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Crystal structure of 2-(2,2,6,6-tetramethylpiperidin-4-yl)-6-[(2,2,6,6-tetramethylpiperidin-4-yl)amino]-1*H*-benz[*de*]isoquinoline-1,3(2*H*)-dione

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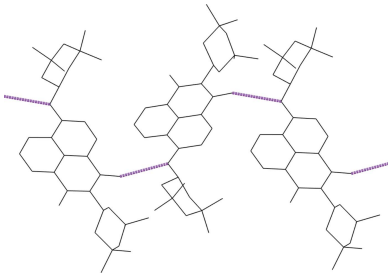
The structure of the title compound, $C_{30}H_{42}N_4O_2$, has orthorhombic (*Pbca*) symmetry. This compound comprises a 4-amino-1,8-naphthalimide core with a 2,2,6,6-tetramethyl-4-piperidinyl substituent bonded to each nitrogen atom. The structure displays N—H···O hydrogen bonding. The structure exhibits disorder of the main molecule.

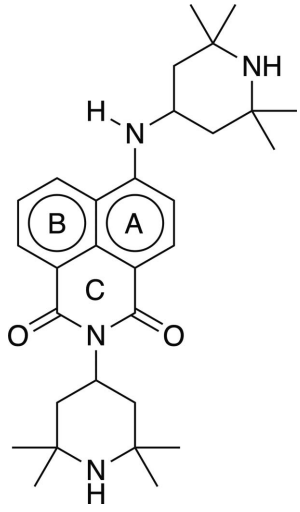
1. Chemical context

The 4-amino-1,8-naphthalimide [6-amino-1*H*-benz[*de*]-isoquinoline-1,3-(2*H*)-dione, **1**] fluorophore has long been recognized as a robust scaffold on which to build fluorescent labels for a wide range of applications. The fluorophore has many desirable properties: (i) unless substituted by a halogen at the 3- position, it is essentially non-toxic to cells, and when substituted by bromine at the 3- position it is highly effective for photochemical inactivation of enveloped viruses such as HIV-1 (Lewis *et al.*, 1993; Chang *et al.*, 1993; Chanh *et al.*, 1993, 1994); (ii) it has a high quantum yield; (iii) it has a large (typically $\geq$100 nm) Stokes shift, which permits its use in fluorescence microscopy with minimal interference from scattering of the excitation radiation (Qian *et al.*, 2010; Srikun *et al.*, 2008); (iv) it is resistant to quenching, including by paramagnetic metal ions such as Cu^{2+} (Mitchell *et al.*, 1998; Veale *et al.*, 2009; Lupo *et al.*, 2010; Wang *et al.*, 2011); (v) it is highly resistant to photochemical bleaching (Sakayori *et al.*, 2005; Bojinov *et al.*, 2009); (vi) its optimal excitation is in the visible, rather than the ultraviolet region; (vii) it is easy to manipulate synthetically, thus allowing a very wide range of reporter ligands to be incorporated into the fluorescent probe (Chang *et al.*, 1999; Zhu *et al.*, 2010; Zheng *et al.*, 2012).

Typically, the groups attached to the aminonaphthalimide fluorophore have been small, allowing relatively easy access of the surroundings to the fluorophore. We have been interested in the synthesis and properties of this fluorophore substituted by sterically hindered groups. One such molecule, 2-(2,2,6,6-tetramethyl-4-piperidinyl)-6-[(2,2,6,6-tetramethyl-4-piperidinyl)amino]-1*H*-benz[*de*]isoquinoline-1,3(2*H*)-dione (designated herein as bis-TMP naphthalimide), was designed, and synthesized by the two-stage reaction between 4-nitro-1,8-naphthalic anhydride and 4-amino-2,2,6,6-tetramethylpiperidine in ethanol then DMF; it was previously reported as a photostable detector for transition-metal cation pollution in



the environment through electron transfer between fluorophore and receptor moieties (Grabchev *et al.*, 2004; Bojinov *et al.*, 2009). In our synthesis, the same compound was obtained by the solvent-free condensation of 4-chloro-1,8-naphthalic anhydride and 4-amino-2,2,6,6-tetramethylpiperidine by fusion of the reaction mixture. The crystal structure of bis-TMP naphthalimide is reported here (Fig. 1).



2. Structural commentary

Evidence of two major resonance contributors to the structure of this *bis*-TMP naphthalimide is provided by the N2—C5 and C1—C2 bond lengths. Direct comparison of the C—N bond lengths of the amine/imide clearly highlight the shortened N2—C5 bond at 1.357 (2) Å compared to the longer N2—C1*A* bond at 1.460 (2) Å, consistent with greater double-bond character of the former. Likewise, direct comparison of the length of the C1—C2 bond at 1.455 (2) Å with the length of the corresponding C12—C10 bond at 1.473 (2) Å is also consistent with greater double-bond character due to resonance of the network along the O1 side of the napthalimide (see Fig. 2). The sole comparison of the bond length of C1—O1 and C12—O2 at 1.233 (2) and 1.224 (2) Å, respectively, indicates a subtle variation in length that reinforces the evidence of resonance in the naphthalimide core increasing the single-bond character of C1—O1 and lengthening it. However, as seen in the discussion of supramolecular features, O1 is also involved in intermolecular hydrogen bonding, which may be a greater contributing factor to reducing the C1—O1 bond order.

3. Supramolecular features

Hydrogen bonding between adjacent molecules repeats in the direction of the *b*-axis with a typical donor-to-acceptor distance of 3.013 (2) Å for N2—H2···O1 and a *D*—H···*A* angle of 165° (Fig. 3, Table 1). Adjacent hydrogen-bonded molecules are rotated by 69.76° with respect to the plane defined by the three fused rings making up the 1*H*-benz[*de*]isoquinoline-1,3(2*H*)-dione (or naphthalimide) core

