Domperidone maleate

K. Vyas, J. Moses Babu and G. Om Reddy

Abstract

Domperidone maleate, 4-[5-chloro-2,3-dihydro-2-oxo-1*H*-benzimidazol-1-yl]-1-[(2,3-dihydro-2-oxo-1*H*- benzimidazol-1-yl)propyl]piperidinium maleate, is an antiemetic drug. The hydrogen bonding interaction between the molecule, maleate group and lattice water molecules confers stability It is Crystallized as hydrate with 2.5 water molecules in the lattice. The piperidine ring assumes a chair conformation with its nitrogen protonated due to salt formation. The maleate ion stacks with one of the benzimidazole moieties. The free carboxylic hydroxyl group of maleate moiety is involved in an intra-molecular hydrogen bound with the carboxylate carbonyl oxygen atom. Staking interaction is between benzimidazole rings related by twofold screw axis confers further stability to the lattice.

Comment

The Domperidone maleate,5-Chloro-1-[1-[3-(2,3-dihydro-2-oxo-1*H*-benzimidazol −1-yl)propyl-4-piperidinyl]-1,3-di-hydro-2*H*-benzimidazol-2-one maleate(I), is an antiemetic drug. The hydrogen bonding interaction between the molecule, maleate group and lattice water molecules confers stability It is Crystallized as hydrate with 2.5 water molecules in the lattice. The piperidine ring assumes a chair conformation with its nitrogen protonated due to salt formation. The maleate ion stacks with one of the benzimidazole moieties. The free carboxylic hydroxyl group of maleate moiety is involved in an intra-molecular hydrogen bound with the carboxylate carbonyl oxygen atom. Staking interaction is between benzimidazole rings related by twofold screw axis confers further 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*.

(qa0146)

Crystal data

$C_{22}H_{25}Cl_1N_5O_2{}^{1+} \cdot C_4H_3O_4{}^{1-} \cdot 2.5H_2O_1$	$V = 2853\ (3)$ Å^3
$M_r = 587.03$	$Z = 4$
Monoclinic, $P2_1/n$	Cu $K\alpha$
$a = 6.676\ (5)$ Å	$\mu = 1.69$ mm^{-1}
$b = 24.324\ (7)$ Å	$T = 298.2$ K
$c = 17.66\ (1)$ Å	$0.5 \times 0.30 \times 0.20$ mm
$\beta = 95.87\ (6)°$	

CIF access

Data collection

Rigaku AFC=7S diffractometer	4047 reflections with $I > 0.9\sigma(I)$
Absorption correction: empirical (using intensity measurements) (DIFABS; Walker & Stuart, 1983)	$R_{int} = 0.068$
$T_{min} = 0.869$, $T_{max} = 1.000$	3 standard reflections
5786 measured reflections	every 150 reflections
5290 independent reflections	intensity decay: -1.0%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$	387 parameters
$wR(F^2) = 0.078$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.81$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
4047 reflections	$\Delta\rho_{min} = -0.32$ e Å^{-3}

References

Molecular Structure Corporation (1992–1997). *TEXSAN*. Single Crystal Structure Analysis Software. Version 1.7. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Molecular Structure Corporation (1994*a*). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Walker, N. & Stuart, D. (1983). *Acta Cryst.* A**39**, 158–166.

Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564.

Scheme 1
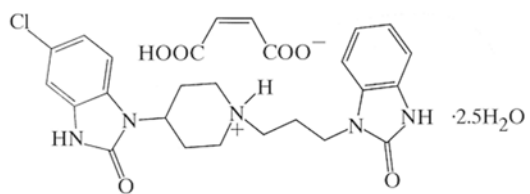
supplementary materials

(qa0146)

Crystal data

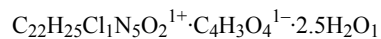|	
$C_{22}H_{25}Cl_1N_5O_2{}^{1+}\cdot C_4H_3O_4{}^{1-}\cdot 2.5H_2O_1$	$F_{000} = 1236.00$
$M_r = 587.03$	$D_x = 1.367$ Mg m^{-3}
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation $\lambda = 1.5418$ Å
$a = 6.676$ (5) Å	Cell parameters from 16 reflections
$b = 24.324$ (7) Å	$\theta = 16.9–28.8º$
$c = 17.66$ (1) Å	$\mu = 1.69$ mm^{-1}
$\beta = 95.87$ (6)º	$T = 298.2$ K
$V = 2853$ (3) Å^3	Block, colorless
$Z = 4$	$0.5 \times 0.30 \times 0.20$ mm

