Acta Cryst. (1999). C**55**, IUC9900105 [**doi:10.1107/S0108270199098868**]

N-tert-Butyl-3-oxo-4-aza-5β,17β-androstane-17-carboxamide methanol solvate, a finasteride impurity

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Abstract

The title compound is isolated during the impurity profiling of the drug Finasteride. This molecule is saturated form of Finasteride with different 'AB' ring fusion. A & B ring junctionis "*cis*". The confirmation of A, B, C and D rings are sofa, chair, chair and envelope respectively. The lattice contains one molecule of methanol. Parallel to the two fold screw along 'a' axis, a train of molecules is formed due to the hydrogen bond between amide N2 atom of the side chain and the carbonyl oxygen atom O1 of the A ring. The amide nitrogen atom N1 forms N—H···O type hydrogen bond with the methanol oxygen atom O3. On the other hand, the methanol donates its hydroxyl hydrogen atom to the carbonyl oxygen O2 of the side chain forming O—H···O type hydrogen bond resulting in a chain molcules parallel to the two fold screw along 'b' axis. The hydrogen bonding interactions between the molecule and lattice water molecules confers stability to the lattice.

Comment

The title compound is isolated during the impurity profiling of the drug Finasteride. This molecule is saturated form of Finasteride with different 'AB' ring fusion. A & B ring junctionis "*cis*". The confirmation of A, B, C and D rings are sofa, chair, chair and envelope respectively. The lattice contains one molecule of methanol. Parallel to the two fold screw along 'a' axis, a train of molecules is formed due to the hydrogen bond between amide N2 atom of the side chain and the carbonyl oxygen atom O1 of the A ring. The amide nitrogen atom N1 forms N—H···O type hydrogen bond with the methanol oxygen atom O3. On the other hand, the methanol donates its hydroxyl hydrogen atom to the carbonyl oxygen O2 of the side chain forming O—H···O type hydrogen bond resulting in a chain molcules parallel to the two fold screw along 'b' axis. The hydrogen bonding interactions between the molecule and lattice water molecules confers stability to the lattice.

Computing details

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1994); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1992-1997); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

(global)

Crystal data

$C_{23}H_{38}N_2O_2 \cdot C_1H_4O_1$	$V = 2437.5\ (9)$ Å^3
$M_r = 406.61$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Cu $K\alpha$
$a = 11.607\ (2)$ Å	$\mu = 0.57$ mm^{-1}

b = 20.097 (5) Å	T = 298.2 K
c = 10.449 (4) Å	0.45 × 0.10 × 0.10 mm

Data collection

Rigaku AFC-7S diffractometer	2152 reflections with $I > 1.1\sigma(I)$
Absorption correction: empirical (using intensity measurements) (DIFABS; Walker & Stuart, 1983)	R_{int} = 0.0000
T_{min} = 0.755, T_{max} = 1.000	3 standard reflections
2635 measured reflections	every 150 reflections
2635 independent reflections	intensity decay: −7.7%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.081	2 restraints
$wR(F^2)$ = 0.114	H atoms treated by a mixture of independent and constrained refinement
S = 1.86	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
2152 reflections	$\Delta\rho_{min}$ = −0.38 e Å^{-3}
266 parameters	

Acknowledgements

The authors acknowledge Dr. A. Venkateswarlu for the interest and encouragement in this work

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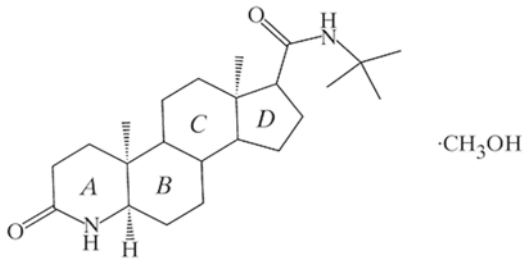
Scheme 1



supplementary materials

(global)

Crystal data

$C_{23}H_{38}N_2O_2 \cdot C_1H_4O_1$	$D_x = 1.108$ Mg m^{-3}
$M_r = 406.61$	Cu $K\alpha$ radiation $\lambda = 1.5418$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 25 reflections
$a = 11.607$ (2) Å	$\theta = 25.2$–32.8º
$b = 20.097$ (5) Å	$\mu = 0.57$ mm^{-1}
$c = 10.449$ (4) Å	$T = 298.2$ K
$V = 2437.5$ (9) Å^3	Block, white
$Z = 4$	0.45 × 0.10 × 0.10 mm
$F_{000} = 896.00$	