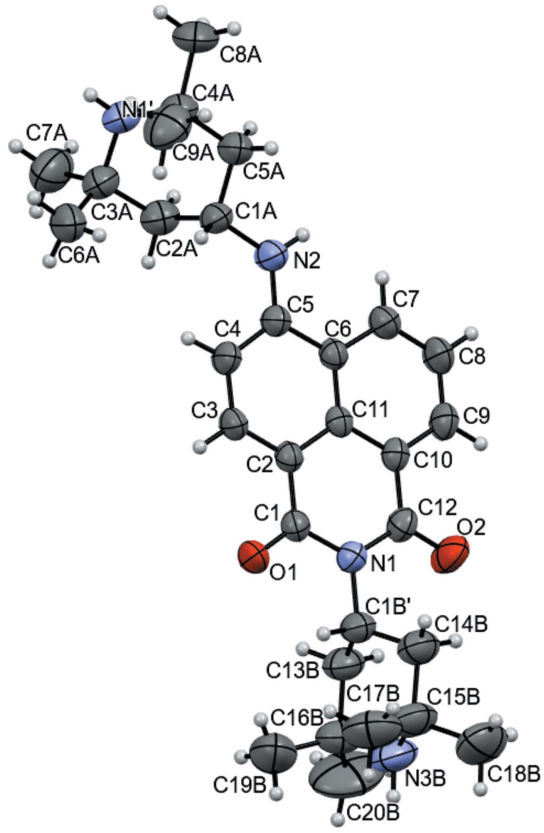


Figure 1
The asymmetric unit of *bis*-TMP naphthalamide represented with displacement ellipsoids at the 50% probability level and disordered TMP omitted for clarity.

in each molecule. While O1 forms a standard hydrogen bond with N2—H2, O2 has close contact with C9—H9 across an inversion center along the path of the *c*-axis such that two close contacts are in parallel with a C9—H9···O2 distance of 3.203 (2) Å and C9—H9···O2 angle of 128°. This relatively close distance and obtuse angle implies that the C9 edge of the fused-ring system carries a significant partial positive charge while O2 carries a significant partial negative charge, resulting in a van der Waals interaction mimicking a hydrogen bond (Arunan *et al.*, 2011).

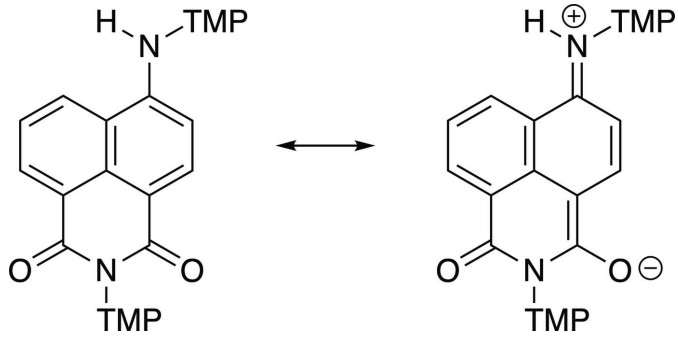


Figure 2
Important resonance contributors to the structure of the *bis*-TMP naphthalimide molecule.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{i}	0.86	2.17	3.0134 (18)	165
C9—H9···O2^{ii}	0.93	2.54	3.203 (2)	128

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (ii) $-x+1, -y+1, -z+1$.

These hydrogen bonds and close dipole attractions organize the naphthalimide cores into sheets parallel to the *bc* plane. The packing along the *a*-axis direction is defined by spatial accommodation of the two bulky TMP moieties of each molecule. It is the steric bulk of these groups that prevents any appreciable π-stacking of the naphthalimide cores. Some T-shaped π-stacking is observed by the C2, C3, C4, C5, C6, C11 edge of the *A*-ring of the naphthalimide ring system to the C7 and C8 edge of the *B*-ring of an adjacent naphthalimide ring system. The distances measured from the centroid of the *A*-ring of the first naphthalimide ring system and atoms C7 and C8 of the *B*-ring of the second naphthalimide system are 4.968 and 5.081 Å, respectively.

4. Database survey

The Cambridge Structural Database (CSD, version 5.42, update of 11/20; Groom *et al.*, 2016) contains many unique 1,8-derivatives of 1*H*-benz[de]isoquinoline-1,3(2*H*)-dione but no examples that contain TMP moieties. A search for $C_{30}H_{42}N_4O_2$ in the database provided seven hits, none of which were the same molecule reported here.

5. Synthesis and crystallization

The title compound was synthesized according to the previously published procedure (Bojinov *et al.*, 2009) and clear, orange rod-like crystals were grown from slow evaporation of an acetone solution.

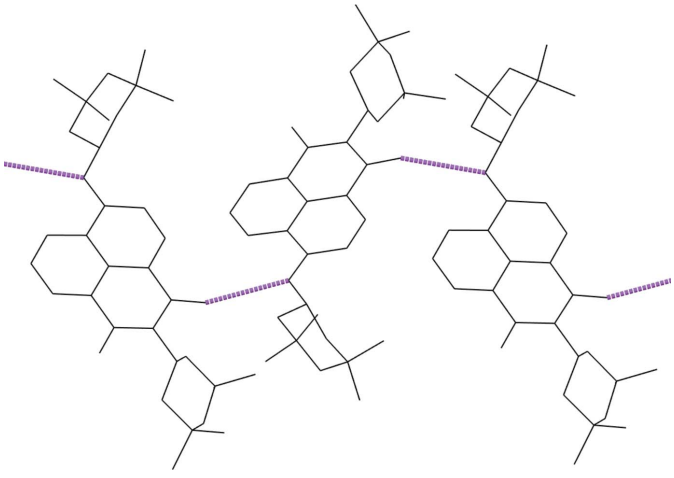


Figure 3
Intermolecular N2—H2···O1 hydrogen bonds linking adjacent molecules are shown as magenta dashed lines (hydrogen atoms and disordered TMP moiety are omitted for clarity).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{30}H_{42}N_4O_2$
M_r	490.67
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	293
a, *b*, *c* (Å)	12.0297 (7), 14.6357 (7), 32.763 (2)
V (Å^3)	5768.4 (6)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	0.07
Crystal size (mm)	0.56 × 0.27 × 0.18
Data collection	
Diffractometer	XtaLAB Mini II
Absorption correction	Analytical [*CrysAlis PRO*; Rigaku OD, 2022; analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by Clark & Reid (1995)]
T_{min}, T_{max}	0.962, 0.990
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	80396, 5164, 3812
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.598
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.049, 0.142, 1.02
No. of reflections	5164
No. of parameters	428
No. of restraints	156
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.15

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), SHELXT (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Disorder of the tetramethylpiperidine (TMP) moiety defined by N3 was refined in two conformations with sufficient restraints and constraints to maintain the typical geometry of the TMP moiety. The disordered components had their ratios set to 0.61 and 0.39. No standard uncertainties are reported as the occupancy ratios were fixed. The reported ratios are the fixed percentages that yielded the best structural model as judged by *RI*, *wR*2, and resolution of any residual electron density. H atoms attached to carbon and nitrogen were positioned geometrically (N—H = 0.86 Å, C—H = 0.93–0.97 Å) and constrained to ride on their parent atoms. U_{iso}(H) values were set to a multiple of U_{eq}(C) [1.2 for CH (*sp*), CH_2 (sp^2), and NH (sp^2) and 1.5 for CH_3 (sp^3)].