Data collection

Rigaku AFC=7S diffractometer	$R_{int} = 0.068$
Radiation source: X-ray tube	$\theta_{max} = 70.1º$
Monochromator: graphite	$\theta_{min} = 2.5º$
$T = 298.2$ K	$h = 0\rightarrow7$
$\omega–2\theta$ scans	$k = 0\rightarrow29$
Absorption correction: empirical (using intensity measurements) (DIFABS; Walker & Stuart, 1983)	$l = -21\rightarrow21$
$T_{min} = 0.869$, $T_{max} = 1.000$	3 standard reflections
5786 measured reflections	every 150 reflections
5290 independent reflections	intensity decay: -1.0%
4047 reflections with $I > 0.9\sigma(I)$	

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 $w = 1/[\sigma^2(F_o) + 0.00051|F_o|^2]$
$R[F^2 > 2\sigma(F^2)] = 0.062$	$(\Delta/\sigma)_{max} = 0.005$
$wR(F^2) = 0.078$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
$S = 1.81$	$\Delta\rho_{min} = -0.32$ e Å^{-3}
4047 reflections	Extinction correction: Zachariasen (1967), equ(3) Acta Cryst. (1968), A24, p. 213
387 parameters	Extinction coefficient: 3.0 (6)E-6

supplementary materials

Special details

Experimental. The scan width was (0.89 + 0.14tanθ)° with an ω scan speed of 16° 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}	Occ. (<1)
Cl1	0.2367 (2)	−0.08175 (5)	1.03494 (5)	0.1011 (3)	
O1	0.9069 (3)	−0.03996 (8)	0.7317 (1)	0.0698 (6)	
O2	0.4661 (3)	0.34519 (8)	0.6263 (1)	0.0713 (6)	
O3	0.1656 (3)	0.1460 (1)	0.7887 (1)	0.0823 (7)	
O4	0.3633 (4)	0.2155 (1)	0.8238 (1)	0.0877 (8)	
O5	0.2173 (4)	0.3122 (1)	1.0138 (1)	0.0957 (9)	
O6	0.3894 (4)	0.2863 (1)	0.9218 (1)	0.0832 (8)	
O7	0.0948 (6)	−0.0836 (1)	0.4753 (2)	0.141 (1)	
O8	0.8404 (8)	−0.0318 (2)	0.5705 (2)	0.181 (2)	
O9	0.439 (2)	−0.0175 (6)	0.5046 (8)	0.207 (6)	0.500
N1	0.7580 (4)	−0.0717 (1)	0.8367 (1)	0.0617 (7)	
N2	0.6132 (3)	−0.00285 (9)	0.7713 (1)	0.0575 (6)	
N3	0.4210 (3)	0.14967 (8)	0.6766 (1)	0.0518 (6)	
N4	0.1660 (3)	0.30858 (9)	0.6581 (1)	0.0639 (7)	
N5	0.3129 (4)	0.3715 (1)	0.7336 (1)	0.0643 (7)	
C1	0.7743 (4)	−0.0388 (1)	0.7753 (2)	0.0583 (8)	
C2	0.5905 (4)	−0.0579 (1)	0.8719 (2)	0.0579 (7)	
C3	0.5145 (5)	−0.0795 (1)	0.9351 (2)	0.0679 (9)	
C4	0.3412 (5)	−0.0554 (1)	0.9562 (2)	0.0708 (9)	
C5	0.2485 (5)	−0.0115 (1)	0.9174 (2)	0.073 (1)	
C6	0.3268 (5)	0.0103 (1)	0.8546 (2)	0.0669 (9)	
C7	0.4979 (4)	−0.0135 (1)	0.8312 (2)	0.0568 (7)	
C8	0.5995 (4)	0.0440 (1)	0.7199 (2)	0.0568 (7)	
C9	0.6571 (4)	0.0962 (1)	0.7636 (2)	0.0593 (8)	
C10	0.3938 (4)	0.0486 (1)	0.6743 (2)	0.0623 (8)	
C11	0.6328 (4)	0.1467 (1)	0.7134 (2)	0.0570 (7)	
C12	0.3763 (4)	0.1008 (1)	0.6266 (2)	0.0614 (8)	
C13	0.3837 (4)	0.2034 (1)	0.6367 (2)	0.0617 (8)	
C14	0.1637 (5)	0.2127 (1)	0.6106 (2)	0.0711 (9)	
C15	0.1239 (5)	0.2733 (1)	0.5924 (2)	0.0730 (9)	
C16	0.3301 (4)	0.3428 (1)	0.6682 (2)	0.0610 (8)	
C17	0.1391 (4)	0.3567 (1)	0.7645 (2)	0.0649 (9)	
C18	0.0551 (6)	0.3736 (1)	0.8281 (2)	0.082 (1)	
C19	−0.1264 (6)	0.3493 (2)	0.8431 (3)	0.099 (1)	
C20	−0.2175 (6)	0.3093 (2)	0.7936 (3)	0.102 (2)	
C21	−0.1333 (5)	0.2927 (1)	0.7307 (3)	0.086 (1)	
C22	0.0459 (4)	0.3162 (1)	0.7162 (2)	0.0655 (9)	
C23	0.2188 (5)	0.1839 (1)	0.8338 (2)	0.0706 (9)	
C24	0.1102 (6)	0.1910 (2)	0.9009 (2)	0.104 (1)	
C25	0.1225 (7)	0.2296 (2)	0.9536 (2)	0.108 (2)	