Data collection

Rigaku AFC-7S diffractometer	$R_{int} = 0.0000$
Radiation source: X-ray tube	$\theta_{max} = 70.1$º
Monochromator: graphite	$\theta_{min} = 2.2$º
$T = 298.2$ K	$h = 0 \rightarrow 14$
ω–2θ scans	$k = 0 \rightarrow 24$
Absorption correction: empirical (using intensity measurements) (DIFABS; Walker & Stuart, 1983)	$l = 0 \rightarrow 12$
$T_{min} = 0.755$, $T_{max} = 1.000$	3 standard reflections
2635 measured reflections	every 150 reflections
2635 independent reflections	intensity decay: −7.7%
2152 reflections with $I > 1.1\sigma(I)$	

Refinement

Refinement on F	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	Weighting scheme based on measured s.u.'s $w = 1/[\sigma^2(F_o) + 0.00176\|F_o\|^2]$
$R[F^2 > 2\sigma(F^2)] = 0.081$	$(\Delta/\sigma)_{max} = 0.003$
$wR(F^2) = 0.114$	$\Delta\rho_{max} = 0.40$ e Å^{-3}
$S = 1.86$	$\Delta\rho_{min} = -0.38$ e Å^{-3}
2152 reflections	Extinction correction: Zachariasen (1967), equ(3) Acta Cryst. (1968), A24, p. 213
266 parameters	Extinction coefficient: 8 (8)E-7
2 restraints	

Special details

Experimental. The scan width was (1.21 + 0.14tanθ)° with an ω scan speed of 0° per minute (up to 5 scans to achieve I/σ(I) > 15). Stationary background counts were recorded at each end of the scan, and the scan time:background time ratio was 2:1.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4600 (4)	0.6252 (2)	0.9962 (4)	0.100 (1)
O2	0.8433 (3)	1.0496 (2)	0.6894 (5)	0.117 (1)
O3	0.1606 (4)	0.6764 (2)	0.9054 (5)	0.127 (2)
N1	0.4038 (3)	0.6812 (2)	0.8250 (4)	0.0638 (9)
N2	0.9501 (3)	0.9767 (2)	0.8012 (4)	0.0668 (9)
C1	0.4808 (4)	0.6452 (2)	0.8886 (5)	0.068 (1)
C2	0.5935 (4)	0.6314 (2)	0.8198 (5)	0.075 (1)
C3	0.5934 (3)	0.6463 (2)	0.6796 (5)	0.069 (1)
C4	0.5334 (3)	0.7123 (2)	0.6453 (4)	0.0577 (8)
C5	0.4101 (3)	0.7057 (2)	0.6917 (4)	0.0628 (9)
C6	0.3418 (3)	0.7690 (2)	0.6814 (5)	0.069 (1)
C7	0.4009 (3)	0.8267 (2)	0.7458 (4)	0.059 (1)
C8	0.5244 (3)	0.8370 (2)	0.6958 (3)	0.0470 (8)
C9	0.5920 (3)	0.7720 (1)	0.7129 (3)	0.0472 (8)
C10	0.7200 (3)	0.7806 (2)	0.6786 (4)	0.0559 (9)
C11	0.7776 (3)	0.8396 (2)	0.7454 (3)	0.0501 (8)
C12	0.7116 (3)	0.9032 (1)	0.7184 (3)	0.0471 (7)
C13	0.5850 (3)	0.8920 (1)	0.7635 (3)	0.0466 (8)
C14	0.5343 (3)	0.9632 (2)	0.7598 (4)	0.066 (1)
C15	0.6349 (4)	1.0074 (2)	0.8008 (5)	0.077 (1)
C16	0.7434 (3)	0.9641 (2)	0.8036 (4)	0.0575 (9)
C17	0.7178 (4)	0.9212 (2)	0.5765 (4)	0.071 (1)
C18	0.5355 (4)	0.7191 (2)	0.5001 (4)	0.077 (1)
C19	0.8495 (4)	1.0014 (2)	0.7609 (4)	0.066 (1)
C20	1.0655 (4)	1.0047 (3)	0.7687 (5)	0.087 (1)
C21	1.1511 (5)	0.9607 (5)	0.833 (1)	0.178 (4)
C22	1.0808 (6)	1.0085 (5)	0.6229 (6)	0.142 (2)
C23	1.0728 (5)	1.0756 (3)	0.8214 (9)	0.136 (3)
C24	0.0592 (7)	0.7164 (5)	0.883 (1)	0.191 (4)
H1	0.3374	0.6937	0.8716	0.075*
H2	0.6129	0.5859	0.8325	0.091*
H3	0.6525	0.6581	0.8605	0.091*
H4	0.5563	0.6110	0.6380	0.084*
H5	0.6720	0.6488	0.6524	0.084*
H6	0.3741	0.6736	0.6396	0.075*
H7	0.2691	0.7625	0.7190	0.081*
H8	0.3329	0.7793	0.5926	0.081*
H9	0.4048	0.8180	0.8353	0.071*
H10	0.3584	0.8659	0.7309	0.071*
H11	0.5202	0.8470	0.6076	0.057*