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supporting information

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Crystal structure of 2-(2,2,6,6-tetramethylpiperidin-4-yl)-6-[(2,2,6,6-tetramethylpiperidin-4-yl)amino]-1*H*-benz[*de*]isoquinoline-1,3(2*H*)-dione

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2022); cell refinement: *CrysAlis PRO* (Rigaku OD, 2022); data reduction: *CrysAlis PRO* (Rigaku OD, 2022); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

2-(2,2,6,6-Tetramethylpiperidin-4-yl)-6-[(2,2,6,6-tetramethylpiperidin-4-yl)amino]-1*H*-benz[*de*]isoquinoline-1,3(2*H*)-dione

Crystal data

$C_{30}H_{42}N_4O_2$
M_r = 490.67
Orthorhombic, *Pbca*
a = 12.0297 (7) Å
b = 14.6357 (7) Å
c = 32.763 (2) Å
V = 5768.4 (6) Å^3
Z = 8
F(000) = 2128
D_x = 1.130 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 6091 reflections
θ = 2.1–23.5°
μ = 0.07 mm^{-1}
T = 293 K
Needle, orange
0.56 × 0.27 × 0.18 mm

Data collection

XtaLAB Mini II diffractometer
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: analytical [CrysAlisPro; Rigaku OD, 2022; analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by Clark & Reid (1995)]
T_{min} = 0.962, T_{max} = 0.990
80396 measured reflections
5164 independent reflections
3812 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.2°, θ_{min} = 2.1°
h = −14→14
k = −17→16
l = −39→39

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.142
S = 1.02
5164 reflections
428 parameters
156 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2 + 1.5942P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Extinction correction: SHELXL-2016/6 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0014 (3)

Special details

Experimental. A clear, orange rod-like crystal of $C_{30}H_{42}N_4O_2$ was grown from slow evaporation of acetone. The crystal of dimensions 0.178 x 0.265 x 0.563 mm was mounted on MiTeGen loop with Parabar oil and diffraction data was collected. Diffraction data was collected with a Rigaku XtaLAB Mini II benchtop X-ray diffractometer with a fine-focus sealed Mo-target X-ray tube (λ = 0.71073 Å) operated at 600 W power (50 kV, 12 mA) and a HyPix-Bantam Hybrid Photon Counting (HPC) Detector. The X-ray intensities were measured at 293 (2) K; the detector was placed at a distance 4.50 cm from the crystal. The collected frames were integrated with the CrysAlisPro 1.171.41.89a (Rigaku Oxford Diffraction, 2022) software package using a narrow-frame algorithm. Data were corrected for absorption effects using a multifaceted crystal analytical numeric absorption correction (Clark & Reid, 1995) and spherical harmonic empirical absorption correction implemented in the SCALE3 ABSPACK scaling algorithm. With the use of a Mo fine focus beam, both standard multi-scan and combined multi-scan/analytical absorption corrections yielding similar results, and the linear absorption coefficient of 0.071 it was surmised that shape anisotropy had negligible influence on absorption and the crystal analyzed showed the highest quality. The space group was assigned using the GRAL algorithm within the CrysAlisPro 1.171.41.89a software package, solved with ShelXT (Sheldrick, 2015a) and refined with ShelXL (Sheldrick, 2015b) and the graphical interface Olex2 v1.3 (Dolomanov *et al.*, 2009). The asymmetric unit includes one unit of the $C_{30}H_{42}N_4O_2$ molecule. All non-hydrogen atoms were refined anisotropically.

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.54190 (10)	0.79035 (8)	0.63165 (4)	0.0600 (4)	
N1	0.48104 (11)	0.68697 (9)	0.58470 (4)	0.0497 (4)	
O2	0.42262 (12)	0.58100 (10)	0.53855 (4)	0.0785 (5)	
N2	0.90392 (13)	0.47902 (10)	0.66263 (5)	0.0620 (4)	
H2	0.908310	0.426096	0.651341	0.074*	
C11	0.65878 (13)	0.56849 (10)	0.60677 (4)	0.0385 (4)	
C2	0.64762 (13)	0.65558 (10)	0.62532 (5)	0.0419 (4)	
C6	0.74695 (14)	0.50901 (11)	0.61780 (5)	0.0429 (4)	
N1′	1.18903 (15)	0.50136 (12)	0.73813 (6)	0.0739 (5)	
C1	0.55558 (14)	0.71571 (11)	0.61494 (5)	0.0450 (4)	
C10	0.58162 (13)	0.54143 (11)	0.57671 (5)	0.0427 (4)	
C5	0.82443 (14)	0.53746 (11)	0.64913 (5)	0.0484 (4)	
C12	0.48992 (14)	0.60266 (12)	0.56483 (5)	0.0501 (4)	
C3	0.72623 (15)	0.68194 (11)	0.65358 (5)	0.0512 (4)	
H3	0.720899	0.739710	0.665246	0.061*	
C4	0.81258 (15)	0.62551 (12)	0.66515 (6)	0.0562 (5)	
H4	0.864195	0.646555	0.684079	0.067*	
C7	0.75413 (16)	0.42440 (12)	0.59757 (6)	0.0559 (5)	
H7	0.810881	0.384085	0.604437	0.067*	
C9	0.59299 (16)	0.45839 (12)	0.55745 (5)	0.0555 (5)	
H9	0.542658	0.441241	0.537315	0.067*	

