Table 81: General Anisotropic Displacement Parameter Expressions (U's) for *rac*-15.

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
O(8)	0.076(1)	0.073(1)	0.0410(8)	-0.0201(9)	-0.0069(8)	0.0160(8)
O(20)	0.0621(9)	0.0371(7)	0.0610(8)	-0.0014(7)	0.0006(7)	-0.0102(7)
O(22)	0.0687(9)	0.0553(9)	0.0468(7)	0.0031(8)	0.0217(6)	0.0039(7)
N(1)	0.0397(8)	0.0340(8)	0.0368(8)	0.0003(7)	0.0006(7)	0.0003(7)
N(3)	0.051(1)	0.0360(8)	0.0391(8)	-0.0003(8)	-0.0042(8)	-0.0027(8)
C(2)	0.044(1)	0.038(1)	0.042(1)	0.0008(9)	-0.0029(9)	-0.0004(9)
C(4)	0.046(1)	0.036(1)	0.040(1)	-0.0048(9)	0.0055(9)	-0.0017(9)
C(5)	0.050(1)	0.0328(9)	0.0345(9)	0.0009(9)	0.0067(8)	0.0040(9)
C(6)	0.052(1)	0.036(1)	0.0326(9)	0.0036(9)	0.0001(9)	0.0012(9)
C(7)	0.051(1)	0.042(1)	0.0344(9)	0.0001(9)	0.0067(9)	-0.0035(9)
C(9)	0.047(1)	0.033(1)	0.039(1)	-0.0009(9)	0.0066(9)	-0.0029(9)
C(10)	0.059(1)	0.039(1)	0.041(1)	-0.003(1)	0.005(1)	-0.0038(9)
C(11)	0.078(2)	0.043(1)	0.048(1)	-0.004(1)	-0.005(1)	-0.006(1)
C(12)	0.057(1)	0.056(1)	0.079(2)	-0.009(1)	-0.008(1)	-0.005(1)
C(13)	0.055(1)	0.073(2)	0.084(2)	-0.011(1)	0.021(1)	-0.005(1)
C(14)	0.056(1)	0.061(1)	0.055(1)	-0.009(1)	0.018(1)	-0.009(1)
C(15)	0.044(1)	0.071(1)	0.063(1)	0.001(1)	0.006(1)	-0.018(1)
C(16)	0.059(2)	0.111(2)	0.112(2)	0.012(1)	0.008(1)	-0.062(2)
C(17)	0.073(2)	0.147(3)	0.088(2)	-0.005(2)	0.039(1)	0.019(2)
C(18)	0.047(1)	0.102(2)	0.093(2)	0.000(1)	0.003(1)	-0.031(2)
C(19)	0.072(2)	0.058(1)	0.050(1)	0.003(1)	-0.016(1)	-0.010(1)
C(21)	0.053(1)	0.034(1)	0.041(1)	0.0015(9)	0.0081(9)	0.0014(9)
C(23)	0.048(1)	0.046(1)	0.043(1)	0.006(1)	0.0076(9)	-0.007(1)
C(24)	0.089(2)	0.049(1)	0.062(1)	0.000(1)	-0.013(1)	0.009(1)
C(25)	0.111(2)	0.071(2)	0.069(2)	0.008(2)	-0.022(2)	0.014(2)
C(26)	0.073(2)	0.128(2)	0.065(2)	0.023(2)	-0.008(1)	0.000(2)
C(27)	0.056(1)	0.180(3)	0.069(2)	-0.041(2)	0.003(1)	-0.010(2)
C(28)	0.063(1)	0.109(2)	0.054(1)	-0.030(1)	0.010(1)	0.005(1)

The form of the anisotropic displacement parameter is:
Exp[-2PI2{h2a2U(1,1) + k2b2U(2,2) + l2c2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)}]
where a, b and c are reciprocal lattice constants.