H12	0.5900	0.7621	0.8026	0.056*
H13	0.7596	0.7412	0.7031	0.067*
H14	0.7255	0.7869	0.5896	0.067*
H15	0.7784	0.8317	0.8353	0.061*
H16	0.8537	0.8438	0.7149	0.061*
H17	0.5895	0.8795	0.8520	0.056*
H18	0.4717	0.9674	0.8179	0.078*
H19	0.5094	0.9741	0.6760	0.078*
H20	0.6213	1.0252	0.8834	0.093*
H21	0.6450	1.0426	0.7412	0.093*
H22	0.7549	0.9489	0.8883	0.068*
H23	0.6875	0.8853	0.5267	0.085*
H24	0.6736	0.9600	0.5607	0.085*
H25	0.7956	0.9286	0.5527	0.085*
H26	0.4977	0.7608	0.4766	0.093*
H27	0.4913	0.6841	0.4622	0.093*
H28	0.6102	0.7193	0.4688	0.093*
H29	0.9481	0.9379	0.8528	0.079*
H30	1.1364	0.9595	0.9250	0.197*
H31	1.1420	0.9154	0.8032	0.197*
H32	1.2266	0.9746	0.8193	0.197*
H33	1.0670	0.9678	0.5857	0.168*
H34	1.1544	1.0255	0.6037	0.168*
H35	1.0239	1.0409	0.5911	0.168*
H36	1.1443	1.0949	0.7962	0.165*
H37	1.0112	1.1012	0.7890	0.165*
H38	1.0691	1.0746	0.9126	0.165*
H39	−0.0011	0.6914	0.8498	0.216*
H40	0.0349	0.7362	0.9639	0.216*
H41	0.0780	0.7525	0.8269	0.216*
H42	0.141 (5)	0.639 (2)	0.854 (5)	0.120*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.118 (3)	0.100 (2)	0.081 (2)	−0.002 (2)	0.008 (2)	0.029 (2)
O2	0.121 (3)	0.082 (2)	0.149 (4)	−0.039 (2)	−0.036 (3)	0.065 (2)
O3	0.117 (3)	0.097 (2)	0.166 (5)	−0.023 (2)	0.046 (3)	−0.033 (3)
N1	0.058 (2)	0.072 (2)	0.062 (2)	−0.007 (1)	0.014 (2)	0.003 (1)
N2	0.061 (1)	0.069 (2)	0.070 (2)	−0.008 (1)	0.001 (2)	0.002 (2)
C1	0.069 (2)	0.058 (2)	0.077 (2)	−0.006 (2)	0.003 (2)	0.000 (2)
C2	0.077 (2)	0.055 (2)	0.093 (2)	0.005 (2)	0.014 (2)	0.004 (2)
C3	0.064 (2)	0.056 (2)	0.089 (2)	−0.006 (1)	0.018 (2)	−0.016 (2)
C4	0.061 (2)	0.058 (2)	0.053 (2)	−0.010 (1)	−0.002 (2)	−0.011 (1)
C5	0.064 (2)	0.067 (2)	0.058 (2)	−0.016 (1)	−0.007 (2)	−0.010 (2)
C6	0.054 (2)	0.078 (2)	0.076 (3)	−0.010 (1)	−0.009 (2)	0.001 (2)
C7	0.048 (1)	0.063 (2)	0.066 (3)	0.004 (1)	−0.004 (2)	0.005 (2)
C8	0.050 (1)	0.055 (1)	0.036 (2)	0.002 (1)	−0.009 (1)	0.000 (1)

