (13)	C23′—C21′—N2′—N1′	1.00 (17)
C6′—C7′—C14′—C15′	174.27 (13)	C22′—C21′—N2′—N1′	−176.29 (15)
C8′—C7′—C14′—C15′	−1.6 (2)	C23′—C21′—N2′—C14′	−170.62 (15)
C6—C7—C14—N2	−1.5 (2)	C22′—C21′—N2′—C14′	12.1 (3)
C8—C7—C14—N2	179.84 (13)	C1′—N1′—N2′—C21′	167.21 (13)
C6—C7—C14—C15	177.75 (13)	C24′—N1′—N2′—C21′	−0.68 (16)
C8—C7—C14—C15	−1.0 (2)	C1′—N1′—N2′—C14′	−19.80 (19)
C7—C14—C15—C16	77.33 (19)	C24′—N1′—N2′—C14′	172.30 (12)
N2—C14—C15—C16	−103.45 (16)	C7′—C14′—N2′—C21′	−173.38 (15)
C7—C14—C15—C20	−101.06 (17)	C15′—C14′—N2′—C21′	9.7 (2)
N2—C14—C15—C20	78.16 (17)	C7′—C14′—N2′—N1′	15.8 (2)
C7′—C14′—C15′—C16′	76.6 (2)	C15′—C14′—N2′—N1′	−161.12 (12)

Hydrogen-bond geometry (Å, º)

Cg1, Cg3, Cg4, Cg11 and Cg12 are the centroids of the N1/N2/C21–C24, C1–C6, C8–C13, C1′–C6′ and C8′–C13′ rings, respectively

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1	0.93	2.22	2.862 (2)	125
C2′—H2′···O1′	0.93	2.22	2.865 (2)	126
C3—H3···O1′^{i}	0.93	2.49	3.381 (2)	162
C3′—H3′···O1^{i}	0.93	2.54	3.456 (2)	170
C11—H11···O1^{ii}	0.93	2.49	3.274 (2)	142
C9—H9···*Cg*1^{iii}	0.93	2.92	3.796 (2)	158
C16—H16···*Cg*3^{iii}	0.93	3.00	3.822 (2)	149
C18—H18···*Cg*12^{iv}	0.93	2.95	3.869 (2)	169
C18′—H18′···*Cg*4^{iv}	0.93	2.98	3.867 (2)	161
C19—H19···*Cg*3^{v}	0.93	2.90	3.685 (2)	143
C19′—H19′···*Cg*11^{vi}	0.93	2.78	3.604 (2)	149

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