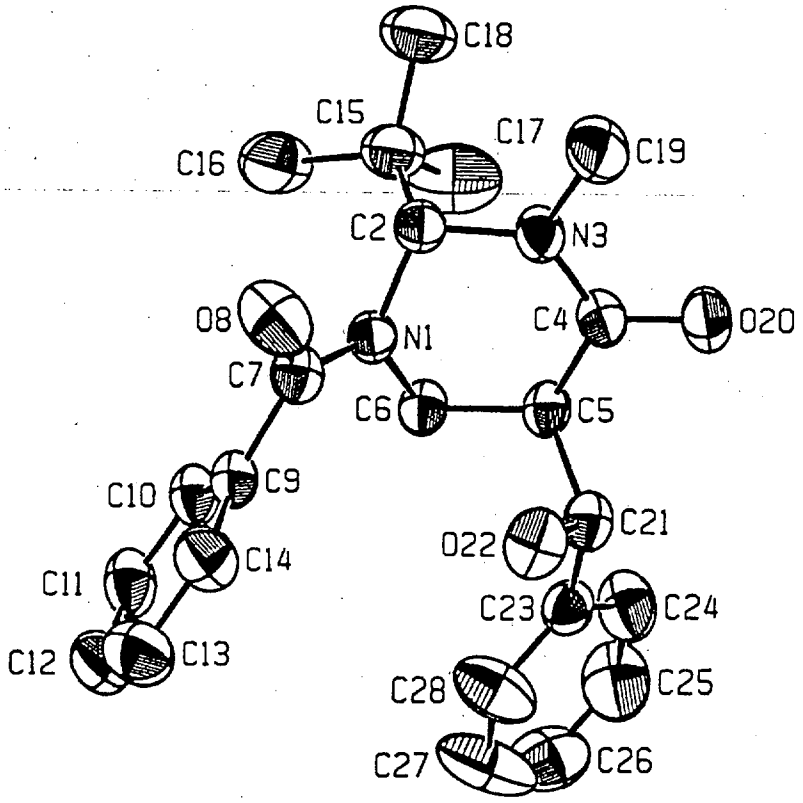

Figure 36. Thermal ellipsoid figure for compound *rac*-15.

Table 82: Crystal data and data collection for compound (2*S*,5*R*)-16.

Identification code	ejmb03	
Empirical formula	$C_{24}H_{30}N_2O_2$	
Formula weight	378.50	
Crystal size	0.45 x 0.2 x 0.2 mm	
Cristal color	colorless	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 6.0840(10) Å	α = 90.00 °
	b = 11.535(2) Å	β = 91.92(3) °
	c = 15.297(3) Å	γ = 90.00 °
Volume	1072.9(3) $Å^3$	
Z	2	
Density (calculated)	1.172 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	408	
Diffractometer used	Enraf-Nonius CAD4	
Radiation and wavelength	MoKα with λ=0.71073 Å	
Scan type	ω/2θ	
Temperature	293(2) K	
2θ range for data collection	4.42 to 49.92°	
Index ranges	$0 \le h \le 7$ $0 \le k \le 13$ $-18 \le l \le 18$	
Reflections collected	2182	
Independent reflections	1987 (R_{int} = 0.0118)	
Observed reflections	1623 (F>4σ(F))	

Table 83: Solution and refinement

Solution	Direct methods
Refinement method	Full-matrix Least-Squares on F^2
Hydrogen atoms	Riding-model, U isotropic
Weighting scheme	$w^{-1}=\sigma^2Fo^2+(0.0736P)^2+0.1489P$
	where $P=(Fo^2+2Fc^2)/3$
Absolute structure	0(2) (Flack H D (1983), Acta Cryst. A39, 876- 881)
Data / restraints / parameters	1987 / 1 / 253
Final R indices [F>4σ(F)]	R1 = 0.0401 , wR2 = 0.1134
R indices (all data)	R1 = 0.0545 , wR2 = 0.1235
Goodness-of-Fit on F^2	1.036