C9	0.049 (1)	0.049 (1)	0.043 (2)	−0.003 (1)	0.004 (1)	−0.004 (1)
C10	0.052 (1)	0.057 (2)	0.059 (2)	−0.002 (1)	0.009 (2)	−0.009 (2)
C11	0.044 (1)	0.055 (1)	0.052 (2)	−0.001 (1)	0.007 (1)	−0.005 (1)
C12	0.051 (1)	0.048 (1)	0.042 (2)	−0.006 (1)	−0.002 (1)	0.003 (1)
C13	0.050 (1)	0.051 (1)	0.039 (2)	0.000 (1)	−0.004 (1)	−0.003 (1)
C14	0.073 (2)	0.051 (1)	0.074 (3)	0.007 (1)	−0.022 (2)	−0.004 (2)
C15	0.075 (2)	0.056 (2)	0.098 (3)	0.003 (1)	−0.023 (3)	−0.015 (2)
C16	0.064 (2)	0.051 (2)	0.057 (2)	−0.007 (1)	−0.006 (2)	−0.005 (2)
C17	0.088 (3)	0.082 (2)	0.043 (2)	−0.024 (2)	0.008 (2)	0.007 (2)
C18	0.076 (2)	0.098 (3)	0.056 (2)	−0.025 (2)	0.008 (2)	−0.023 (2)
C19	0.067 (2)	0.056 (2)	0.076 (3)	−0.014 (1)	−0.011 (2)	−0.004 (2)
C20	0.073 (2)	0.105 (2)	0.084 (3)	−0.033 (2)	0.016 (2)	−0.006 (2)
C21	0.052 (2)	0.213 (8)	0.27 (1)	0.024 (4)	0.008 (4)	0.114 (8)
C22	0.115 (4)	0.223 (8)	0.088 (3)	−0.065 (5)	0.037 (4)	−0.022 (5)
C23	0.091 (3)	0.117 (4)	0.201 (8)	−0.037 (3)	0.009 (5)	−0.062 (5)
C24	0.148 (7)	0.202 (8)	0.22 (1)	0.069 (6)	0.020 (8)	−0.010 (9)

Geometric parameters (Å, °)

O1—C1	1.219 (8)	C11—H15	0.95
O2—C19	1.225 (7)	C11—H16	0.94
O3—C24	1.445 (8)	C12—C13	1.560 (6)
O3—H42	0.952 (9)	C12—C16	1.557 (6)
N1—C1	1.328 (7)	C12—C17	1.528 (7)
N1—C5	1.479 (8)	C13—C14	1.546 (6)
N1—H1	0.95	C13—H17	0.96
N2—C19	1.337 (7)	C14—C15	1.529 (8)
N2—C20	1.493 (7)	C14—H18	0.95
N2—H29	0.95	C14—H19	0.95
C1—C2	1.518 (8)	C15—C16	1.531 (8)
C2—C3	1.50 (1)	C15—H20	0.95
C2—H2	0.95	C15—H21	0.95
C2—H3	0.97	C16—C19	1.509 (7)
C3—C4	1.540 (7)	C16—H22	0.95
C3—H4	0.94	C17—H23	0.96
C3—H5	0.96	C17—H24	0.95
C4—C5	1.517 (7)	C17—H25	0.95
C4—C9	1.550 (6)	C18—H26	0.98
C4—C18	1.523 (8)	C18—H27	0.96
C5—C6	1.502 (8)	C18—H28	0.93
C5—H6	0.94	C20—C21	1.49 (1)
C6—C7	1.506 (8)	C20—C22	1.54 (1)
C6—H7	0.94	C20—C23	1.53 (1)
C6—H8	0.96	C21—H30	0.98
C7—C8	1.541 (7)	C21—H31	0.97
C7—H9	0.95	C21—H32	0.93
C7—H10	0.94	C22—H33	0.92
C8—C9	1.534 (6)	C22—H34	0.94
C8—C13	1.489 (6)	C22—H35	0.99