C26	0.2465 (5)	0.2794 (2)	0.9636 (2)	0.074 (1)
H1	0.846 (6)	−0.104 (1)	0.846 (2)	0.10 (1)*
H2	0.5764	−0.1091	0.9627	0.078*
H3	0.1301	0.0038	0.9335	0.085*
H4	0.2654	0.0406	0.8281	0.075*
H5	0.6971	0.0385	0.6847	0.065*
H6	0.5720	0.0997	0.8036	0.067*
H7	0.7929	0.0935	0.7848	0.067*
H8	0.2923	0.0486	0.7085	0.073*
H9	0.3738	0.0175	0.6414	0.073*
H10	0.6621	0.1785	0.7439	0.066*
H11	0.7229	0.1445	0.6756	0.066*
H12	0.2441	0.1036	0.6019	0.072*
H13	0.4706	0.0993	0.5900	0.072*
H14	0.328 (4)	0.149 (1)	0.717 (2)	0.064 (8)*
H15	0.4580	0.2042	0.5938	0.071*
H16	0.4295	0.2323	0.6709	0.071*
H17	0.0842	0.2015	0.6500	0.085*
H18	0.1266	0.1913	0.5664	0.085*
H19	−0.0140	0.2777	0.5738	0.086*
H20	0.2065	0.2845	0.5549	0.086*
H21	0.401 (6)	0.399 (1)	0.746 (2)	0.10 (1)*
H22	0.1201	0.4013	0.8608	0.093*
H23	−0.1883	0.3597	0.8864	0.115*
H24	−0.3410	0.2935	0.8037	0.117*
H25	−0.1946	0.2652	0.6976	0.096*
H26	0.0124	0.1629	0.9061	0.124*
H27	0.0346	0.2242	0.9923	0.131*
H28	0.409 (8)	0.257 (2)	0.886 (3)	0.16 (2)*
H29	0.1418	−0.1153	0.4896	0.145*
H30	0.2085	−0.0650	0.4981	0.140*
H31	0.8502	−0.0676	0.5627	0.145*
H32	1.0010	−0.0281	0.6007	0.222*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1185 (8)	0.1171 (8)	0.0699 (5)	−0.0344 (6)	0.0203 (5)	0.0056 (5)
O1	0.062 (1)	0.069 (1)	0.080 (1)	0.013 (1)	0.012 (1)	0.012 (1)
O2	0.067 (1)	0.065 (1)	0.081 (1)	−0.009 (1)	0.002 (1)	−0.005 (1)
O3	0.081 (1)	0.081 (1)	0.087 (2)	−0.011 (1)	0.020 (1)	−0.014 (1)
O4	0.086 (2)	0.097 (2)	0.086 (2)	−0.023 (1)	0.033 (1)	−0.016 (1)
O5	0.098 (2)	0.110 (2)	0.080 (2)	0.005 (1)	0.015 (1)	−0.020 (1)
O6	0.080 (2)	0.093 (2)	0.078 (1)	−0.013 (1)	0.017 (1)	−0.010 (1)
O7	0.157 (3)	0.109 (2)	0.153 (3)	0.001 (2)	−0.003 (2)	0.008 (2)
O8	0.237 (5)	0.192 (4)	0.121 (3)	0.036 (4)	0.048 (3)	0.030 (3)
O9	0.19 (1)	0.26 (2)	0.180 (8)	−0.016 (9)	0.044 (9)	−0.04 (1)
N1	0.060 (1)	0.054 (1)	0.070 (2)	0.003 (1)	0.001 (1)	0.009 (1)