Table 84: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (2*S*,5*R*)-16. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	-1758(3)	489(2)	2491.1(13)	33.8(5)
C(2)	-1257(4)	1391(3)	3132.3(19)	37.8(6)
N(3)	-1285(4)	866(2)	4009.1(15)	41.1(6)
C(4)	-2394(5)	-104(3)	4225.1(19)	47.4(8)
C(5)	-3713(5)	-760(2)	3519.2(19)	37.2(6)
C(6)	-3786(4)	-156(3)	2629.8(17)	35.0(6)
C(7)	-337(4)	308(3)	1836.6(18)	37.5(6)
O(8)	1438(3)	820(2)	1817.1(15)	51.8(6)
C(9)	-953(5)	-520(3)	1130.1(18)	43.1(7)
C(10)	530(6)	-1387(4)	915(2)	63.2(10)
C(11)	26(8)	-2147(5)	251(3)	84.0(14)
C(12)	-1910(8)	-2067(5)	-223(3)	81.2(14)
C(13)	-3372(7)	-1210(4)	-38(2)	69.5(11)
C(14)	-2924(6)	-440(4)	635.5(19)	54.2(9)
C(15)	-2695(5)	2511(3)	3017(2)	46.7(8)
C(16)	-3222(9)	2711(4)	2053(3)	79.5(13)
C(17)	-1363(7)	3555(4)	3352(4)	81.5(14)
C(18)	-4824(6)	2473(4)	3514(3)	64.1(10)
C(19)	22(6)	1432(4)	4711(2)	54.2(9)
O(20)	-2308(5)	-471(3)	4974.6(15)	80.6(9)
C(21)	-6089(5)	-852(3)	3835(2)	54.0(9)
C(22)	-2614(5)	-1980(3)	3457(2)	48.4(8)
C(23)	-3981(6)	-2867(3)	2973(2)	48.2(8)
C(24)	-5475(7)	-3523(3)	3421(3)	66.3(11)
C(25)	-6879(8)	-4284(4)	2998(3)	81.3(13)
C(26)	-6813(9)	-4416(4)	2113(4)	89.0(15)
C(27)	-5272(9)	-3816(4)	1650(3)	81.8(13)
C(28)	-3846(7)	-3047(3)	2086(3)	62.4(10)
H(2A)	234	1625	3045	80
H(6A)	-3994	-722	2175	80
H(6B)	-5011	369	2598	80
H(10A)	1924	-1440	1226	80
H(11A)	1042	-2757	126	80
H(12A)	-2228	-2606	-688	80
H(13A)	-4701	-1144	-390	80
H(14A)	-3987	145	765	80
H(16A)	-4112	3393	1976	80
H(16B)	-1877	2807	1750	80
H(16C)	-4005	2051	1820	80
H(17A)	-2219	4250	3287	80
H(17B)	-966	3440	3959	80
H(17C)	-54	3624	3022	80
H(18A)	-5628	3179	3413	80

H(18B)	-5699	1827	3312	80
H(18C)	-4489	2388	4128	80
H(19A)	-128	1019	5251	80
H(19B)	1540	1441	4559	80
H(19C)	-490	2213	4778	80
H(21A)	-6723	-91	3867	80
H(21B)	-6950	-1317	3432	80
H(21C)	-6070	-1205	4403	80
H(22A)	-2271	-2257	4037	80
H(22B)	-1254	-1895	3163	80
H(24A)	-5549	-3420	4042	80
H(25A)	-7850	-4753	3331	80
H(26A)	-7863	-4908	1812	80
H(27A)	-5201	-3920	1029	80
H(28A)	-2740	-2649	1769	80

Table 85: Bond lengths [Å], bond angles and torsion angles [°] for (2*S*,5*R*)-16.