C1A	0.98242 (15)	0.50075 (12)	0.69519 (6)	0.0561 (5)	
H1A	0.943213	0.536848	0.715863	0.067*	
C1B′	0.386 (3)	0.7491 (18)	0.5753 (6)	0.0582 (9)	0.39
C8	0.67939 (17)	0.40020 (13)	0.56801 (6)	0.0638 (5)	
H8	0.686560	0.344196	0.554862	0.077*	
C5A	1.02551 (18)	0.41457 (13)	0.71540 (7)	0.0674 (6)	
H5AA	1.065081	0.378156	0.695379	0.081*	
H5AB	0.963128	0.378804	0.725231	0.081*	
C2A	1.08065 (17)	0.55632 (14)	0.68009 (7)	0.0682 (6)	
H2AA	1.053570	0.610657	0.666361	0.082*	
H2AB	1.122249	0.520536	0.660405	0.082*	
C4A	1.10345 (18)	0.43604 (13)	0.75119 (7)	0.0688 (6)	
C3A	1.15818 (17)	0.58465 (14)	0.71509 (7)	0.0708 (6)	
C6A	1.1047 (2)	0.65994 (15)	0.74091 (8)	0.0918 (8)	
H6AA	1.032065	0.640762	0.749458	0.138*	
H6AB	1.098644	0.714763	0.724982	0.138*	
H6AC	1.150006	0.671495	0.764482	0.138*	
C8A	1.1671 (2)	0.34944 (16)	0.76296 (10)	0.1126 (11)	
H8AA	1.209770	0.328589	0.740009	0.169*	
H8AB	1.115442	0.302784	0.770945	0.169*	
H8AC	1.216185	0.362631	0.785316	0.169*	
C16B	0.3244 (8)	0.8717 (5)	0.5282 (2)	0.0769 (8)	0.39
C9A	1.0374 (2)	0.4680 (2)	0.78833 (8)	0.1004 (8)	
H9AA	1.087714	0.484540	0.809835	0.151*	
H9AB	0.989720	0.419561	0.797492	0.151*	
H9AC	0.993090	0.520090	0.781022	0.151*	
C7A	1.2668 (2)	0.6219 (2)	0.69801 (10)	0.1129 (10)	
H7AA	1.316345	0.636092	0.720086	0.169*	
H7AB	1.252150	0.676229	0.682504	0.169*	
H7AC	1.300436	0.576826	0.680659	0.169*	
C15B	0.1852 (5)	0.7834 (5)	0.5713 (3)	0.0908 (19)	0.39
C13B	0.4103 (6)	0.7963 (5)	0.5371 (2)	0.0734 (15)	0.39
H13A	0.410160	0.752463	0.514920	0.088*	0.39
H13B	0.483811	0.823225	0.538643	0.088*	0.39
C14B	0.2731 (4)	0.7072 (4)	0.5771 (2)	0.0772 (14)	0.39
H14A	0.262301	0.677489	0.603306	0.093*	0.39
H14B	0.265368	0.661575	0.555842	0.093*	0.39
C17B	0.1659 (9)	0.8375 (7)	0.6110 (3)	0.120 (3)	0.39
H17A	0.137450	0.797248	0.631645	0.180*	0.39
H17B	0.113354	0.885591	0.606075	0.180*	0.39
H17C	0.235004	0.863374	0.620072	0.180*	0.39
C18B	0.0732 (6)	0.7362 (7)	0.5625 (4)	0.127 (3)	0.39
H18A	0.081066	0.696025	0.539565	0.191*	0.39
H18B	0.017887	0.781617	0.556578	0.191*	0.39
H18C	0.050719	0.701631	0.586031	0.191*	0.39
C1A′	0.3888 (17)	0.7484 (11)	0.5710 (4)	0.0582 (8)	0.61
H1A′	0.352130	0.716321	0.548459	0.070*	0.61
C14A	0.3019 (3)	0.7590 (3)	0.60353 (11)	0.0649 (8)	0.61

H14C	0.334600	0.790061	0.626759	0.078*	0.61
H14D	0.278571	0.698843	0.612531	0.078*	0.61
C15A	0.1991 (3)	0.8127 (3)	0.58943 (13)	0.0769 (8)	0.61
C18A	0.1236 (5)	0.7516 (4)	0.5629 (2)	0.116 (2)	0.61
H18D	0.166708	0.724795	0.541377	0.174*	0.61
H18E	0.065057	0.787957	0.551396	0.174*	0.61
H18F	0.092089	0.704175	0.579508	0.174*	0.61
C17A	0.1309 (6)	0.8422 (5)	0.62700 (18)	0.1162 (19)	0.61
H17D	0.107125	0.788960	0.641754	0.174*	0.61
H17E	0.066979	0.876227	0.618248	0.174*	0.61
H17F	0.176017	0.879688	0.644407	0.174*	0.61
N3A	0.2379 (3)	0.8959 (2)	0.56933 (10)	0.0702 (7)	0.61
C19A	0.3559 (5)	0.9944 (3)	0.5302 (2)	0.151 (3)	0.61
H19A	0.293617	1.027895	0.519594	0.227*	0.61
H19B	0.415350	0.995374	0.510615	0.227*	0.61
H19C	0.380507	1.022024	0.555158	0.227*	0.61
C13A	0.4234 (3)	0.8408 (3)	0.55399 (13)	0.0711 (10)	0.61
H13C	0.475435	0.831970	0.531738	0.085*	0.61
H13D	0.460498	0.875789	0.575132	0.085*	0.61
C20A	0.2847 (6)	0.8554 (5)	0.49672 (15)	0.153 (4)	0.61
H20A	0.342869	0.864610	0.477088	0.229*	0.61
H20B	0.218459	0.885891	0.487692	0.229*	0.61
H20C	0.270180	0.791181	0.499477	0.229*	0.61
N3B	0.2136 (4)	0.8350 (4)	0.53552 (19)	0.0963 (15)	0.39
H3B	0.163899	0.875434	0.530133	0.116*	0.39
C19B	0.3506 (7)	0.9570 (5)	0.5541 (3)	0.126 (3)	0.39
H19D	0.375302	0.938363	0.580689	0.189*	0.39
H19E	0.284770	0.993621	0.556705	0.189*	0.39
H19F	0.407880	0.991982	0.541031	0.189*	0.39
C20B	0.3297 (13)	0.8977 (11)	0.4826 (3)	0.176 (7)	0.39
H20D	0.303123	0.847607	0.466422	0.264*	0.39
H20E	0.405137	0.911249	0.475269	0.264*	0.39
H20F	0.284057	0.950434	0.477849	0.264*	0.39
H1′	1.230 (3)	0.513 (2)	0.7596 (10)	0.156 (13)*	
H1B′	0.388 (4)	0.792 (2)	0.5982 (8)	0.049 (12)*	0.39
C16A	0.3210 (5)	0.8948 (3)	0.53838 (14)	0.0769 (8)	0.61
H3A	0.189 (3)	0.932 (3)	0.5619 (12)	0.088 (13)*	0.61