N2	0.054 (1)	0.053 (1)	0.066 (1)	0.007 (1)	0.007 (1)	0.008 (1)
N3	0.051 (1)	0.048 (1)	0.056 (1)	−0.001 (1)	0.003 (1)	0.0018 (9)
N4	0.055 (1)	0.049 (1)	0.084 (2)	−0.005 (1)	−0.010 (1)	0.000 (1)
N5	0.054 (1)	0.061 (1)	0.076 (2)	−0.007 (1)	−0.002 (1)	−0.003 (1)
C1	0.053 (2)	0.055 (1)	0.066 (2)	0.003 (1)	0.003 (1)	0.004 (1)
C2	0.059 (2)	0.051 (1)	0.062 (2)	−0.005 (1)	−0.002 (1)	0.000 (1)
C3	0.079 (2)	0.060 (2)	0.062 (2)	−0.012 (1)	−0.004 (2)	0.005 (1)
C4	0.075 (2)	0.076 (2)	0.061 (2)	−0.021 (2)	0.006 (2)	−0.002 (1)
C5	0.070 (2)	0.077 (2)	0.074 (2)	−0.007 (2)	0.012 (2)	−0.009 (2)
C6	0.063 (2)	0.067 (2)	0.072 (2)	0.003 (1)	0.009 (1)	0.000 (1)
C7	0.057 (2)	0.052 (1)	0.061 (2)	−0.001 (1)	0.005 (1)	0.000 (1)
C8	0.059 (2)	0.051 (1)	0.060 (2)	0.006 (1)	0.007 (1)	0.007 (1)
C9	0.051 (1)	0.059 (1)	0.067 (2)	−0.001 (1)	−0.001 (1)	0.007 (1)
C10	0.069 (2)	0.051 (1)	0.064 (2)	0.001 (1)	−0.007 (1)	−0.004 (1)
C11	0.050 (1)	0.055 (1)	0.066 (2)	−0.004 (1)	0.002 (1)	0.004 (1)
C12	0.070 (2)	0.054 (1)	0.058 (2)	0.004 (1)	−0.003 (1)	−0.004 (1)
C13	0.066 (2)	0.050 (1)	0.069 (2)	−0.001 (1)	0.004 (1)	0.009 (1)
C14	0.073 (2)	0.050 (1)	0.085 (2)	−0.002 (1)	−0.018 (2)	0.003 (1)
C15	0.074 (2)	0.051 (1)	0.087 (2)	0.000 (1)	−0.023 (2)	0.000 (1)
C16	0.053 (2)	0.054 (1)	0.074 (2)	−0.002 (1)	−0.005 (1)	0.002 (1)
C17	0.055 (2)	0.063 (2)	0.076 (2)	0.002 (1)	0.000 (1)	0.010 (1)
C18	0.077 (2)	0.081 (2)	0.087 (2)	0.007 (2)	0.005 (2)	0.010 (2)
C19	0.088 (3)	0.105 (3)	0.107 (3)	0.024 (2)	0.027 (2)	0.028 (2)
C20	0.073 (2)	0.091 (3)	0.144 (4)	0.001 (2)	0.019 (3)	0.034 (3)
C21	0.060 (2)	0.073 (2)	0.124 (3)	−0.006 (2)	0.000 (2)	0.019 (2)
C22	0.052 (2)	0.053 (1)	0.089 (2)	−0.002 (1)	−0.007 (2)	0.011 (1)
C23	0.063 (2)	0.075 (2)	0.076 (2)	−0.002 (2)	0.014 (2)	0.001 (2)
C24	0.102 (3)	0.113 (3)	0.105 (3)	−0.042 (2)	0.054 (2)	−0.025 (2)
C25	0.108 (3)	0.123 (3)	0.101 (3)	−0.035 (3)	0.052 (2)	−0.030 (3)
C26	0.068 (2)	0.093 (2)	0.062 (2)	0.002 (2)	0.007 (2)	−0.001 (2)

Geometric parameters (Å, °)