N(1)-C(7)	1.361(3)	N(1)-C(2)	1.455(4)
N(1)-C(6)	1.462(3)	C(2)-N(3)	1.472(4)
C(2)-C(15)	1.566(4)	N(3)-C(4)	1.353(4)
N(3)-C(19)	1.467(4)	C(4)-O(20)	1.222(4)
C(4)-C(5)	1.525(4)	C(5)-C(6)	1.528(4)
C(5)-C(21)	1.543(4)	C(5)-C(22)	1.563(4)
C(7)-O(8)	1.232(3)	C(7)-C(9)	1.482(4)
C(9)-C(10)	1.393(5)	C(9)-C(14)	1.399(4)
C(10)-C(11)	1.370(6)	C(11)-C(12)	1.365(7)
C(12)-C(13)	1.366(7)	C(13)-C(14)	1.380(5)
C(15)-C(16)	1.517(5)	C(15)-C(18)	1.524(5)
C(15)-C(17)	1.530(5)	C(22)-C(23)	1.498(5)
C(23)-C(28)	1.378(5)	C(23)-C(24)	1.382(5)
C(24)-C(25)	1.372(6)	C(25)-C(26)	1.364(7)
C(26)-C(27)	1.380(7)	C(27)-C(28)	1.395(6)
C(7)-N(1)-C(2)	118.8(2)	C(7)-N(1)-C(6)	126.1(2)
C(2)-N(1)-C(6)	115.1(2)	N(1)-C(2)-N(3)	108.2(2)
N(1)-C(2)-C(15)	114.2(2)	N(3)-C(2)-C(15)	114.7(2)
C(4)-N(3)-C(19)	116.8(3)	C(4)-N(3)-C(2)	125.7(2)
C(19)-N(3)-C(2)	117.5(3)	O(20)-C(4)-N(3)	120.7(3)
O(20)-C(4)-C(5)	119.8(3)	N(3)-C(4)-C(5)	119.5(2)
C(4)-C(5)-C(6)	113.8(2)	C(4)-C(5)-C(21)	106.8(3)
C(6)-C(5)-C(21)	108.1(2)	C(4)-C(5)-C(22)	105.9(2)
C(6)-C(5)-C(22)	110.9(3)	C(21)-C(5)-C(22)	111.4(3)

N(1)-C(6)-C(5)	111.2(2)	O(8)-C(7)-N(1)	121.6(3)
O(8)-C(7)-C(9)	119.5(3)	N(1)-C(7)-C(9)	118.9(2)
C(10)-C(9)-C(14)	118.0(3)	C(10)-C(9)-C(7)	119.0(3)
C(14)-C(9)-C(7)	122.9(3)	C(11)-C(10)-C(9)	120.2(4)
C(12)-C(11)-C(10)	121.2(4)	C(11)-C(12)-C(13)	119.7(4)
C(12)-C(13)-C(14)	120.5(4)	C(13)-C(14)-C(9)	120.3(4)
C(16)-C(15)-C(18)	109.5(3)	C(16)-C(15)-C(17)	107.3(4)
C(18)-C(15)-C(17)	107.8(3)	C(16)-C(15)-C(2)	109.5(3)
C(18)-C(15)-C(2)	113.6(3)	C(17)-C(15)-C(2)	108.9(3)
C(23)-C(22)-C(5)	114.4(2)	C(28)-C(23)-C(24)	117.8(3)
C(28)-C(23)-C(22)	122.6(3)	C(24)-C(23)-C(22)	119.6(3)
C(25)-C(24)-C(23)	121.8(4)	C(26)-C(25)-C(24)	120.1(4)
C(25)-C(26)-C(27)	119.8(4)	C(26)-C(27)-C(28)	119.7(4)
C(23)-C(28)-C(27)	120.7(4)		

