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N-[1,4,4-Trimethyltricyclo[6.3.1.$0^{3,9}$]dodec-8(12)-en-2-yl]acetamide

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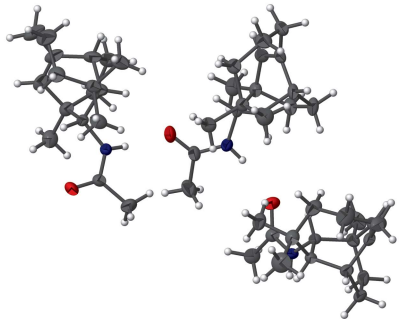
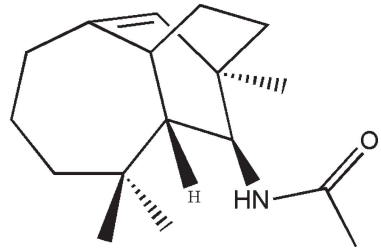
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{17}H_{27}NO$, crystallizes with three independent molecules in the asymmetric unit with almost identical conformations. Each molecule is built up from a seven-membered ring to which a bridged six-membered ring is fused. In each of the three molecules, the seven-membered rings have a twist-chair conformation, while the cyclohexenyl rings display perfect boat conformations. In the crystal, N—H···O hydrogen bonds link the molecules into zigzag chains running along the *b*-axis direction.

3D view



Chemical scheme



Structure description

The bicyclic sesquiterpene α-himachalene is a constituent (20%) of the essential oil of the Atlas cedar (*Cedrus Atlantica*) (El Haib *et al.*, 2010; Loubidi *et al.*, 2014). The reactivity of this sesquiterpene and its derivatives has been studied extensively by our team (El Jamili *et al.*, 2002; El Haib *et al.*, 2011; Loubidi *et al.*, 2014; Benharref *et al.*, 2016, 2017) in order to prepare new products with biological properties. Indeed, these compounds have been tested, using the food-poisoning technique, for their potential antifungal activity against the phytopathogen *Botrytis cinerea* (Daoubi *et al.*, 2004). Herein, we report the synthesis and crystal structure of the title compound, synthesized by the reaction of 6α,7α- epoxyhimachalene with BF_3OEt in acetonitrile under argon.

The asymmetric unit of this new compound contains three independent molecules with similar conformations. Each molecule is built up from a seven-membered ring, which is fused to a bridged cyclohexenyl ring as shown in Fig. 1. In each of the three molecules, the seven-membered ring displays a twist-chair conformation as indicated by the total puckering amplitude Q_T = 0.864 (3) Å, a spherical polar angle θ = 39.60 (2)°; φ2 =

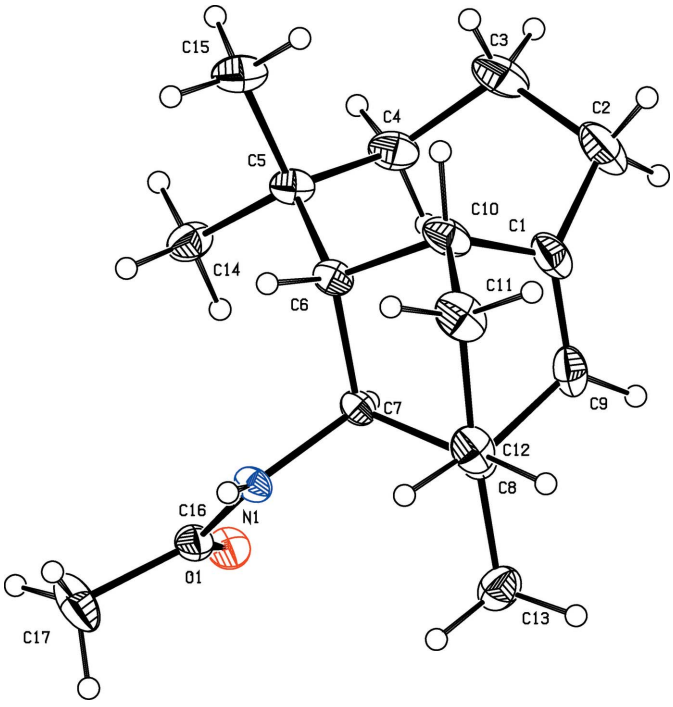


Figure 1
The molecular structure of one of the three unique molecules the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The other two molecules are labelled similarly but with the suffix A or B.

342.4 (3)° and $\varphi 3$ = 301.6 (3)°, whereas the cyclohexenyl ring shows a perfect boat conformation with Q_T = 0.865 (3) Å, a spherical polar angle θ = 88.7 (2)° and $\varphi 2$ = 125.08 (18)°.

In the crystal, the three molecules are linked by N—H···O hydrogen bonds, forming zigzag chains running along the *b*-axis direction (Fig. 2 and Table 1). Adjacent chains form sheets of molecules in the *bc* plane (Fig. 3).

Synthesis and crystallization

2 g (9 mmol) of 8,9-epoxy-2methylene-6,6,9-triméthylbicyclo [5.4.0^{1},^{7}]undecane (Lassaba *et al.*, 1998) was dissolved in 30 ml

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	2.04	2.893 (2)	173
N2—H2···O3	0.86	2.11	2.956 (3)	167
N3—H3···O1^{i}	0.86	2.06	2.909 (2)	169

Symmetry code: (i) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{27}NO$
M_r	261.39
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	180
a, *b*, *c* (Å)	9.0275 (4), 16.9076 (7), 30.7411 (11)
V (Å^3)	4692.1 (3)
Z	12
Radiation type	Mo *Kα*
μ (mm^{-1})	0.07
Crystal size (mm)	0.50 × 0.25 × 0.12
Data collection	
Diffractometer	Rigaku Oxford Diffraction Xcalibur Eos Gemini ultra
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku Oxford Diffraction, 2015)
T_{min}, T_{max}	0.911, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26928, 9534, 8730
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.043, 0.102, 1.07
No. of reflections	9534
No. of parameters	526
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.15
Absolute structure	Flack *x* determined using 3320 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.3 (5)

Computer programs: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

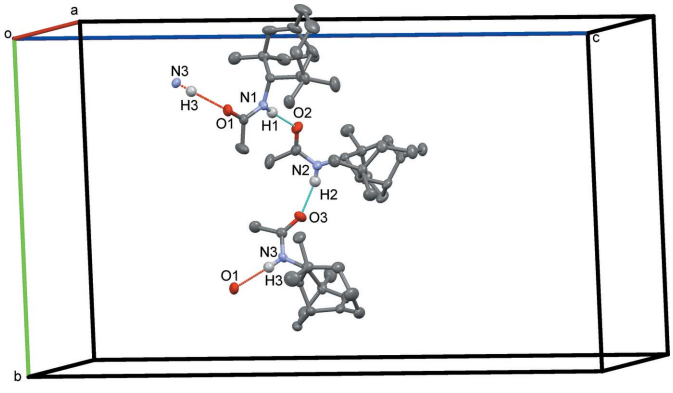


Figure 2
A view of the three molecules in the asymmetric unit, linked by N—H···O hydrogen bonds (see Table 1). **A and B molecules should be indicated**