Cl1—C4	1.740 (3)	C6—H4	0.94
O1—C1	1.231 (4)	C8—C9	1.515 (4)
O2—C16	1.230 (4)	C8—C10	1.523 (4)
O3—C23	1.247 (4)	C8—H5	0.95
O4—C23	1.258 (4)	C9—C11	1.515 (4)
O5—C26	1.223 (4)	C9—H6	0.95
O6—C26	1.276 (4)	C9—H7	0.95
O6—H28	0.97 (5)	C10—C12	1.521 (4)
O7—H29	0.86	C10—H8	0.95
O7—H30	0.94	C10—H9	0.96
O8—H31	0.88	C11—H10	0.95
O8—H32	1.15	C11—H11	0.94
O9—O9^i	1.20 (2)	C12—H12	0.95
N1—C1	1.360 (4)	C12—H13	0.95
N1—C2	1.375 (4)	C13—C14	1.511 (4)
N1—H1	0.98 (4)	C13—H15	0.95

N2—C1	1.383 (4)	C13—H16	0.96
N2—C7	1.395 (4)	C14—C15	1.527 (4)
N2—C8	1.454 (3)	C14—H17	0.96
N3—C11	1.495 (3)	C14—H18	0.95
N3—C12	1.493 (3)	C15—H19	0.95
N3—C13	1.495 (3)	C15—H20	0.94
N3—H14	0.99 (3)	C17—C18	1.369 (5)
N4—C15	1.447 (4)	C17—C22	1.406 (4)
N4—C16	1.373 (4)	C18—C19	1.397 (5)
N4—C22	1.378 (4)	C18—H22	0.96
N5—C16	1.365 (4)	C19—C20	1.404 (6)
N5—C17	1.379 (4)	C19—H23	0.94
N5—H21	0.91 (4)	C20—C21	1.357 (6)
C2—C3	1.377 (4)	C20—H24	0.94
C2—C7	1.405 (4)	C21—C22	1.374 (5)
C3—C4	1.381 (5)	C21—H25	0.95
C3—H2	0.94	C23—C24	1.461 (5)
C4—C5	1.383 (5)	C24—C25	1.320 (5)
C5—C6	1.380 (4)	C24—H26	0.96
C5—H3	0.94	C25—C26	1.468 (5)
C6—C7	1.382 (4)	C25—H27	0.95
Cl1···O2^{ii}	3.509 (2)	O8···O8^{xiv}	3.770 (9)
Cl1···C9^{iii}	3.574 (3)	O8···C12^{i}	3.999 (5)
Cl1···C7^{iii}	3.639 (3)	O9···C12^{i}	3.40 (2)
Cl1···C6^{iii}	3.763 (4)	O9···C10	3.44 (1)
Cl1···C24^{iv}	3.774 (4)	O9···C10^{i}	3.54 (1)
Cl1···C2^{iii}	3.898 (3)	O9···C12	3.65 (2)
O1···O8	2.844 (5)	O9···C18^{ii}	3.97 (2)
O1···N5^{v}	2.877 (3)	O9···C8^{i}	4.00 (1)
O1···C19^{ii}	3.465 (4)	N1···C16^{v}	3.457 (4)
O1···C6^{vi}	3.580 (4)	N1···C22^{ii}	3.469 (4)
O1···C16^{v}	3.702 (3)	N1···C17^{ii}	3.506 (4)
O1···O2^{v}	3.791 (3)	N1···N5^{v}	3.520 (4)
O1···C18^{ii}	3.793 (4)	N1···C21^{ii}	3.577 (4)
O1···C5^{vi}	3.860 (4)	N1···C18^{ii}	3.657 (4)
O1···C20^{ii}	3.889 (5)	N1···C20^{ii}	3.691 (5)
O1···C17^{v}	3.933 (4)	N1···C5^{vi}	3.734 (4)
O2···N1^{vii}	2.768 (3)	N1···C19^{ii}	3.739 (5)
O2···C21^{vi}	3.343 (4)	N2···C18^{ii}	3.603 (4)
O2···C4^{viii}	3.401 (4)	N2···C17^{ii}	3.833 (4)
O2···C20^{vi}	3.560 (5)	N3···C23	3.314 (4)
O2···C1^{vii}	3.656 (3)	N4···C3^{viii}	3.342 (4)
O2···C3^{viii}	3.758 (4)	N4···C2^{viii}	3.684 (3)
O2···C2^{vii}	3.781 (4)	N4···C4^{viii}	3.873 (4)