C(7)-N(1)-C(2)-N(3)	-125.6(3)	O(8)-C(7)-C(9)-C(14)	-125.4(3)
C(6)-N(1)-C(2)-N(3)	53.7(3)	N(1)-C(7)-C(9)-C(14)	54.2(4)
C(7)-N(1)-C(2)-C(15)	105.4(3)	C(14)-C(9)-C(10)-C(11)	-1.4(6)
C(6)-N(1)-C(2)-C(15)	-75.3(3)	C(7)-C(9)-C(10)-C(11)	-178.4(4)
N(1)-C(2)-N(3)-C(4)	-24.3(4)	C(9)-C(10)-C(11)-C(12)	0.9(7)
C(15)-C(2)-N(3)-C(4)	104.4(3)	C(10)-C(11)-C(12)-C(13)	0.5(8)
N(1)-C(2)-N(3)-C(19)	154.9(2)	C(11)-C(12)-C(13)-C(14)	-1.3(7)
C(15)-C(2)-N(3)-C(19)	-76.4(3)	C(12)-C(13)-C(14)-C(9)	0.7(6)
C(19)-N(3)-C(4)-O(20)	0.7(5)	C(10)-C(9)-C(14)-C(13)	0.6(5)
C(2)-N(3)-C(4)-O(20)	179.9(3)	C(7)-C(9)-C(14)-C(13)	177.4(3)
C(19)-N(3)-C(4)-C(5)	-177.7(3)	N(1)-C(2)-C(15)-C(16)	-33.6(4)
C(2)-N(3)-C(4)-C(5)	1.5(4)	N(3)-C(2)-C(15)-C(16)	-159.2(3)
O(20)-C(4)-C(5)-C(6)	176.4(3)	N(1)-C(2)-C(15)-C(18)	89.2(3)
N(3)-C(4)-C(5)-C(6)	-5.3(4)	N(3)-C(2)-C(15)-C(18)	-36.4(4)
O(20)-C(4)-C(5)-C(21)	57.2(4)	N(1)-C(2)-C(15)-C(17)	-150.7(3)
N(3)-C(4)-C(5)-C(21)	-124.4(3)	N(3)-C(2)-C(15)-C(17)	83.7(3)
O(20)-C(4)-C(5)-C(22)	-61.6(4)	C(4)-C(5)-C(22)-C(23)	164.9(3)
N(3)-C(4)-C(5)-C(22)	116.8(3)	C(6)-C(5)-C(22)-C(23)	-71.2(3)
C(7)-N(1)-C(6)-C(5)	119.6(3)	C(21)-C(5)-C(22)-C(23)	49.2(4)
C(2)-N(1)-C(6)-C(5)	-59.6(3)	C(5)-C(22)-C(23)-C(28)	91.0(4)
C(4)-C(5)-C(6)-N(1)	32.2(3)	C(5)-C(22)-C(23)-C(24)	-87.7(4)
C(21)-C(5)-C(6)-N(1)	150.6(3)	C(28)-C(23)-C(24)-C(25)	-3.7(6)
C(22)-C(5)-C(6)-N(1)	-87.1(3)	C(22)-C(23)-C(24)-C(25)	175.1(4)
C(2)-N(1)-C(7)-O(8)	6.1(4)	C(23)-C(24)-C(25)-C(26)	0.5(8)
C(6)-N(1)-C(7)-O(8)	-173.1(3)	C(24)-C(25)-C(26)-C(27)	2.5(8)
C(2)-N(1)-C(7)-C(9)	-173.6(3)	C(25)-C(26)-C(27)-C(28)	-2.3(8)
C(6)-N(1)-C(7)-C(9)	7.3(4)	C(24)-C(23)-C(28)-C(27)	4.0(6)
O(8)-C(7)-C(9)-C(10)	51.3(4)	C(22)-C(23)-C(28)-C(27)	-174.8(4)
N(1)-C(7)-C(9)-C(10)	-129.0(3)	C(26)-C(27)-C(28)-C(23)	-1.1(7)

Table 86: Anisotropic displacement parameters [Å^2 x 10^3] for (2*S*,5*R*)-16.