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0614 (8)	0.0420 (7)	0.0765 (9)	0.0064 (6)	−0.0148 (7)	−0.0154 (6)
N1	0.0488 (8)	0.0465 (8)	0.0539 (8)	0.0030 (6)	−0.0119 (7)	−0.0058 (6)
O2	0.0732 (9)	0.0864 (10)	0.0759 (9)	0.0147 (8)	−0.0352 (8)	−0.0298 (8)
N2	0.0676 (10)	0.0485 (9)	0.0699 (10)	0.0146 (8)	−0.0251 (8)	−0.0177 (7)
C11	0.0439 (8)	0.0363 (8)	0.0354 (8)	−0.0046 (7)	0.0012 (7)	−0.0020 (6)
C2	0.0484 (9)	0.0368 (8)	0.0404 (8)	−0.0024 (7)	−0.0042 (7)	−0.0036 (7)
C6	0.0479 (9)	0.0378 (8)	0.0429 (8)	−0.0026 (7)	−0.0020 (7)	−0.0046 (7)

N1′	0.0624 (11)	0.0655 (11)	0.0938 (14)	0.0067 (9)	−0.0289 (10)	0.0072 (10)
C1	0.0480 (9)	0.0388 (9)	0.0482 (9)	−0.0044 (7)	−0.0034 (7)	−0.0014 (7)
C10	0.0447 (9)	0.0440 (9)	0.0394 (8)	−0.0058 (7)	−0.0012 (7)	−0.0042 (7)
C5	0.0519 (10)	0.0437 (9)	0.0495 (9)	0.0029 (8)	−0.0095 (8)	−0.0054 (7)
C12	0.0496 (10)	0.0556 (11)	0.0450 (9)	−0.0036 (8)	−0.0068 (8)	−0.0067 (8)
C3	0.0619 (11)	0.0366 (9)	0.0550 (10)	0.0025 (8)	−0.0139 (9)	−0.0114 (7)
C4	0.0609 (11)	0.0471 (10)	0.0604 (11)	0.0038 (9)	−0.0230 (9)	−0.0145 (8)
C7	0.0611 (11)	0.0445 (10)	0.0622 (11)	0.0063 (8)	−0.0090 (9)	−0.0120 (8)
C9	0.0588 (11)	0.0535 (10)	0.0543 (10)	−0.0052 (9)	−0.0117 (9)	−0.0155 (8)
C1A	0.0568 (11)	0.0509 (10)	0.0607 (11)	0.0090 (9)	−0.0184 (9)	−0.0078 (8)
C1B′	0.0549 (12)	0.0563 (13)	0.064 (2)	0.0103 (11)	−0.0130 (18)	−0.0010 (15)
C8	0.0727 (13)	0.0472 (10)	0.0716 (12)	0.0049 (9)	−0.0137 (10)	−0.0236 (9)
C5A	0.0678 (12)	0.0518 (11)	0.0825 (14)	0.0083 (10)	−0.0217 (11)	−0.0027 (10)
C2A	0.0664 (13)	0.0653 (13)	0.0730 (13)	0.0063 (10)	−0.0119 (11)	0.0037 (10)
C4A	0.0690 (13)	0.0555 (11)	0.0817 (14)	0.0073 (10)	−0.0262 (11)	0.0087 (10)
C3A	0.0605 (12)	0.0657 (13)	0.0863 (15)	−0.0003 (10)	−0.0237 (11)	0.0095 (11)
C6A	0.1029 (18)	0.0602 (13)	0.1121 (19)	0.0030 (13)	−0.0456 (16)	−0.0121 (13)
C8A	0.110 (2)	0.0690 (15)	0.159 (3)	0.0135 (14)	−0.060 (2)	0.0283 (16)
C16B	0.0726 (11)	0.0780 (18)	0.0800 (19)	0.0214 (12)	−0.0034 (12)	0.0157 (13)
C9A	0.106 (2)	0.121 (2)	0.0738 (16)	−0.0005 (17)	−0.0189 (15)	0.0094 (15)
C7A	0.0765 (17)	0.112 (2)	0.150 (3)	−0.0180 (16)	−0.0271 (17)	0.030 (2)
C15B	0.053 (2)	0.098 (5)	0.122 (5)	0.019 (2)	−0.007 (3)	0.023 (3)
C13B	0.065 (3)	0.073 (3)	0.082 (4)	0.008 (3)	−0.014 (3)	0.020 (3)
C14B	0.057 (2)	0.076 (3)	0.099 (4)	0.0080 (19)	−0.009 (3)	0.015 (3)
C17B	0.100 (8)	0.127 (6)	0.133 (5)	0.051 (5)	−0.005 (5)	0.008 (5)
C18B	0.055 (3)	0.124 (6)	0.202 (9)	0.009 (3)	−0.014 (5)	0.023 (5)
C1A′	0.0548 (11)	0.0563 (12)	0.063 (2)	0.0096 (10)	−0.0128 (17)	−0.0008 (15)
C14A	0.0532 (16)	0.064 (2)	0.077 (2)	0.0032 (14)	−0.0037 (14)	0.0146 (16)
C15A	0.0726 (11)	0.0780 (18)	0.0800 (19)	0.0214 (12)	−0.0034 (12)	0.0157 (13)
C18A	0.055 (3)	0.096 (3)	0.197 (5)	0.013 (2)	−0.036 (3)	−0.006 (3)
C17A	0.085 (4)	0.145 (5)	0.119 (3)	0.039 (3)	0.034 (3)	0.028 (3)
N3A	0.0652 (16)	0.0639 (16)	0.0816 (19)	0.0207 (13)	−0.0055 (13)	0.0049 (13)
C19A	0.121 (4)	0.102 (3)	0.232 (8)	0.032 (3)	0.033 (4)	0.100 (4)
C13A	0.069 (2)	0.068 (2)	0.076 (3)	0.0194 (18)	0.0102 (19)	0.0203 (18)
C20A	0.185 (8)	0.215 (8)	0.058 (3)	0.123 (7)	−0.019 (4)	0.017 (4)
N3B	0.0698 (19)	0.099 (4)	0.120 (4)	0.013 (2)	−0.030 (2)	0.030 (3)
C19B	0.101 (5)	0.087 (4)	0.191 (8)	0.023 (4)	−0.042 (6)	−0.015 (4)
C20B	0.192 (13)	0.214 (14)	0.121 (9)	0.030 (10)	−0.032 (9)	0.098 (9)
C16A	0.0726 (11)	0.0780 (18)	0.0800 (19)	0.0214 (12)	−0.0034 (12)	0.0157 (13)

Geometric parameters (Å, º)