O2···C25^{ix}	3.789 (5)	N5···C1^{vii}	3.531 (4)
O2···C5^{viii}	3.819 (4)	N5···C20^{vi}	3.544 (5)
O3···N3	2.743 (4)	N5···C2^{viii}	3.556 (4)
O3···C13	3.476 (4)	N5···C7^{viii}	3.599 (4)
O3···C12	3.494 (4)	N5···C3^{viii}	3.708 (4)
O3···C11	3.514 (4)	N5···C6^{viii}	3.795 (4)
O3···C14	3.537 (4)	N5···C4^{viii}	3.841 (4)
O3···C10	3.556 (4)	N5···C5^{viii}	3.894 (4)
O3···C9	3.568 (4)	C1···C18^{ii}	3.449 (4)
O3···C9^{x}	3.589 (4)	C1···C19^{ii}	3.512 (5)
O3···C6	3.625 (4)	C1···C17^{ii}	3.765 (4)
O3···C11^{x}	3.669 (4)	C1···C5^{vi}	3.890 (5)
O4···N3	3.110 (3)	C1···C20^{ii}	3.895 (5)
O4···C11	3.249 (4)	C1···C16^{v}	3.965 (4)
O4···C13	3.334 (4)	C1···C6^{vi}	3.992 (5)
O4···C22	3.645 (4)	C2···C17^{ii}	3.422 (4)
O4···C20^{vi}	3.693 (5)	C2···C22^{ii}	3.512 (4)
O4···C9	3.719 (4)	C2···C16^{ii}	3.717 (4)
O4···N4	3.827 (3)	C2···C18^{ii}	3.937 (4)
O4···C17	3.850 (4)	C3···C16^{ii}	3.368 (4)
O4···C14	3.864 (4)	C3···C5^{iii}	3.652 (4)
O5···O7^{viii}	2.826 (4)	C3···C22^{ii}	3.677 (4)
O5···C13^{xi}	3.287 (4)	C3···C15^{ii}	3.718 (4)
O5···C14^{xii}	3.336 (4)	C3···C4^{iii}	3.873 (4)
O5···C15^{xii}	3.585 (4)	C3···C17^{ii}	3.892 (4)
O5···C18	3.665 (4)	C4···C16^{ii}	3.428 (4)
O5···C19	3.708 (5)	C4···C4^{iii}	3.673 (6)
O5···C11^{xi}	3.761 (4)	C4···C5^{iii}	3.726 (4)
O5···N3^{xi}	3.769 (4)	C4···C6^{iii}	3.971 (4)
O5···C12^{xi}	3.816 (4)	C5···C16^{ii}	3.869 (4)
O6···C18	3.386 (4)	C7···C17^{ii}	3.652 (4)
O6···C17	3.535 (4)	C7···C18^{ii}	3.921 (4)
O6···C15^{xii}	3.559 (4)	C9···C23	3.924 (5)
O6···C14^{xii}	3.637 (4)	C11···C23	3.766 (5)
O6···O7^{viii}	3.645 (4)	C11···C21^{vi}	3.877 (4)
O6···C20^{vi}	3.680 (6)	C13···C23	3.786 (4)
O6···C19	3.893 (5)	C14···C26^{xv}	3.614 (4)
O6···N5	3.905 (4)	C14···C23	3.982 (4)
O6···C19^{vi}	3.956 (5)	C15···C26^{xv}	3.463 (4)
O7···O8^{x}	2.807 (6)	C15···C25^{xv}	3.943 (6)
O7···O9	2.81 (1)	C16···C20^{vi}	3.650 (5)