	U11	U22	U33	U23	U13	U12
N(1)	28.7(11)	41.0(13)	31.6(11)	-2.9(10)	0.9(9)	-6.1(10)
C(2)	28.1(13)	43.6(16)	41.8(15)	-4.0(13)	2.4(11)	-7.7(13)
N(3)	37.3(12)	49.3(14)	36.3(12)	-3.4(11)	-3.0(10)	-3.8(12)
C(4)	50.5(18)	54.0(19)	37.5(15)	-2.0(14)	-1.1(13)	-2.7(16)
C(5)	34.4(13)	37.9(16)	39.4(14)	2.5(12)	2.9(11)	-2.8(12)
C(6)	29.0(13)	40.3(15)	35.7(13)	1.7(13)	-0.5(10)	-5.6(12)
C(7)	31.1(14)	47.3(17)	33.9(13)	8.0(13)	1.5(10)	0.2(13)
O(8)	35.9(11)	66.6(15)	53.6(12)	-3.4(12)	10.2(9)	-9.5(11)
C(9)	43.4(15)	51.5(18)	35.1(14)	2.8(14)	10.2(12)	-3.1(15)
C(10)	48.6(19)	82(3)	60(2)	-17(2)	11.9(16)	5.6(19)
C(11)	81(3)	89(3)	84(3)	-37(3)	26(3)	8(3)
C(12)	100(3)	92(3)	51(2)	-30(2)	12(2)	-9(3)
C(13)	84(3)	85(3)	38.6(18)	-7(2)	-10.1(17)	-13(3)
C(14)	63(2)	61(2)	38.7(15)	1.5(16)	-6.0(14)	-0.9(18)
C(15)	42.9(16)	40.4(17)	56.7(18)	-5.1(15)	-0.9(14)	-3.7(14)
C(16)	106(3)	64(3)	68(3)	16(2)	-1(2)	20(3)
C(17)	66(3)	43(2)	134(4)	-5(2)	-10(3)	-13(2)
C(18)	47.9(19)	55(2)	90(3)	-9(2)	7.9(19)	6.9(18)
C(19)	49.7(17)	68(2)	44.7(17)	-18.7(17)	-1.1(14)	-10.2(17)
O(20)	122(2)	83(2)	36.9(12)	9.3(14)	-7.7(13)	-32.4(19)
C(21)	45.8(17)	52(2)	65(2)	3.1(16)	19.8(15)	-4.9(16)
C(22)	44.2(16)	45.2(18)	55.6(19)	6.8(15)	-3.2(14)	3.1(15)
C(23)	52.3(18)	37.2(18)	55.3(18)	2.4(14)	6.9(14)	1.5(15)
C(24)	86(3)	43(2)	72(2)	-1.8(18)	24(2)	-18(2)
C(25)	95(3)	52(2)	98(3)	-12(2)	29(3)	-29(2)
C(26)	96(3)	55(3)	115(4)	-17(3)	-10(3)	-28(3)
C(27)	130(4)	48(2)	67(3)	-12(2)	-1(2)	-9(3)
C(28)	85(3)	43.1(18)	60(2)	-4.2(17)	18.2(19)	-6.7(19)