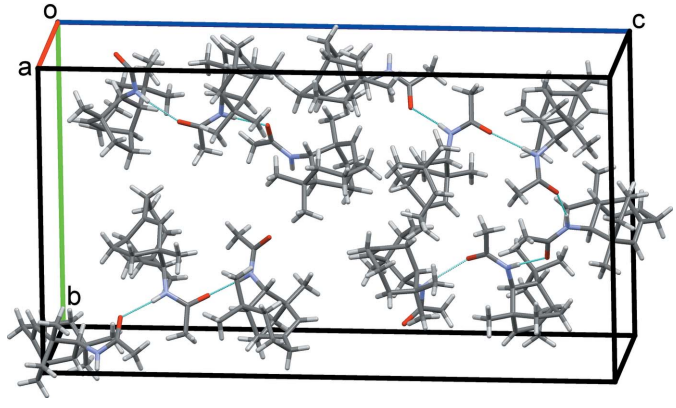


Figure 3
Overall packing of the title compound viewed along *a*.

of CH_3CN and stirred at 273 K under argon. BF_3OEt (3% mmol) was added and the reaction mixture was stirred and monitored by TLC. After the completion of reaction, the solvent was removed and the residue obtained was chromatographed on silica, eluting with hexane–ethylacetate (90:10), which allowed the isolation of the title compound (yield: 1.5 g, 5.7 mmol, 64%).

Refinement

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

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full crystallographic data

IUCrData (2017). **2**, x170805 [https://doi.org/10.1107/S2414314617008057]

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Crystal data

$C_{17}H_{27}NO$
M_r = 261.39
Orthorhombic, $P2_12_12_1$
a = 9.0275 (4) Å
b = 16.9076 (7) Å
c = 30.7411 (11) Å
V = 4692.1 (3) Å^3
Z = 12
F(000) = 1728
D_x = 1.110 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9534 reflections
θ = 3–26.4°
μ = 0.07 mm^{-1}
T = 180 K
Rectangular plate, colourless
0.50 × 0.25 × 0.12 mm

Data collection

Rigaku Oxford Diffraction Xcalibur Eos Gemini ultra diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1978 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku Oxford Diffraction, 2015)
T_{min} = 0.911, T_{max} = 1.000
26928 measured reflections
9534 independent reflections
8730 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.4°, θ_{min} = 3.0°
h = −10→11
k = −21→20
l = −38→37

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.102
S = 1.07
9534 reflections
526 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.5238P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack x determined using 3320 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.3 (5)

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. All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.99 Å (methylene), 0.98 Å (methyl), 1.0Å (methine) with $U_{iso}(H) = 1.2U_{eq}$(CH and CH_2) or $U_{iso}(H) = 1.5U_{eq}(CH_3)$. The coordinates of H atoms attached to N atoms were freely refined with $U_{iso}(H) = 1.2U_{eq}(N)$ and the H attached to hydroxyl O atoms were fixed geometrically and treated as riding with O—H = 0.84Å and $U_{iso}(H) = 1.5U_{eq}(O)$.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.2729 (2)	0.27939 (10)	0.21957 (5)	0.0355 (4)
O3	0.8062 (2)	0.57328 (10)	0.39222 (5)	0.0367 (4)
N1	1.2026 (2)	0.26183 (11)	0.28991 (6)	0.0271 (4)
H1	1.1510	0.2811	0.3109	0.033*
O2	1.0471 (2)	0.32177 (11)	0.36531 (5)	0.0435 (4)
N2	0.9937 (2)	0.43161 (11)	0.40406 (6)	0.0286 (4)
H2	0.9476	0.4761	0.4041	0.034*
N3	0.8069 (2)	0.69312 (11)	0.35888 (6)	0.0267 (4)
H3	0.7722	0.7201	0.3374	0.032*
C8A	0.9896 (2)	0.38980 (14)	0.48235 (7)	0.0288 (5)
C10A	1.1816 (3)	0.49735 (13)	0.50212 (7)	0.0297 (5)
H10A	1.2557	0.5363	0.5113	0.036*
C5A	1.3599 (3)	0.46297 (14)	0.43902 (7)	0.0291 (5)
C5B	1.1863 (3)	0.74100 (14)	0.35737 (8)	0.0330 (5)
C6	1.3768 (3)	0.18714 (14)	0.33651 (7)	0.0286 (5)
H6	1.3453	0.2319	0.3545	0.034*
C1B	1.0646 (3)	0.85866 (14)	0.42509 (8)	0.0346 (6)
C16B	0.7589 (2)	0.61863 (13)	0.36388 (7)	0.0282 (5)
C17B	0.6396 (3)	0.59381 (15)	0.33209 (8)	0.0370 (6)
H17A	0.6745	0.5501	0.3150	0.056*
H17B	0.6162	0.6374	0.3133	0.056*
H17C	0.5525	0.5782	0.3478	0.056*
C6B	1.0294 (3)	0.77820 (12)	0.35998 (7)	0.0253 (5)
H6B	0.9908	0.7802	0.3302	0.030*
C7A	1.0855 (2)	0.41177 (12)	0.44174 (7)	0.0237 (4)
H7A	1.1438	0.3649	0.4340	0.028*
C1A	1.2051 (3)	0.41964 (15)	0.52530 (7)	0.0310 (5)
C6A	1.1968 (2)	0.47923 (13)	0.45294 (7)	0.0250 (4)
H6A	1.1640	0.5265	0.4372	0.030*
C7	1.2724 (2)	0.18478 (13)	0.29605 (7)	0.0252 (5)
H7	1.3346	0.1749	0.2705	0.030*
C7B	0.9144 (2)	0.73141 (13)	0.38758 (7)	0.0249 (5)
H7B	0.9673	0.6901	0.4036	0.030*
C12A	0.9095 (3)	0.46473 (16)	0.49821 (8)	0.0362 (6)
H12A	0.8473	0.4519	0.5230	0.043*