C8—H11	0.94	C23—H36	0.95
C9—C10	1.538 (6)	C23—H37	0.94
C9—H12	0.96	C23—H38	0.95
C10—C11	1.530 (7)	C24—H39	0.93
C10—H13	0.95	C24—H40	0.98
C10—H14	0.94	C24—H41	0.96
C11—C12	1.518 (6)		
O1···N2^{i}	2.947 (7)	O2···O3^{ii}	2.734 (7)
O1···C21^{i}	3.33 (1)	O3···N1	2.948 (7)
O1···C11^{i}	3.503 (7)		
C24—O3—H42	99 (5)	C13—C12—C16	99.4 (4)
C1—N1—C5	128.2 (5)	C13—C12—C17	111.8 (4)
C1—N1—H1	115.9	C16—C12—C17	111.0 (4)
C5—N1—H1	115.9	C8—C13—C12	114.1 (4)
C19—N2—C20	124.9 (5)	C8—C13—C14	119.6 (4)
C19—N2—H29	117.6	C8—C13—H17	106.8
C20—N2—H29	117.5	C12—C13—C14	102.6 (4)
O1—C1—N1	120.6 (6)	C12—C13—H17	106.2
O1—C1—C2	123.1 (6)	C14—C13—H17	106.7
N1—C1—C2	116.3 (6)	C13—C14—C15	103.8 (4)
C1—C2—C3	115.2 (6)	C13—C14—H18	111.0
C1—C2—H2	108.3	C13—C14—H19	110.7
C1—C2—H3	107.5	C15—C14—H18	110.6
C3—C2—H2	109.1	C15—C14—H19	110.9
C3—C2—H3	108.7	H18—C14—H19	109.6
H2—C2—H3	107.8	C14—C15—C16	107.7 (4)
C2—C3—C4	113.6 (5)	C14—C15—H20	110.4
C2—C3—H4	107.7	C14—C15—H21	110.1
C2—C3—H5	107.5	C16—C15—H20	109.5
C4—C3—H4	109.7	C16—C15—H21	109.5
C4—C3—H5	108.4	H20—C15—H21	109.6
H4—C3—H5	109.9	C12—C16—C15	103.9 (4)
C3—C4—C5	106.1 (4)	C12—C16—C19	114.5 (5)
C3—C4—C9	111.3 (4)	C12—C16—H22	108.4
C3—C4—C18	107.6 (5)	C15—C16—C19	112.6 (4)
C5—C4—C9	109.6 (4)	C15—C16—H22	108.5
C5—C4—C18	109.9 (5)	C19—C16—H22	108.8
C9—C4—C18	112.2 (4)	C12—C17—H23	109.3
N1—C5—C4	112.1 (5)	C12—C17—H24	109.7
N1—C5—C6	108.9 (5)	C12—C17—H25	109.6
N1—C5—H6	107.1	H23—C17—H24	109.2
C4—C5—C6	113.7 (4)	H23—C17—H25	109.0
C4—C5—H6	107.0	H24—C17—H25	110.0
C6—C5—H6	107.7	C4—C18—H26	108.7
C5—C6—C7	112.3 (4)	C4—C18—H27	109.7
C5—C6—H7	109.1	C4—C18—H28	111.5
C5—C6—H8	108.1	H26—C18—H27	106.7
C7—C6—H7	109.2	H26—C18—H28	109.1