O1—C1	1.2328 (19)	C9A—H9AA	0.9600
N1—C1	1.401 (2)	C9A—H9AB	0.9600
N1—C12	1.399 (2)	C9A—H9AC	0.9600
N1—C1B′	1.49 (3)	C7A—H7AA	0.9600
N1—C1A′	1.497 (19)	C7A—H7AB	0.9600
O2—C12	1.224 (2)	C7A—H7AC	0.9600

N2—H2	0.8600	C15B—C14B	1.549 (9)
N2—C5	1.357 (2)	C15B—C17B	1.542 (3)
N2—C1A	1.460 (2)	C15B—C18B	1.542 (3)
C11—C2	1.418 (2)	C15B—N3B	1.434 (9)
C11—C6	1.419 (2)	C13B—H13A	0.9700
C11—C10	1.410 (2)	C13B—H13B	0.9700
C2—C1	1.455 (2)	C14B—H14A	0.9700
C2—C3	1.379 (2)	C14B—H14B	0.9700
C6—C5	1.448 (2)	C17B—H17A	0.9600
C6—C7	1.407 (2)	C17B—H17B	0.9600
N1′—C4A	1.469 (3)	C17B—H17C	0.9600
N1′—C3A	1.481 (3)	C18B—H18A	0.9600
N1′—H1′	0.87 (3)	C18B—H18B	0.9600
C10—C12	1.473 (2)	C18B—H18C	0.9600
C10—C9	1.376 (2)	C1A′—H1A′	0.9800
C5—C4	1.399 (2)	C1A′—C14A	1.500 (14)
C3—H3	0.9300	C1A′—C13A	1.522 (17)
C3—C4	1.380 (2)	C14A—H14C	0.9700
C4—H4	0.9300	C14A—H14D	0.9700
C7—H7	0.9300	C14A—C15A	1.536 (5)
C7—C8	1.368 (3)	C15A—C18A	1.542 (3)
C9—H9	0.9300	C15A—C17A	1.541 (3)
C9—C8	1.387 (3)	C15A—N3A	1.462 (5)
C1A—H1A	0.9800	C18A—H18D	0.9600
C1A—C5A	1.516 (3)	C18A—H18E	0.9600
C1A—C2A	1.517 (3)	C18A—H18F	0.9600
C1B′—C13B	1.46 (2)	C17A—H17D	0.9600
C1B′—C14B	1.49 (3)	C17A—H17E	0.9600
C1B′—H1B′	0.9800 (11)	C17A—H17F	0.9600
C8—H8	0.9300	N3A—C16A	1.424 (6)
C5A—H5AA	0.9700	N3A—H3A	0.83 (4)
C5A—H5AB	0.9700	C19A—H19A	0.9600
C5A—C4A	1.534 (3)	C19A—H19B	0.9600
C2A—H2AA	0.9700	C19A—H19C	0.9600
C2A—H2AB	0.9700	C19A—C16A	1.541 (3)
C2A—C3A	1.535 (3)	C13A—H13C	0.9700
C4A—C8A	1.530 (3)	C13A—H13D	0.9700
C4A—C9A	1.527 (3)	C13A—C16A	1.549 (7)
C3A—C6A	1.531 (3)	C20A—H20A	0.9600
C3A—C7A	1.522 (3)	C20A—H20B	0.9600
C6A—H6AA	0.9600	C20A—H20C	0.9600
C6A—H6AB	0.9600	C20A—C16A	1.545 (3)
C6A—H6AC	0.9600	N3B—H3B	0.8602
C8A—H8AA	0.9600	C19B—H19D	0.9600
C8A—H8AB	0.9600	C19B—H19E	0.9600
C8A—H8AC	0.9600	C19B—H19F	0.9600
C16B—C13B	1.539 (10)	C20B—H20D	0.9600
C16B—N3B	1.457 (10)	C20B—H20E	0.9600

C16B—C19B	1.542 (3)	C20B—H20F	0.9600
C16B—C20B	1.542 (3)		
C1—N1—C1B′	116.9 (10)	C3A—C7A—H7AB	109.5
C1—N1—C1A′	120.4 (7)	C3A—C7A—H7AC	109.5
C12—N1—C1	123.02 (14)	H7AA—C7A—H7AB	109.5
C12—N1—C1B′	120.0 (11)	H7AA—C7A—H7AC	109.5
C12—N1—C1A′	116.5 (6)	H7AB—C7A—H7AC	109.5
C5—N2—H2	118.1	C17B—C15B—C14B	111.6 (7)
C5—N2—C1A	123.83 (14)	C17B—C15B—C18B	104.8 (8)
C1A—N2—H2	118.1	C18B—C15B—C14B	107.3 (6)
C2—C11—C6	120.85 (14)	N3B—C15B—C14B	108.5 (5)
C10—C11—C2	119.30 (14)	N3B—C15B—C17B	117.1 (7)
C10—C11—C6	119.85 (14)	N3B—C15B—C18B	107.0 (7)
C11—C2—C1	121.03 (14)	C1B′—C13B—C16B	111.7 (12)
C3—C2—C11	118.32 (15)	C1B′—C13B—H13A	109.3
C3—C2—C1	120.65 (14)	C1B′—C13B—H13B	109.3
C11—C6—C5	119.04 (14)	C16B—C13B—H13A	109.3
C7—C6—C11	117.76 (14)	C16B—C13B—H13B	109.3
C7—C6—C5	123.20 (15)	H13A—C13B—H13B	107.9
C4A—N1′—C3A	120.58 (16)	C1B′—C14B—C15B	108.7 (11)
C4A—N1′—H1′	107 (2)	C1B′—C14B—H14A	109.9
C3A—N1′—H1′	113 (2)	C1B′—C14B—H14B	109.9
O1—C1—N1	119.64 (15)	C15B—C14B—H14A	109.9
O1—C1—C2	122.27 (15)	C15B—C14B—H14B	109.9
N1—C1—C2	118.09 (14)	H14A—C14B—H14B	108.3
C11—C10—C12	120.43 (14)	C15B—C17B—H17A	109.5
C9—C10—C11	120.18 (16)	C15B—C17B—H17B	109.5
C9—C10—C12	119.37 (15)	C15B—C17B—H17C	109.5
N2—C5—C6	120.23 (15)	H17A—C17B—H17B	109.5
N2—C5—C4	122.02 (15)	H17A—C17B—H17C	109.5
C4—C5—C6	117.74 (15)	H17B—C17B—H17C	109.5
N1—C12—C10	118.07 (14)	C15B—C18B—H18A	109.5
O2—C12—N1	120.35 (16)	C15B—C18B—H18B	109.5
O2—C12—C10	121.58 (16)	C15B—C18B—H18C	109.5
C2—C3—H3	118.9	H18A—C18B—H18B	109.5
C2—C3—C4	122.22 (15)	H18A—C18B—H18C	109.5
C4—C3—H3	118.9	H18B—C18B—H18C	109.5
C5—C4—H4	119.2	N1—C1A′—H1A′	105.8
C3—C4—C5	121.67 (15)	N1—C1A′—C14A	111.5 (9)
C3—C4—H4	119.2	N1—C1A′—C13A	116.1 (13)
C6—C7—H7	119.3	C14A—C1A′—H1A′	105.8
C8—C7—C6	121.40 (17)	C14A—C1A′—C13A	111.0 (10)
C8—C7—H7	119.3	C13A—C1A′—H1A′	105.8
C10—C9—H9	119.9	C1A′—C14A—H14C	108.8
C10—C9—C8	120.15 (16)	C1A′—C14A—H14D	108.8
C8—C9—H9	119.9	C1A′—C14A—C15A	113.6 (7)
N2—C1A—H1A	108.1	H14C—C14A—H14D	107.7