H12B	0.8466	0.4852	0.4752	0.043*
C10B	1.0316 (3)	0.86401 (13)	0.37708 (7)	0.0313 (5)
H10B	1.1075	0.8952	0.3621	0.038*
C4	1.6173 (3)	0.12822 (17)	0.30345 (9)	0.0412 (6)
H4A	1.7144	0.1447	0.2934	0.049*
H4B	1.5595	0.1148	0.2779	0.049*
C9B	0.9623 (3)	0.82009 (16)	0.44760 (8)	0.0372 (6)
H9B	0.9682	0.8140	0.4776	0.045*
C5	1.5432 (3)	0.20015 (15)	0.32539 (7)	0.0336 (5)
C14B	1.1719 (3)	0.65226 (15)	0.34653 (9)	0.0398 (6)
H14A	1.1050	0.6456	0.3225	0.060*
H14B	1.1343	0.6245	0.3714	0.060*
H14C	1.2673	0.6315	0.3389	0.060*
C16A	0.9779 (3)	0.38418 (15)	0.36961 (7)	0.0333 (5)
C8	1.1602 (3)	0.11518 (14)	0.29940 (8)	0.0318 (5)
C3A	1.4772 (3)	0.41685 (18)	0.51402 (8)	0.0415 (6)
H3A1	1.5095	0.4715	0.5160	0.050*
H3A2	1.5601	0.3838	0.5225	0.050*
C12B	0.7612 (3)	0.85432 (16)	0.39610 (8)	0.0396 (6)
H12C	0.6880	0.8328	0.3763	0.048*
H12D	0.7111	0.8895	0.4162	0.048*
C11A	1.0239 (3)	0.52780 (16)	0.51135 (9)	0.0386 (6)
H11A	1.0138	0.5398	0.5421	0.046*
H11B	1.0064	0.5760	0.4950	0.046*
C2A	1.3501 (3)	0.40409 (17)	0.54694 (8)	0.0384 (6)
H2A1	1.3526	0.3502	0.5577	0.046*
H2A2	1.3624	0.4396	0.5715	0.046*
C13A	0.8812 (3)	0.32349 (16)	0.47200 (9)	0.0426 (6)
H13A	0.9347	0.2782	0.4616	0.064*
H13B	0.8129	0.3409	0.4501	0.064*
H13C	0.8276	0.3095	0.4978	0.064*
C13	1.0527 (3)	0.11491 (17)	0.26134 (9)	0.0419 (6)
H13D	1.1072	0.1127	0.2345	0.063*
H13E	0.9940	0.1622	0.2620	0.063*
H13F	0.9891	0.0696	0.2634	0.063*
C10	1.3475 (3)	0.11117 (15)	0.36304 (8)	0.0392 (6)
H10	1.4194	0.1062	0.3868	0.047*
C8B	0.8356 (3)	0.78670 (15)	0.42139 (7)	0.0327 (5)
C17A	0.8678 (3)	0.41232 (19)	0.33585 (9)	0.0514 (7)
H17D	0.8667	0.3760	0.3118	0.077*
H17E	0.8961	0.4639	0.3257	0.077*
H17F	0.7708	0.4149	0.3486	0.077*
C12	1.0776 (3)	0.12117 (16)	0.34338 (8)	0.0394 (6)
H12E	1.0257	0.1713	0.3451	0.047*
H12F	1.0050	0.0790	0.3455	0.047*
C14	1.5592 (3)	0.27036 (16)	0.29424 (8)	0.0390 (6)
H14D	1.5104	0.3157	0.3064	0.058*
H14E	1.5149	0.2574	0.2668	0.058*

H14F	1.6623	0.2820	0.2901	0.058*
C9	1.2618 (3)	0.04393 (14)	0.29990 (9)	0.0401 (6)
H9	1.2543	0.0034	0.2796	0.048*
C4A	1.4388 (3)	0.39866 (15)	0.46613 (7)	0.0338 (5)
H4A1	1.3770	0.3518	0.4658	0.041*
H4A2	1.5303	0.3853	0.4513	0.041*
C16	1.2149 (3)	0.30401 (14)	0.25332 (7)	0.0317 (5)
C9A	1.1030 (3)	0.36573 (15)	0.51578 (7)	0.0325 (5)
H9A	1.1016	0.3162	0.5289	0.039*
C1	1.3629 (3)	0.04340 (15)	0.33164 (9)	0.0419 (6)
C15A	1.4470 (3)	0.54094 (16)	0.44141 (9)	0.0439 (6)
H15A	1.5490	0.5313	0.4343	0.066*
H15B	1.4405	0.5621	0.4703	0.066*
H15C	1.4060	0.5781	0.4211	0.066*
C2B	1.2171 (3)	0.87902 (16)	0.44012 (9)	0.0451 (7)
H2B1	1.2262	0.8684	0.4710	0.054*
H2B2	1.2358	0.9348	0.4354	0.054*
C15	1.6263 (3)	0.22284 (19)	0.36732 (9)	0.0481 (7)
H15D	1.7295	0.2301	0.3609	0.072*
H15E	1.6152	0.1814	0.3884	0.072*
H15F	1.5860	0.2711	0.3787	0.072*
C4B	1.2783 (3)	0.74766 (15)	0.39976 (9)	0.0400 (6)
H4B1	1.2199	0.7248	0.4231	0.048*
H4B2	1.3655	0.7148	0.3963	0.048*
C14A	1.3623 (3)	0.43624 (16)	0.39113 (8)	0.0365 (6)
H14G	1.3110	0.4744	0.3736	0.055*
H14H	1.3144	0.3858	0.3886	0.055*
H14I	1.4630	0.4319	0.3814	0.055*
C3B	1.3303 (3)	0.82954 (18)	0.41482 (11)	0.0523 (8)
H3B1	1.4172	0.8226	0.4330	0.063*
H3B2	1.3605	0.8594	0.3894	0.063*
C17	1.1539 (4)	0.38749 (16)	0.25564 (9)	0.0561 (8)
H17G	1.2232	0.4235	0.2427	0.084*
H17H	1.1383	0.4018	0.2855	0.084*
H17I	1.0615	0.3900	0.2402	0.084*
C13B	0.7265 (3)	0.7406 (2)	0.44942 (9)	0.0511 (7)
H13G	0.7768	0.6972	0.4631	0.077*
H13H	0.6478	0.7206	0.4315	0.077*
H13I	0.6860	0.7749	0.4713	0.077*
C11	1.1887 (3)	0.11465 (18)	0.38117 (8)	0.0462 (7)
H11C	1.1785	0.1600	0.4002	0.055*
H11D	1.1684	0.0673	0.3980	0.055*
C3	1.6374 (3)	0.05218 (19)	0.33059 (11)	0.0560 (8)
H3A	1.7218	0.0234	0.3192	0.067*
H3B	1.6609	0.0673	0.3602	0.067*
C11B	0.8777 (3)	0.90048 (14)	0.37048 (8)	0.0390 (6)
H11E	0.8786	0.9551	0.3801	0.047*
H11F	0.8527	0.8998	0.3398	0.047*