C7—C6—H8	108.4	H27—C18—H28	111.0
H7—C6—H8	109.7	O2—C19—N2	122.5 (6)
C6—C7—C8	112.1 (5)	O2—C19—C16	121.7 (6)
C6—C7—H9	108.7	N2—C19—C16	115.8 (5)
C6—C7—H10	109.4	N2—C20—C21	105.8 (6)
C8—C7—H9	108.2	N2—C20—C22	110.4 (6)
C8—C7—H10	108.5	N2—C20—C23	108.6 (6)
H9—C7—H10	109.9	C21—C20—C22	114 (1)
C7—C8—C9	108.7 (4)	C21—C20—C23	110.8 (9)
C7—C8—C13	112.3 (4)	C22—C20—C23	107.7 (9)
C7—C8—H11	108.1	C20—C21—H30	109.9
C9—C8—C13	109.6 (4)	C20—C21—H31	110.0
C9—C8—H11	108.7	C20—C21—H32	112.4
C13—C8—H11	109.3	H30—C21—H31	105.8
C4—C9—C8	112.5 (4)	H30—C21—H32	108.8
C4—C9—C10	113.8 (4)	H31—C21—H32	109.7
C4—C9—H12	105.9	C20—C22—H33	110.8
C8—C9—C10	111.8 (4)	C20—C22—H34	109.5
C8—C9—H12	106.2	C20—C22—H35	106.8
C10—C9—H12	105.9	H33—C22—H34	113.0
C9—C10—C11	113.8 (4)	H33—C22—H35	109.1
C9—C10—H13	108.2	H34—C22—H35	107.3
C9—C10—H14	108.1	C20—C23—H36	109.1
C11—C10—H13	108.1	C20—C23—H37	109.7
C11—C10—H14	108.5	C20—C23—H38	109.7
H13—C10—H14	110.2	H36—C23—H37	109.8
C10—C11—C12	110.3 (4)	H36—C23—H38	108.9
C10—C11—H15	109.0	H37—C23—H38	109.7
C10—C11—H16	109.0	O3—C24—H39	111.9
C12—C11—H15	109.2	O3—C24—H40	108.6
C12—C11—H16	109.4	O3—C24—H41	109.6
H15—C11—H16	109.9	H39—C24—H40	109.0
C11—C12—C13	107.3 (3)	H39—C24—H41	110.8
C11—C12—C16	115.9 (4)	H40—C24—H41	106.7
C11—C12—C17	110.9 (4)		
O1—C1—N1—C5	−175.3 (5)	C7—C8—C13—C12	178.6 (4)
O1—C1—C2—C3	166.6 (5)	C7—C8—C13—C14	−59.5 (6)
O2—C19—N2—C20	2(1)	C8—C9—C4—C18	67.4 (6)
O2—C19—C16—C12	93.0 (7)	C8—C9—C10—C11	51.1 (6)
O2—C19—C16—C15	−25.4 (9)	C8—C13—C12—C11	−61.1 (5)
N1—C1—C2—C3	−13.6 (7)	C8—C13—C12—C16	177.9 (4)
N1—C5—C4—C3	48.7 (5)	C8—C13—C12—C17	60.7 (5)
N1—C5—C4—C9	−71.5 (5)	C8—C13—C14—C15	−163.0 (5)
N1—C5—C4—C18	164.7 (4)	C9—C8—C13—C12	57.6 (5)
N1—C5—C6—C7	72.4 (6)	C9—C8—C13—C14	179.5 (4)
N2—C19—C16—C12	−84.0 (6)	C9—C10—C11—C12	−55.2 (6)
N2—C19—C16—C15	157.6 (5)	C10—C9—C4—C18	−61.1 (6)
C1—N1—C5—C4	−24.8 (7)	C10—C9—C8—C13	−50.7 (6)
C1—N1—C5—C6	−151.4 (5)	C10—C11—C12—C13	56.9 (5)

C1—C2—C3—C4	42.9 (7)	C10—C11—C12—C16	166.8 (4)
C2—C1—N1—C5	4.9 (8)	C10—C11—C12—C17	−65.5 (5)
C2—C3—C4—C5	−60.0 (6)	C11—C12—C13—C14	168.0 (4)
C2—C3—C4—C9	59.1 (6)	C11—C12—C16—C15	−155.2 (5)
C2—C3—C4—C18	−177.6 (5)	C11—C12—C16—C19	81.6 (6)
C3—C4—C5—C6	172.7 (5)	C12—C13—C14—C15	−35.5 (6)
C3—C4—C9—C8	−172.0 (4)	C12—C16—C15—C14	19.7 (7)
C3—C4—C9—C10	59.5 (6)	C13—C12—C16—C15	−40.6 (5)
C4—C5—C6—C7	−53.4 (7)	C13—C12—C16—C19	−163.8 (4)
C4—C9—C8—C7	56.6 (5)	C13—C14—C15—C16	9.8 (7)
C4—C9—C8—C13	179.7 (4)	C14—C13—C12—C16	47.0 (5)
C4—C9—C10—C11	−180.0 (4)	C14—C13—C12—C17	−70.2 (5)
C5—C4—C9—C8	−55.0 (6)	C14—C15—C16—C19	144.1 (6)
C5—C4—C9—C10	176.5 (4)	C15—C16—C12—C17	77.2 (6)
C5—C6—C7—C8	54.7 (7)	C16—C19—N2—C20	178.8 (6)
C6—C5—C4—C9	52.4 (7)	C17—C12—C16—C19	−46.0 (6)
C6—C5—C4—C18	−71.3 (6)	C19—N2—C20—C21	−179.2 (9)
C6—C7—C8—C9	−55.9 (6)	C19—N2—C20—C22	−56 (1)
C6—C7—C8—C13	−177.3 (4)	C19—N2—C20—C23	61.8 (9)
C7—C8—C9—C10	−173.8 (4)		

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