N2—C1A—C5A	111.05 (15)	C15A—C14A—H14C	108.8
N2—C1A—C2A	112.48 (16)	C15A—C14A—H14D	108.8
C5A—C1A—H1A	108.1	C14A—C15A—C18A	110.3 (4)
C5A—C1A—C2A	108.79 (16)	C14A—C15A—C17A	109.4 (4)
C2A—C1A—H1A	108.1	C17A—C15A—C18A	107.4 (5)
N1—C1B′—C14B	116.0 (17)	N3A—C15A—C14A	107.7 (3)
N1—C1B′—H1B′	102 (3)	N3A—C15A—C18A	114.7 (4)
C13B—C1B′—N1	108.3 (16)	N3A—C15A—C17A	107.2 (4)
C13B—C1B′—C14B	114.2 (19)	C15A—C18A—H18D	109.5
C13B—C1B′—H1B′	110 (3)	C15A—C18A—H18E	109.5
C14B—C1B′—H1B′	105 (3)	C15A—C18A—H18F	109.5
C7—C8—C9	120.65 (16)	H18D—C18A—H18E	109.5
C7—C8—H8	119.7	H18D—C18A—H18F	109.5
C9—C8—H8	119.7	H18E—C18A—H18F	109.5
C1A—C5A—H5AA	109.2	C15A—C17A—H17D	109.5
C1A—C5A—H5AB	109.2	C15A—C17A—H17E	109.5
C1A—C5A—C4A	111.87 (15)	C15A—C17A—H17F	109.5
H5AA—C5A—H5AB	107.9	H17D—C17A—H17E	109.5
C4A—C5A—H5AA	109.2	H17D—C17A—H17F	109.5
C4A—C5A—H5AB	109.2	H17E—C17A—H17F	109.5
C1A—C2A—H2AA	109.2	C15A—N3A—H3A	115 (3)
C1A—C2A—H2AB	109.2	C16A—N3A—C15A	122.3 (3)
C1A—C2A—C3A	112.00 (17)	C16A—N3A—H3A	108 (3)
H2AA—C2A—H2AB	107.9	H19A—C19A—H19B	109.5
C3A—C2A—H2AA	109.2	H19A—C19A—H19C	109.5
C3A—C2A—H2AB	109.2	H19B—C19A—H19C	109.5
N1′—C4A—C5A	109.81 (18)	C16A—C19A—H19A	109.5
N1′—C4A—C8A	105.17 (18)	C16A—C19A—H19B	109.5
N1′—C4A—C9A	113.4 (2)	C16A—C19A—H19C	109.5
C8A—C4A—C5A	109.21 (18)	C1A′—C13A—H13C	109.5
C9A—C4A—C5A	110.71 (19)	C1A′—C13A—H13D	109.5
C9A—C4A—C8A	108.3 (2)	C1A′—C13A—C16A	110.9 (8)
N1′—C3A—C2A	108.10 (17)	H13C—C13A—H13D	108.1
N1′—C3A—C6A	114.6 (2)	C16A—C13A—H13C	109.5
N1′—C3A—C7A	105.48 (18)	C16A—C13A—H13D	109.5
C6A—C3A—C2A	110.61 (17)	H20A—C20A—H20B	109.5
C7A—C3A—C2A	110.1 (2)	H20A—C20A—H20C	109.5
C7A—C3A—C6A	107.8 (2)	H20B—C20A—H20C	109.5
C3A—C6A—H6AA	109.5	C16A—C20A—H20A	109.5
C3A—C6A—H6AB	109.5	C16A—C20A—H20B	109.5
C3A—C6A—H6AC	109.5	C16A—C20A—H20C	109.5
H6AA—C6A—H6AB	109.5	C16B—N3B—H3B	110.4
H6AA—C6A—H6AC	109.5	C15B—N3B—C16B	123.1 (6)
H6AB—C6A—H6AC	109.5	C15B—N3B—H3B	111.4
C4A—C8A—H8AA	109.5	C16B—C19B—H19D	109.5
C4A—C8A—H8AB	109.5	C16B—C19B—H19E	109.5
C4A—C8A—H8AC	109.5	C16B—C19B—H19F	109.5
H8AA—C8A—H8AB	109.5	H19D—C19B—H19E	109.5

H8AA—C8A—H8AC	109.5	H19D—C19B—H19F	109.5
H8AB—C8A—H8AC	109.5	H19E—C19B—H19F	109.5
C13B—C16B—C19B	109.8 (6)	C16B—C20B—H20D	109.5
C13B—C16B—C20B	109.5 (7)	C16B—C20B—H20E	109.5
N3B—C16B—C13B	108.5 (6)	C16B—C20B—H20F	109.5
N3B—C16B—C19B	113.2 (7)	H20D—C20B—H20E	109.5
N3B—C16B—C20B	106.8 (8)	H20D—C20B—H20F	109.5
C20B—C16B—C19B	108.9 (9)	H20E—C20B—H20F	109.5
C4A—C9A—H9AA	109.5	N3A—C16A—C19A	107.7 (4)
C4A—C9A—H9AB	109.5	N3A—C16A—C13A	109.2 (4)
C4A—C9A—H9AC	109.5	N3A—C16A—C20A	115.8 (5)
H9AA—C9A—H9AB	109.5	C19A—C16A—C13A	108.8 (4)
H9AA—C9A—H9AC	109.5	C19A—C16A—C20A	106.0 (6)
H9AB—C9A—H9AC	109.5	C20A—C16A—C13A	109.1 (4)
C3A—C7A—H7AA	109.5		