C2	1.5042 (4)	−0.00377 (18)	0.33162 (13)	0.0609 (9)
H2A	1.5066	−0.0382	0.3064	0.073*
H2B	1.5087	−0.0365	0.3575	0.073*
C15B	1.2701 (4)	0.7791 (2)	0.31947 (10)	0.0560 (8)
H15G	1.2692	0.8355	0.3228	0.084*
H15H	1.2231	0.7650	0.2925	0.084*
H15I	1.3707	0.7606	0.3193	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0459 (10)	0.0391 (9)	0.0216 (7)	0.0015 (8)	−0.0010 (7)	0.0004 (7)
O3	0.0387 (10)	0.0300 (9)	0.0415 (9)	−0.0002 (8)	−0.0025 (8)	0.0102 (7)
N1	0.0313 (10)	0.0275 (9)	0.0224 (8)	0.0074 (8)	0.0003 (8)	−0.0010 (7)
O2	0.0565 (12)	0.0402 (10)	0.0340 (9)	0.0088 (9)	−0.0016 (9)	−0.0137 (8)
N2	0.0301 (10)	0.0257 (10)	0.0301 (9)	0.0055 (8)	−0.0051 (8)	−0.0045 (8)
N3	0.0273 (10)	0.0264 (9)	0.0264 (9)	0.0000 (8)	−0.0048 (8)	0.0054 (7)
C8A	0.0236 (11)	0.0316 (12)	0.0311 (11)	−0.0007 (10)	0.0048 (9)	−0.0039 (9)
C10A	0.0255 (11)	0.0303 (12)	0.0332 (12)	0.0015 (10)	−0.0016 (9)	−0.0128 (9)
C5A	0.0264 (12)	0.0319 (12)	0.0289 (11)	0.0004 (10)	0.0026 (9)	−0.0003 (9)
C5B	0.0269 (12)	0.0324 (12)	0.0396 (13)	−0.0013 (10)	0.0030 (10)	−0.0017 (10)
C6	0.0302 (12)	0.0330 (12)	0.0226 (10)	0.0043 (10)	0.0018 (9)	0.0035 (9)
C1B	0.0418 (14)	0.0254 (11)	0.0366 (13)	0.0078 (11)	−0.0141 (11)	−0.0079 (10)
C16B	0.0231 (11)	0.0295 (11)	0.0319 (11)	−0.0003 (10)	0.0035 (9)	0.0024 (9)
C17B	0.0320 (13)	0.0358 (13)	0.0432 (13)	−0.0086 (11)	−0.0018 (11)	0.0028 (11)
C6B	0.0302 (12)	0.0237 (11)	0.0221 (9)	0.0015 (9)	−0.0019 (9)	0.0016 (8)
C7A	0.0240 (11)	0.0214 (10)	0.0256 (10)	0.0043 (9)	−0.0006 (8)	−0.0039 (8)
C1A	0.0303 (12)	0.0417 (13)	0.0210 (10)	0.0070 (11)	0.0037 (9)	−0.0059 (9)
C6A	0.0252 (11)	0.0226 (10)	0.0273 (10)	0.0017 (9)	−0.0008 (9)	−0.0011 (8)
C7	0.0265 (11)	0.0248 (10)	0.0242 (10)	0.0046 (9)	0.0023 (9)	0.0014 (8)
C7B	0.0245 (11)	0.0258 (11)	0.0245 (10)	0.0045 (9)	−0.0035 (8)	0.0017 (8)
C12A	0.0245 (12)	0.0459 (15)	0.0383 (13)	0.0031 (11)	0.0033 (10)	−0.0119 (11)
C10B	0.0376 (14)	0.0233 (11)	0.0329 (12)	−0.0001 (10)	−0.0074 (10)	0.0015 (9)
C4	0.0266 (13)	0.0525 (16)	0.0446 (14)	0.0081 (12)	0.0025 (11)	0.0027 (12)
C9B	0.0435 (15)	0.0421 (14)	0.0260 (11)	0.0123 (13)	−0.0071 (11)	−0.0072 (10)
C5	0.0288 (13)	0.0429 (14)	0.0291 (11)	0.0019 (11)	−0.0017 (10)	0.0040 (10)
C14B	0.0318 (14)	0.0392 (14)	0.0484 (15)	0.0080 (12)	−0.0007 (12)	−0.0116 (11)
C16A	0.0352 (13)	0.0351 (13)	0.0294 (11)	0.0017 (11)	0.0000 (10)	−0.0072 (10)
C8	0.0279 (12)	0.0304 (12)	0.0370 (12)	0.0010 (10)	0.0053 (10)	0.0019 (10)
C3A	0.0280 (13)	0.0565 (17)	0.0399 (13)	0.0077 (13)	−0.0060 (11)	−0.0006 (12)
C12B	0.0362 (14)	0.0440 (14)	0.0386 (13)	0.0182 (12)	−0.0085 (11)	−0.0160 (11)
C11A	0.0313 (13)	0.0401 (14)	0.0446 (14)	0.0076 (12)	0.0015 (11)	−0.0183 (11)
C2A	0.0382 (14)	0.0492 (15)	0.0277 (11)	0.0109 (12)	−0.0032 (10)	−0.0054 (11)
C13A	0.0349 (14)	0.0417 (15)	0.0513 (15)	−0.0085 (12)	0.0064 (12)	−0.0058 (12)
C13	0.0334 (13)	0.0435 (15)	0.0488 (15)	−0.0061 (12)	0.0011 (11)	−0.0051 (12)
C10	0.0380 (14)	0.0459 (15)	0.0336 (12)	0.0066 (12)	0.0019 (11)	0.0174 (11)
C8B	0.0305 (13)	0.0423 (14)	0.0251 (10)	0.0077 (11)	0.0002 (9)	−0.0019 (10)
C17A	0.0530 (17)	0.0627 (19)	0.0384 (14)	0.0055 (15)	−0.0157 (13)	−0.0141 (13)