O7···O8[i]	2.965 (6)	C16···C21[vi]	3.838 (5)
O7···C12[xiii]	3.486 (5)	C17···C26	3.988 (4)
O7···C26[ii]	3.627 (5)	C18···C26	3.461 (5)
O7···C14[xiii]	3.822 (4)	C19···C26	3.540 (5)
O7···O9[i]	3.95 (1)	C19···C25	3.792 (6)
O8···O9[i]	2.49 (2)	C20···C25	3.947 (7)
O8···O9	2.83 (2)	C20···C24	3.977 (7)
O8···C19[ii]	3.630 (6)	C21···C23	3.868 (5)
O8···C1	3.693 (5)	C22···C23	3.938 (4)
O8···C8	3.717 (5)		
C26—O6—H28	116 (3)	N3—C11—H11	109.8
H29—O7—H30	92.9	C9—C11—H10	108.9
H31—O8—H32	93.9	C9—C11—H11	109.2
C1—N1—C2	110.6 (2)	H10—C11—H11	109.8
C1—N1—H1	120 (2)	N3—C12—C10	109.8 (2)
C2—N1—H1	128 (2)	N3—C12—H12	109.6
C1—N2—C7	109.3 (2)	N3—C12—H13	109.1
C1—N2—C8	121.7 (2)	C10—C12—H12	109.4
C7—N2—C8	128.0 (2)	C10—C12—H13	109.1
C11—N3—C12	110.0 (2)	H12—C12—H13	109.9
C11—N3—C13	110.5 (2)	N3—C13—C14	112.6 (2)
C11—N3—H14	109 (2)	N3—C13—H15	108.6
C12—N3—C13	113.8 (2)	N3—C13—H16	108.5
C12—N3—H14	108 (2)	C14—C13—H15	109.0
C13—N3—H14	106 (2)	C14—C13—H16	108.8
C15—N4—C16	123.4 (3)	H15—C13—H16	109.3
C15—N4—C22	126.6 (2)	C13—C14—C15	110.5 (2)
C16—N4—C22	109.8 (2)	C13—C14—H17	109.3
C16—N5—C17	110.4 (3)	C13—C14—H18	109.5
C16—N5—H21	118 (2)	C15—C14—H17	109.3
C17—N5—H21	131 (2)	C15—C14—H18	109.2
O1—C1—N1	127.3 (3)	H17—C14—H18	109.0
O1—C1—N2	126.0 (3)	N4—C15—C14	112.9 (2)
N1—C1—N2	106.7 (3)	N4—C15—H19	108.1
N1—C2—C3	131.2 (3)	N4—C15—H20	108.2
N1—C2—C7	106.9 (2)	C14—C15—H19	108.9
C3—C2—C7	121.9 (3)	C14—C15—H20	109.0
C2—C3—C4	116.5 (3)	H19—C15—H20	109.8
C2—C3—H2	122.1	O2—C16—N4	125.4 (3)
C4—C3—H2	121.4	O2—C16—N5	128.0 (3)
Cl1—C4—C3	118.4 (3)	N4—C16—N5	106.6 (3)
Cl1—C4—C5	119.0 (3)	N5—C17—C18	132.7 (3)
C3—C4—C5	122.6 (3)	N5—C17—C22	106.4 (3)
C4—C5—C6	120.6 (3)	C18—C17—C22	120.9 (3)
C4—C5—H3	120.2	C17—C18—C19	117.7 (4)
C6—C5—H3	119.2	C17—C18—H22	120.3
C5—C6—C7	118.1 (3)	C19—C18—H22	122.0