N1—C1B′—C13B—C16B	−172.0 (11)	C9—C10—C12—O2	0.9 (3)
N1—C1B′—C14B—C15B	173.9 (11)	C1A—N2—C5—C6	−177.46 (16)
N1—C1A′—C14A—C15A	−173.6 (8)	C1A—N2—C5—C4	1.3 (3)
N1—C1A′—C13A—C16A	176.2 (6)	C1A—C5A—C4A—N1′	−50.5 (2)
N2—C5—C4—C3	−174.82 (18)	C1A—C5A—C4A—C8A	−165.3 (2)
N2—C1A—C5A—C4A	−177.00 (17)	C1A—C5A—C4A—C9A	75.5 (2)
N2—C1A—C2A—C3A	175.87 (16)	C1A—C2A—C3A—N1′	53.1 (2)
C11—C2—C1—O1	177.45 (16)	C1A—C2A—C3A—C6A	−73.0 (2)
C11—C2—C1—N1	−2.9 (2)	C1A—C2A—C3A—C7A	167.90 (19)
C11—C2—C3—C4	−2.0 (3)	C1B′—N1—C1—O1	−1.6 (10)
C11—C6—C5—N2	174.59 (16)	C1B′—N1—C1—C2	178.7 (10)
C11—C6—C5—C4	−4.2 (2)	C1B′—N1—C12—O2	2.9 (11)
C11—C6—C7—C8	0.5 (3)	C1B′—N1—C12—C10	−176.7 (10)
C11—C10—C12—N1	−1.1 (2)	C5A—C1A—C2A—C3A	−60.7 (2)
C11—C10—C12—O2	179.29 (17)	C2A—C1A—C5A—C4A	58.7 (2)
C11—C10—C9—C8	1.1 (3)	C4A—N1′—C3A—C2A	−48.5 (3)
C2—C11—C6—C5	1.5 (2)	C4A—N1′—C3A—C6A	75.3 (3)
C2—C11—C6—C7	−178.78 (15)	C4A—N1′—C3A—C7A	−166.3 (2)
C2—C11—C10—C12	−0.4 (2)	C3A—N1′—C4A—C5A	47.5 (3)
C2—C11—C10—C9	178.00 (16)	C3A—N1′—C4A—C8A	164.9 (2)
C2—C3—C4—C5	−0.8 (3)	C3A—N1′—C4A—C9A	−76.9 (3)
C6—C11—C2—C1	−178.24 (14)	C13B—C1B′—C14B—C15B	−59.1 (17)
C6—C11—C2—C3	1.6 (2)	C13B—C16B—N3B—C15B	46.5 (9)
C6—C11—C10—C12	−179.75 (15)	C14B—C1B′—C13B—C16B	57.1 (18)
C6—C11—C10—C9	−1.4 (2)	C14B—C15B—N3B—C16B	−49.9 (9)
C6—C5—C4—C3	3.9 (3)	C17B—C15B—C14B—C1B′	−79.7 (11)
C6—C7—C8—C9	−0.8 (3)	C17B—C15B—N3B—C16B	77.5 (9)
C1—N1—C12—O2	−179.84 (17)	C18B—C15B—C14B—C1B′	166.1 (11)
C1—N1—C12—C10	0.5 (2)	C18B—C15B—N3B—C16B	−165.3 (7)
C1—N1—C1B′—C13B	103.3 (14)	C1A′—N1—C1—O1	3.3 (7)
C1—N1—C1B′—C14B	−126.8 (12)	C1A′—N1—C1—C2	−176.4 (7)
C1—N1—C1A′—C14A	−70.1 (13)	C1A′—N1—C12—O2	−2.0 (7)

C1—N1—C1A′—C13A	58.4 (9)	C1A′—N1—C12—C10	178.4 (6)
C1—C2—C3—C4	177.84 (17)	C1A′—C14A—C15A—C18A	77.3 (9)
C10—C11—C2—C1	2.4 (2)	C1A′—C14A—C15A—C17A	−164.8 (9)
C10—C11—C2—C3	−177.74 (15)	C1A′—C14A—C15A—N3A	−48.6 (9)
C10—C11—C6—C5	−179.15 (15)	C1A′—C13A—C16A—N3A	50.7 (7)
C10—C11—C6—C7	0.6 (2)	C1A′—C13A—C16A—C19A	168.0 (7)
C10—C9—C8—C7	0.0 (3)	C1A′—C13A—C16A—C20A	−76.8 (7)
C5—N2—C1A—C5A	155.91 (18)	C14A—C1A′—C13A—C16A	−55.0 (12)
C5—N2—C1A—C2A	−81.9 (2)	C14A—C15A—N3A—C16A	49.8 (5)
C5—C6—C7—C8	−179.77 (18)	C15A—N3A—C16A—C19A	−169.7 (4)
C12—N1—C1—O1	−178.93 (16)	C15A—N3A—C16A—C13A	−51.6 (5)
C12—N1—C1—C2	1.4 (2)	C15A—N3A—C16A—C20A	71.9 (6)
C12—N1—C1B′—C13B	−79.3 (19)	C18A—C15A—N3A—C16A	−73.5 (5)
C12—N1—C1B′—C14B	50.7 (15)	C17A—C15A—N3A—C16A	167.4 (5)
C12—N1—C1A′—C14A	112.0 (9)	C13A—C1A′—C14A—C15A	55.2 (13)
C12—N1—C1A′—C13A	−119.5 (9)	N3B—C16B—C13B—C1B′	−45.7 (15)
C12—C10—C9—C8	179.47 (17)	N3B—C15B—C14B—C1B′	50.8 (11)
C3—C2—C1—O1	−2.4 (3)	C19B—C16B—C13B—C1B′	78.6 (15)
C3—C2—C1—N1	177.21 (16)	C19B—C16B—N3B—C15B	−75.7 (10)
C7—C6—C5—N2	−5.1 (3)	C20B—C16B—C13B—C1B′	−161.9 (15)
C7—C6—C5—C4	176.09 (17)	C20B—C16B—N3B—C15B	164.5 (8)
C9—C10—C12—N1	−179.46 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.86	2.17	3.0134 (18)	165
C9—H9···O2^{ii}	0.93	2.54	3.203 (2)	128

Symmetry codes: (i) −*x*+3/2, *y*−1/2, *z*; (ii) −*x*+1, −*y*+1, −*z*+1.