C12	0.0340 (14)	0.0393 (14)	0.0448 (14)	0.0000 (12)	0.0141 (11)	0.0097 (11)
C14	0.0326 (13)	0.0481 (15)	0.0361 (12)	−0.0103 (12)	−0.0035 (11)	0.0053 (11)
C9	0.0409 (15)	0.0241 (12)	0.0552 (16)	−0.0012 (11)	0.0120 (13)	0.0033 (11)
C4A	0.0243 (12)	0.0423 (14)	0.0346 (12)	0.0062 (11)	0.0049 (10)	−0.0018 (10)
C16	0.0376 (13)	0.0311 (12)	0.0264 (11)	0.0018 (11)	−0.0066 (10)	0.0004 (9)
C9A	0.0350 (13)	0.0364 (13)	0.0262 (11)	0.0022 (11)	0.0079 (9)	0.0032 (9)
C1	0.0379 (15)	0.0310 (13)	0.0567 (16)	0.0054 (12)	0.0079 (13)	0.0180 (12)
C15A	0.0369 (14)	0.0412 (15)	0.0537 (15)	−0.0080 (12)	0.0031 (13)	0.0015 (12)
C2B	0.0493 (16)	0.0342 (13)	0.0519 (15)	−0.0029 (13)	−0.0228 (13)	−0.0033 (12)
C15	0.0397 (15)	0.0674 (19)	0.0372 (13)	0.0018 (14)	−0.0103 (12)	0.0048 (13)
C4B	0.0267 (13)	0.0362 (13)	0.0571 (16)	0.0038 (11)	−0.0092 (11)	−0.0017 (12)
C14A	0.0344 (13)	0.0430 (14)	0.0321 (12)	0.0017 (12)	0.0091 (10)	0.0032 (10)
C3B	0.0338 (15)	0.0462 (16)	0.077 (2)	−0.0071 (13)	−0.0166 (15)	−0.0071 (15)
C17	0.092 (2)	0.0357 (15)	0.0405 (14)	0.0197 (16)	0.0053 (15)	0.0097 (12)
C13B	0.0403 (16)	0.077 (2)	0.0364 (14)	0.0018 (15)	0.0126 (12)	−0.0001 (14)
C11	0.0485 (16)	0.0532 (17)	0.0367 (13)	0.0033 (14)	0.0145 (12)	0.0176 (12)
C3	0.0401 (16)	0.061 (2)	0.068 (2)	0.0253 (15)	−0.0007 (15)	0.0083 (16)
C11B	0.0510 (16)	0.0275 (12)	0.0386 (13)	0.0123 (12)	−0.0172 (12)	−0.0046 (10)
C2	0.058 (2)	0.0407 (17)	0.084 (2)	0.0197 (15)	0.0040 (17)	0.0197 (15)
C15B	0.0428 (17)	0.064 (2)	0.0610 (18)	−0.0049 (16)	0.0189 (14)	0.0049 (15)

Geometric parameters (Å, º)

O1—C16	1.234 (3)	C3A—C2A	1.545 (4)
O3—C16B	1.237 (3)	C3A—H3A1	0.9700
N1—C16	1.336 (3)	C3A—H3A2	0.9700
N1—C7	1.459 (3)	C12B—C11B	1.528 (4)
N1—H1	0.8600	C12B—C8B	1.537 (3)
O2—C16A	1.233 (3)	C12B—H12C	0.9700
N2—C16A	1.336 (3)	C12B—H12D	0.9700
N2—C7A	1.463 (3)	C11A—H11A	0.9700
N2—H2	0.8600	C11A—H11B	0.9700
N3—C16B	1.341 (3)	C2A—H2A1	0.9700
N3—C7B	1.463 (3)	C2A—H2A2	0.9700
N3—H3	0.8600	C13A—H13A	0.9600
C8A—C9A	1.506 (3)	C13A—H13B	0.9600
C8A—C13A	1.522 (3)	C13A—H13C	0.9600
C8A—C12A	1.538 (3)	C13—H13D	0.9600
C8A—C7A	1.564 (3)	C13—H13E	0.9600
C10A—C1A	1.510 (3)	C13—H13F	0.9600
C10A—C11A	1.540 (3)	C10—C1	1.505 (4)
C10A—C6A	1.549 (3)	C10—C11	1.539 (4)
C10A—H10A	0.9800	C10—H10	0.9800
C5A—C15A	1.537 (3)	C8B—C13B	1.524 (4)
C5A—C14A	1.540 (3)	C17A—H17D	0.9600
C5A—C4A	1.544 (3)	C17A—H17E	0.9600
C5A—C6A	1.558 (3)	C17A—H17F	0.9600
C5B—C15B	1.531 (4)	C12—C11	1.539 (4)

C5B—C14B	1.542 (3)	C12—H12E	0.9700
C5B—C4B	1.549 (4)	C12—H12F	0.9700
C5B—C6B	1.552 (3)	C14—H14D	0.9600
C6—C10	1.544 (3)	C14—H14E	0.9600
C6—C5	1.557 (3)	C14—H14F	0.9600
C6—C7	1.561 (3)	C9—C1	1.336 (4)
C6—H6	0.9800	C9—H9	0.9300
C1B—C9B	1.326 (4)	C4A—H4A1	0.9700
C1B—C2B	1.492 (4)	C4A—H4A2	0.9700
C1B—C10B	1.508 (3)	C16—C17	1.517 (4)
C16B—C17B	1.514 (3)	C9A—H9A	0.9300
C17B—H17A	0.9600	C1—C2	1.504 (4)
C17B—H17B	0.9600	C15A—H15A	0.9600
C17B—H17C	0.9600	C15A—H15B	0.9600
C6B—C10B	1.543 (3)	C15A—H15C	0.9600
C6B—C7B	1.557 (3)	C2B—C3B	1.533 (4)
C6B—H6B	0.9800	C2B—H2B1	0.9700
C7A—C6A	1.558 (3)	C2B—H2B2	0.9700
C7A—H7A	0.9800	C15—H15D	0.9600
C1A—C9A	1.329 (4)	C15—H15E	0.9600
C1A—C2A	1.492 (3)	C15—H15F	0.9600
C6A—H6A	0.9800	C4B—C3B	1.533 (4)
C7—C8	1.556 (3)	C4B—H4B1	0.9700
C7—H7	0.9800	C4B—H4B2	0.9700
C7B—C8B	1.568 (3)	C14A—H14G	0.9600
C7B—H7B	0.9800	C14A—H14H	0.9600
C12A—C11A	1.539 (4)	C14A—H14I	0.9600
C12A—H12A	0.9700	C3B—H3B1	0.9700
C12A—H12B	0.9700	C3B—H3B2	0.9700
C10B—C11B	1.533 (4)	C17—H17G	0.9600
C10B—H10B	0.9800	C17—H17H	0.9600
C4—C5	1.543 (4)	C17—H17I	0.9600
C4—C3	1.543 (4)	C13B—H13G	0.9600
C4—H4A	0.9700	C13B—H13H	0.9600
C4—H4B	0.9700	C13B—H13I	0.9600
C9B—C8B	1.509 (3)	C11—H11C	0.9700
C9B—H9B	0.9300	C11—H11D	0.9700
C5—C14	1.532 (3)	C3—C2	1.530 (5)
C5—C15	1.540 (3)	C3—H3A	0.9700
C14B—H14A	0.9600	C3—H3B	0.9700
C14B—H14B	0.9600	C11B—H11E	0.9700
C14B—H14C	0.9600	C11B—H11F	0.9700
C16A—C17A	1.514 (4)	C2—H2A	0.9700
C8—C9	1.514 (3)	C2—H2B	0.9700
C8—C13	1.520 (3)	C15B—H15G	0.9600
C8—C12	1.547 (3)	C15B—H15H	0.9600
C3A—C4A	1.543 (3)	C15B—H15I	0.9600