C5—C6—H4	121.2	C18—C19—C20	120.2 (4)
C7—C6—H4	120.7	C18—C19—H23	120.2
N2—C7—C2	106.5 (2)	C20—C19—H23	119.6
N2—C7—C6	133.2 (3)	C19—C20—C21	121.8 (4)
C2—C7—C6	120.3 (3)	C19—C20—H24	119.8
N2—C8—C9	110.0 (2)	C21—C20—H24	118.4
N2—C8—C10	112.5 (2)	C20—C21—C22	118.0 (4)
N2—C8—H5	107.1	C20—C21—H25	121.6
C9—C8—C10	112.1 (2)	C22—C21—H25	120.4
C9—C8—H5	107.1	N4—C22—C17	106.9 (3)
C10—C8—H5	107.8	N4—C22—C21	131.8 (3)
C8—C9—C11	112.1 (2)	C17—C22—C21	121.3 (4)
C8—C9—H6	108.3	O3—C23—O4	122.3 (3)
C8—C9—H7	109.1	O3—C23—C24	118.1 (3)
C11—C9—H6	108.8	O4—C23—C24	119.5 (3)
C11—C9—H7	109.2	C23—C24—C25	131.0 (4)
H6—C9—H7	109.3	C23—C24—H26	113.3
C8—C10—C12	111.6 (2)	C25—C24—H26	115.7
C8—C10—H8	109.1	C24—C25—C26	131.8 (4)
C8—C10—H9	109.1	C24—C25—H27	114.1
C12—C10—H8	109.3	C26—C25—H27	114.1
C12—C10—H9	109.0	O5—C26—O6	121.2 (3)
H8—C10—H9	108.8	O5—C26—C25	119.7 (3)
N3—C11—C9	109.4 (2)	O6—C26—C25	119.0 (3)
N3—C11—H10	109.8		
Cl1—C4—C3—C2	179.1 (2)	C1—N2—C7—C6	178.5 (3)
Cl1—C4—C5—C6	−179.8 (2)	C1—N2—C8—C9	−102.2 (3)
O1—C1—N1—C2	179.6 (3)	C1—N2—C8—C10	132.1 (3)
O1—C1—N2—C7	−178.9 (3)	C2—C3—C4—C5	−1.0 (4)
O1—C1—N2—C8	−9.3 (4)	C2—C7—N2—C8	−169.7 (2)
O2—C16—N4—C15	−4.9 (4)	C2—C7—C6—C5	−1.4 (4)
O2—C16—N4—C22	179.1 (3)	C3—C2—C7—C6	0.7 (4)
O2—C16—N5—C17	−179.4 (3)	C3—C4—C5—C6	0.3 (5)
O3—C23—C24—C25	−173.6 (5)	C4—C3—C2—C7	0.5 (4)
O4—C23—C24—C25	7.4 (8)	C4—C5—C6—C7	0.9 (4)
O5—C26—C25—C24	173.0 (5)	C6—C7—N2—C8	9.7 (5)
O6—C26—C25—C24	−10.3 (8)	C7—N2—C8—C9	65.3 (3)
N1—C1—N2—C7	0.4 (3)	C7—N2—C8—C10	−60.4 (3)
N1—C1—N2—C8	170.0 (2)	C9—C8—C10—C12	50.0 (3)
N1—C2—C3—C4	179.4 (3)	C9—C11—N3—C12	−62.3 (3)
N1—C2—C7—N2	1.1 (3)	C9—C11—N3—C13	171.1 (2)
N1—C2—C7—C6	−178.4 (2)	C10—C8—C9—C11	−50.5 (3)
N2—C1—N1—C2	0.3 (3)	C10—C12—N3—C11	62.3 (3)
N2—C7—C2—C3	−179.7 (2)	C10—C12—N3—C13	−173.0 (2)
N2—C7—C6—C5	179.2 (3)	C11—N3—C13—C14	−169.9 (2)
N2—C8—C9—C11	−176.4 (2)	C12—N3—C13—C14	65.8 (3)
N2—C8—C10—C12	174.5 (2)	C14—C15—N4—C16	107.0 (3)
N3—C11—C9—C8	56.3 (3)	C14—C15—N4—C22	−77.8 (4)
N3—C12—C10—C8	−55.7 (3)	C15—N4—C22—C17	−175.9 (2)

N3—C13—C14—C15	163.0 (3)	C15—N4—C22—C21	3.2 (5)
N4—C15—C14—C13	−62.7 (4)	C16—N4—C22—C17	−0.1 (3)
N4—C16—N5—C17	−0.9 (3)	C16—N4—C22—C21	179.0 (3)
N4—C22—C17—N5	−0.5 (3)	C16—N5—C17—C18	−179.6 (3)
N4—C22—C17—C18	179.9 (3)	C16—N5—C17—C22	0.9 (3)
N4—C22—C21—C20	−179.5 (3)	C17—C18—C19—C20	−0.4 (5)
N5—C16—N4—C15	176.6 (2)	C17—C22—C21—C20	−0.5 (5)
N5—C16—N4—C22	0.6 (3)	C18—C17—C22—C21	0.7 (4)
N5—C17—C18—C19	−179.7 (3)	C18—C19—C20—C21	0.6 (6)
N5—C17—C22—C21	−179.7 (3)	C19—C18—C17—C22	−0.2 (5)
C1—N1—C2—C3	−179.9 (3)	C19—C20—C21—C22	−0.1 (6)
C1—N1—C2—C7	−0.9 (3)	C23—C24—C25—C26	1(1)
C1—N2—C7—C2	−1.0 (3)		

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2; (iii) −*x*+1, −*y*, −*z*+2; (iv) −*x*, −*y*, −*z*+2; (v) −*x*+3/2, *y*−1/2, −*z*+3/2; (vi) *x*+1, *y*, *z*; (vii) −*x*+3/2, *y*+1/2, −*z*+3/2; (viii) −*x*+1/2, *y*+1/2, −*z*+3/2; (ix) *x*+1/2, −*y*+1/2, *z*−1/2; (x) *x*−1, *y*, *z*; (xi) *x*−1/2, −*y*+1/2, *z*+1/2; (xii) *x*+1/2, −*y*+1/2, *z*+1/2; (xiii) −*x*, −*y*, −*z*+1; (xiv) −*x*+2, −*y*, −*z*+1; (xv) *x*−1/2, −*y*+1/2, *z*−1/2.