C16—N1—C7	123.34 (18)	C1A—C2A—C3A	109.58 (19)
C16—N1—H1	118.3	C1A—C2A—H2A1	109.8
C7—N1—H1	118.3	C3A—C2A—H2A1	109.8
C16A—N2—C7A	123.41 (19)	C1A—C2A—H2A2	109.8
C16A—N2—H2	118.3	C3A—C2A—H2A2	109.8
C7A—N2—H2	118.3	H2A1—C2A—H2A2	108.2
C16B—N3—C7B	124.11 (18)	C8A—C13A—H13A	109.5
C16B—N3—H3	117.9	C8A—C13A—H13B	109.5
C7B—N3—H3	117.9	H13A—C13A—H13B	109.5
C9A—C8A—C13A	112.4 (2)	C8A—C13A—H13C	109.5
C9A—C8A—C12A	109.02 (19)	H13A—C13A—H13C	109.5
C13A—C8A—C12A	111.75 (19)	H13B—C13A—H13C	109.5
C9A—C8A—C7A	103.46 (17)	C8—C13—H13D	109.5
C13A—C8A—C7A	111.35 (18)	C8—C13—H13E	109.5
C12A—C8A—C7A	108.52 (19)	H13D—C13—H13E	109.5
C1A—C10A—C11A	109.5 (2)	C8—C13—H13F	109.5
C1A—C10A—C6A	106.04 (17)	H13D—C13—H13F	109.5
C11A—C10A—C6A	109.11 (19)	H13E—C13—H13F	109.5
C1A—C10A—H10A	110.7	C1—C10—C11	110.4 (2)
C11A—C10A—H10A	110.7	C1—C10—C6	106.18 (19)
C6A—C10A—H10A	110.7	C11—C10—C6	108.6 (2)
C15A—C5A—C14A	106.9 (2)	C1—C10—H10	110.5
C15A—C5A—C4A	110.0 (2)	C11—C10—H10	110.5
C14A—C5A—C4A	107.63 (19)	C6—C10—H10	110.5
C15A—C5A—C6A	108.62 (19)	C9B—C8B—C13B	112.3 (2)
C14A—C5A—C6A	109.12 (19)	C9B—C8B—C12B	108.8 (2)
C4A—C5A—C6A	114.34 (19)	C13B—C8B—C12B	112.6 (2)
C15B—C5B—C14B	106.6 (2)	C9B—C8B—C7B	103.50 (18)
C15B—C5B—C4B	110.1 (2)	C13B—C8B—C7B	111.3 (2)
C14B—C5B—C4B	107.3 (2)	C12B—C8B—C7B	107.83 (18)
C15B—C5B—C6B	108.7 (2)	C16A—C17A—H17D	109.5
C14B—C5B—C6B	109.17 (19)	C16A—C17A—H17E	109.5
C4B—C5B—C6B	114.59 (19)	H17D—C17A—H17E	109.5
C10—C6—C5	113.5 (2)	C16A—C17A—H17F	109.5
C10—C6—C7	107.23 (19)	H17D—C17A—H17F	109.5
C5—C6—C7	114.29 (17)	H17E—C17A—H17F	109.5
C10—C6—H6	107.1	C11—C12—C8	109.9 (2)
C5—C6—H6	107.1	C11—C12—H12E	109.7
C7—C6—H6	107.1	C8—C12—H12E	109.7
C9B—C1B—C2B	126.5 (2)	C11—C12—H12F	109.7
C9B—C1B—C10B	113.7 (2)	C8—C12—H12F	109.7
C2B—C1B—C10B	118.1 (2)	H12E—C12—H12F	108.2
O3—C16B—N3	123.5 (2)	C5—C14—H14D	109.5
O3—C16B—C17B	121.9 (2)	C5—C14—H14E	109.5
N3—C16B—C17B	114.6 (2)	H14D—C14—H14E	109.5
C16B—C17B—H17A	109.5	C5—C14—H14F	109.5
C16B—C17B—H17B	109.5	H14D—C14—H14F	109.5
H17A—C17B—H17B	109.5	H14E—C14—H14F	109.5

C16B—C17B—H17C	109.5	C1—C9—C8	115.3 (2)
H17A—C17B—H17C	109.5	C1—C9—H9	122.4
H17B—C17B—H17C	109.5	C8—C9—H9	122.4
C10B—C6B—C5B	112.75 (19)	C3A—C4A—C5A	118.6 (2)
C10B—C6B—C7B	107.50 (18)	C3A—C4A—H4A1	107.7
C5B—C6B—C7B	115.53 (17)	C5A—C4A—H4A1	107.7
C10B—C6B—H6B	106.9	C3A—C4A—H4A2	107.7
C5B—C6B—H6B	106.9	C5A—C4A—H4A2	107.7
C7B—C6B—H6B	106.9	H4A1—C4A—H4A2	107.1
N2—C7A—C6A	111.84 (17)	O1—C16—N1	124.2 (2)
N2—C7A—C8A	111.92 (17)	O1—C16—C17	120.5 (2)
C6A—C7A—C8A	110.75 (17)	N1—C16—C17	115.3 (2)
N2—C7A—H7A	107.4	C1A—C9A—C8A	115.9 (2)
C6A—C7A—H7A	107.4	C1A—C9A—H9A	122.1
C8A—C7A—H7A	107.4	C8A—C9A—H9A	122.1
C9A—C1A—C2A	125.9 (2)	C9—C1—C2	125.6 (3)
C9A—C1A—C10A	113.3 (2)	C9—C1—C10	113.6 (2)
C2A—C1A—C10A	119.1 (2)	C2—C1—C10	118.8 (3)
C10A—C6A—C5A	112.72 (18)	C5A—C15A—H15A	109.5
C10A—C6A—C7A	107.68 (17)	C5A—C15A—H15B	109.5
C5A—C6A—C7A	114.81 (17)	H15A—C15A—H15B	109.5
C10A—C6A—H6A	107.1	C5A—C15A—H15C	109.5
C5A—C6A—H6A	107.1	H15A—C15A—H15C	109.5
C7A—C6A—H6A	107.1	H15B—C15A—H15C	109.5
N1—C7—C8	113.79 (18)	C1B—C2B—C3B	109.4 (2)
N1—C7—C6	109.92 (17)	C1B—C2B—H2B1	109.8
C8—C7—C6	111.06 (17)	C3B—C2B—H2B1	109.8
N1—C7—H7	107.3	C1B—C2B—H2B2	109.8
C8—C7—H7	107.3	C3B—C2B—H2B2	109.8
C6—C7—H7	107.3	H2B1—C2B—H2B2	108.2
N3—C7B—C6B	109.80 (16)	C5—C15—H15D	109.5
N3—C7B—C8B	111.28 (18)	C5—C15—H15E	109.5
C6B—C7B—C8B	111.14 (18)	H15D—C15—H15E	109.5
N3—C7B—H7B	108.2	C5—C15—H15F	109.5
C6B—C7B—H7B	108.2	H15D—C15—H15F	109.5
C8B—C7B—H7B	108.2	H15E—C15—H15F	109.5
C8A—C12A—C11A	109.77 (18)	C3B—C4B—C5B	118.9 (2)
C8A—C12A—H12A	109.7	C3B—C4B—H4B1	107.6
C11A—C12A—H12A	109.7	C5B—C4B—H4B1	107.6
C8A—C12A—H12B	109.7	C3B—C4B—H4B2	107.6
C11A—C12A—H12B	109.7	C5B—C4B—H4B2	107.6
H12A—C12A—H12B	108.2	H4B1—C4B—H4B2	107.0
C1B—C10B—C11B	109.4 (2)	C5A—C14A—H14G	109.5
C1B—C10B—C6B	106.23 (18)	C5A—C14A—H14H	109.5
C11B—C10B—C6B	108.7 (2)	H14G—C14A—H14H	109.5
C1B—C10B—H10B	110.8	C5A—C14A—H14I	109.5
C11B—C10B—H10B	110.8	H14G—C14A—H14I	109.5
C6B—C10B—H10B	110.8	H14H—C14A—H14I	109.5

C5—C4—C3	118.1 (2)	C2B—C3B—C4B	116.2 (2)
C5—C4—H4A	107.8	C2B—C3B—H3B1	108.2
C3—C4—H4A	107.8	C4B—C3B—H3B1	108.2
C5—C4—H4B	107.8	C2B—C3B—H3B2	108.2
C3—C4—H4B	107.8	C4B—C3B—H3B2	108.2
H4A—C4—H4B	107.1	H3B1—C3B—H3B2	107.4
C1B—C9B—C8B	115.7 (2)	C16—C17—H17G	109.5
C1B—C9B—H9B	122.2	C16—C17—H17H	109.5
C8B—C9B—H9B	122.2	H17G—C17—H17H	109.5
C14—C5—C15	106.5 (2)	C16—C17—H17I	109.5
C14—C5—C4	107.3 (2)	H17G—C17—H17I	109.5
C15—C5—C4	110.6 (2)	H17H—C17—H17I	109.5
C14—C5—C6	109.7 (2)	C8B—C13B—H13G	109.5
C15—C5—C6	108.7 (2)	C8B—C13B—H13H	109.5
C4—C5—C6	113.8 (2)	H13G—C13B—H13H	109.5
C5B—C14B—H14A	109.5	C8B—C13B—H13I	109.5
C5B—C14B—H14B	109.5	H13G—C13B—H13I	109.5
H14A—C14B—H14B	109.5	H13H—C13B—H13I	109.5
C5B—C14B—H14C	109.5	C10—C11—C12	109.66 (19)
H14A—C14B—H14C	109.5	C10—C11—H11C	109.7
H14B—C14B—H14C	109.5	C12—C11—H11C	109.7
O2—C16A—N2	123.0 (2)	C10—C11—H11D	109.7
O2—C16A—C17A	121.9 (2)	C12—C11—H11D	109.7
N2—C16A—C17A	115.2 (2)	H11C—C11—H11D	108.2
C9—C8—C13	113.1 (2)	C2—C3—C4	115.7 (2)
C9—C8—C12	109.6 (2)	C2—C3—H3A	108.3
C13—C8—C12	111.4 (2)	C4—C3—H3A	108.3
C9—C8—C7	102.04 (17)	C2—C3—H3B	108.3
C13—C8—C7	111.51 (19)	C4—C3—H3B	108.3
C12—C8—C7	108.78 (19)	H3A—C3—H3B	107.4
C4A—C3A—C2A	115.5 (2)	C12B—C11B—C10B	110.48 (19)
C4A—C3A—H3A1	108.4	C12B—C11B—H11E	109.6
C2A—C3A—H3A1	108.4	C10B—C11B—H11E	109.6
C4A—C3A—H3A2	108.4	C12B—C11B—H11F	109.6
C2A—C3A—H3A2	108.4	C10B—C11B—H11F	109.6
H3A1—C3A—H3A2	107.5	H11E—C11B—H11F	108.1
C11B—C12B—C8B	109.9 (2)	C1—C2—C3	109.8 (2)
C11B—C12B—H12C	109.7	C1—C2—H2A	109.7
C8B—C12B—H12C	109.7	C3—C2—H2A	109.7
C11B—C12B—H12D	109.7	C1—C2—H2B	109.7
C8B—C12B—H12D	109.7	C3—C2—H2B	109.7
H12C—C12B—H12D	108.2	H2A—C2—H2B	108.2
C12A—C11A—C10A	109.92 (19)	C5B—C15B—H15G	109.5
C12A—C11A—H11A	109.7	C5B—C15B—H15H	109.5
C10A—C11A—H11A	109.7	H15G—C15B—H15H	109.5
C12A—C11A—H11B	109.7	C5B—C15B—H15I	109.5
C10A—C11A—H11B	109.7	H15G—C15B—H15I	109.5
H11A—C11A—H11B	108.2	H15H—C15B—H15I	109.5

C7B—N3—C16B—O3	−3.5 (3)	C7A—N2—C16A—C17A	174.9 (2)
C7B—N3—C16B—C17B	175.87 (19)	N1—C7—C8—C9	173.33 (19)
C15B—C5B—C6B—C10B	−72.3 (3)	C6—C7—C8—C9	−62.0 (2)
C14B—C5B—C6B—C10B	171.80 (19)	N1—C7—C8—C13	52.3 (2)
C4B—C5B—C6B—C10B	51.4 (3)	C6—C7—C8—C13	177.01 (19)
C15B—C5B—C6B—C7B	163.6 (2)	N1—C7—C8—C12	−70.9 (2)
C14B—C5B—C6B—C7B	47.6 (3)	C6—C7—C8—C12	53.7 (2)
C4B—C5B—C6B—C7B	−72.7 (2)	C8A—C12A—C11A—C10A	3.0 (3)
C16A—N2—C7A—C6A	128.1 (2)	C1A—C10A—C11A—C12A	−55.8 (3)
C16A—N2—C7A—C8A	−106.9 (2)	C6A—C10A—C11A—C12A	59.9 (3)
C9A—C8A—C7A—N2	175.83 (18)	C9A—C1A—C2A—C3A	110.7 (3)
C13A—C8A—C7A—N2	54.9 (2)	C10A—C1A—C2A—C3A	−53.5 (3)
C12A—C8A—C7A—N2	−68.5 (2)	C4A—C3A—C2A—C1A	−30.7 (3)
C9A—C8A—C7A—C6A	−58.6 (2)	C5—C6—C10—C1	−74.6 (3)
C13A—C8A—C7A—C6A	−179.54 (19)	C7—C6—C10—C1	52.6 (2)
C12A—C8A—C7A—C6A	57.1 (2)	C5—C6—C10—C11	166.7 (2)
C11A—C10A—C1A—C9A	54.5 (2)	C7—C6—C10—C11	−66.1 (2)
C6A—C10A—C1A—C9A	−63.1 (2)	C1B—C9B—C8B—C13B	177.7 (2)
C11A—C10A—C1A—C2A	−139.4 (2)	C1B—C9B—C8B—C12B	−56.9 (3)
C6A—C10A—C1A—C2A	103.0 (2)	C1B—C9B—C8B—C7B	57.6 (3)
C1A—C10A—C6A—C5A	−72.7 (2)	C11B—C12B—C8B—C9B	52.1 (2)
C11A—C10A—C6A—C5A	169.4 (2)	C11B—C12B—C8B—C13B	177.3 (2)
C1A—C10A—C6A—C7A	54.9 (2)	C11B—C12B—C8B—C7B	−59.6 (2)
C11A—C10A—C6A—C7A	−62.9 (2)	N3—C7B—C8B—C9B	179.91 (18)
C15A—C5A—C6A—C10A	−70.3 (2)	C6B—C7B—C8B—C9B	−57.4 (2)
C14A—C5A—C6A—C10A	173.54 (19)	N3—C7B—C8B—C13B	59.1 (2)
C4A—C5A—C6A—C10A	53.0 (3)	C6B—C7B—C8B—C13B	−178.22 (19)
C15A—C5A—C6A—C7A	165.91 (19)	N3—C7B—C8B—C12B	−64.9 (2)
C14A—C5A—C6A—C7A	49.7 (2)	C6B—C7B—C8B—C12B	57.8 (2)
C4A—C5A—C6A—C7A	−70.8 (2)	C9—C8—C12—C11	49.7 (3)
N2—C7A—C6A—C10A	129.69 (18)	C13—C8—C12—C11	175.5 (2)
C8A—C7A—C6A—C10A	4.1 (2)	C7—C8—C12—C11	−61.1 (3)
N2—C7A—C6A—C5A	−103.9 (2)	C13—C8—C9—C1	177.0 (2)
C8A—C7A—C6A—C5A	130.54 (19)	C12—C8—C9—C1	−58.0 (3)
C16—N1—C7—C8	−112.4 (2)	C7—C8—C9—C1	57.1 (3)
C16—N1—C7—C6	122.3 (2)	C2A—C3A—C4A—C5A	83.0 (3)
C10—C6—C7—N1	135.11 (19)	C15A—C5A—C4A—C3A	53.1 (3)
C5—C6—C7—N1	−98.2 (2)	C14A—C5A—C4A—C3A	169.2 (2)
C10—C6—C7—C8	8.3 (2)	C6A—C5A—C4A—C3A	−69.4 (3)
C5—C6—C7—C8	135.0 (2)	C7—N1—C16—O1	7.7 (4)
C16B—N3—C7B—C6B	136.5 (2)	C7—N1—C16—C17	−171.3 (2)
C16B—N3—C7B—C8B	−100.0 (2)	C2A—C1A—C9A—C8A	−161.7 (2)
C10B—C6B—C7B—N3	126.08 (18)	C10A—C1A—C9A—C8A	3.3 (3)
C5B—C6B—C7B—N3	−107.1 (2)	C13A—C8A—C9A—C1A	177.5 (2)
C10B—C6B—C7B—C8B	2.5 (2)	C12A—C8A—C9A—C1A	−58.0 (3)
C5B—C6B—C7B—C8B	129.40 (19)	C7A—C8A—C9A—C1A	57.3 (2)
C9A—C8A—C12A—C11A	51.1 (3)	C8—C9—C1—C2	−159.1 (2)

C13A—C8A—C12A—C11A	176.0 (2)	C8—C9—C1—C10	4.8 (3)
C7A—C8A—C12A—C11A	−60.9 (2)	C11—C10—C1—C9	53.5 (3)
C9B—C1B—C10B—C11B	54.7 (3)	C6—C10—C1—C9	−64.0 (3)
C2B—C1B—C10B—C11B	−138.9 (2)	C11—C10—C1—C2	−141.5 (2)
C9B—C1B—C10B—C6B	−62.5 (3)	C6—C10—C1—C2	101.0 (3)
C2B—C1B—C10B—C6B	103.8 (2)	C9B—C1B—C2B—C3B	110.3 (3)
C5B—C6B—C10B—C1B	−72.8 (2)	C10B—C1B—C2B—C3B	−54.0 (3)
C7B—C6B—C10B—C1B	55.7 (2)	C15B—C5B—C4B—C3B	55.3 (3)
C5B—C6B—C10B—C11B	169.54 (19)	C14B—C5B—C4B—C3B	171.0 (2)
C7B—C6B—C10B—C11B	−62.0 (2)	C6B—C5B—C4B—C3B	−67.6 (3)
C2B—C1B—C9B—C8B	−163.1 (2)	C1B—C2B—C3B—C4B	−30.3 (4)
C10B—C1B—C9B—C8B	1.9 (3)	C5B—C4B—C3B—C2B	82.4 (3)
C3—C4—C5—C14	171.3 (2)	C1—C10—C11—C12	−56.6 (3)
C3—C4—C5—C15	55.5 (3)	C6—C10—C11—C12	59.4 (3)
C3—C4—C5—C6	−67.2 (3)	C8—C12—C11—C10	4.6 (3)
C10—C6—C5—C14	172.6 (2)	C5—C4—C3—C2	85.2 (4)
C7—C6—C5—C14	49.2 (3)	C8B—C12B—C11B—C10B	1.3 (3)
C10—C6—C5—C15	−71.2 (3)	C1B—C10B—C11B—C12B	−54.3 (3)
C7—C6—C5—C15	165.4 (2)	C6B—C10B—C11B—C12B	61.3 (2)
C10—C6—C5—C4	52.5 (3)	C9—C1—C2—C3	114.8 (3)
C7—C6—C5—C4	−70.9 (3)	C10—C1—C2—C3	−48.3 (4)
C7A—N2—C16A—O2	−4.9 (4)	C4—C3—C2—C1	−35.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	2.04	2.893 (2)	173
N2—H2···O3	0.86	2.11	2.956 (3)	167
N3—H3···O1^{i}	0.86	2.06	2.909 (2)	169

Symmetry code: (i) −*x*+2, *y*+1/2, −*z*+1/2.