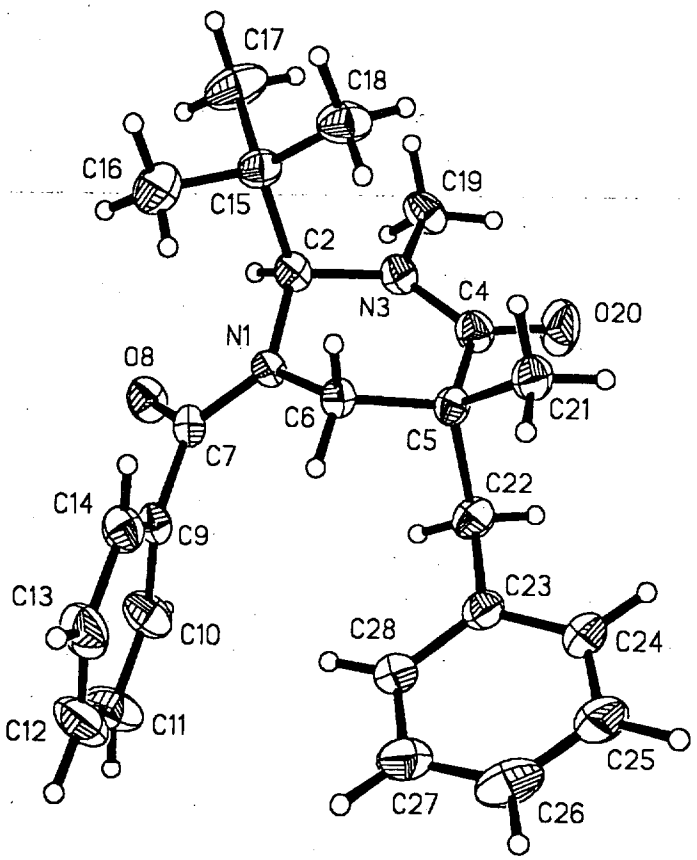

Figure 37. Thermal ellipsoid figure for compound (2*S*,5*R*)-16.

Table 87: Crystal data and data collection for compound (2*S*,5*R*)-17.

Identification code	ejmb05	
Empirical formula	$C_{21}\ H_{32}\ N_2\ O_2$	
Formula weight	344.49	
Crystal size	0.3 x 0.2 x 0.15 mm	
Cristal color	colorless	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.873(2) Å	α = 90.00 °
	b = 10.616(2) Å	β = 108.39(2) °
	c = 11.269(2) Å	γ = 90.00 °
Volume	1007.3(3) $Å^3$	
Z	2	
Density (calculated)	1.136 Mg/m^3	
Absorption coefficient	0.073 mm^{-1}	
F(000)	376	
Diffractometer used	Enraf-Nonius CAD4	
Radiation and wavelength	MoKα with λ=0.71073 Å	
Scan type	ω/2θ	
Temperature	293(2) K	
2θ range for data collection	4.84 to 43.94°	
Index ranges	$-10 \le h \le 1$ $-12 \le k \le 12$ $-13 \le l \le 13$	
Reflections collected	3059	
Independent reflections	2475 (R_{int} = 0.0424)	
Observed reflections	1337 (F>4σ(F))	

Table 88: Solution and refinement

Solution	Direct methods
Refinement method	Full-matrix Least-Squares on F^2
Extinction correction	SHELXL
Extinction coefficients	0.025(5)
Hydrogen atoms	riding model, fixed isotropic U
Weighting scheme	$w^{-1}=\sigma^2Fo^2+(0.0658P)^2+0.0195P$ where $P=(Fo^2+2Fc^2)/3$
Absolute structure	0(3) (Flack H D (1983), Acta Cryst. A39, 876-881)
Data / restraints / parameters	2475 / 1 / 227
Final R indices [F>4σ(F)]	R1 = 0.0428 , wR2 = 0.1125
R indices (all data)	R1 = 0.1306 , wR2 = 0.1413
Goodness-of-Fit on F^2	1.027

Table 89: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for (2*S*,5*R*)-17. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	-4658(4)	-9579(3)	-1366(3)	41.4(10)
C(2)	-5368(6)	-10015(4)	-2635(4)	51.8(13)
N(3)	-4366(5)	-9630(4)	-3378(3)	61.7(12)
C(4)	-3368(7)	-8623(5)	-3116(5)	66.4(16)
C(5)	-3027(6)	-7940(4)	-1882(4)	54.7(13)
C(6)	-4253(5)	-8264(4)	-1244(4)	46.4(12)
C(7)	-4148(6)	-10465(5)	-457(4)	48.5(13)
O(8)	-4261(5)	-11596(3)	-692(3)	69.2(11)
C(9)	-3440(5)	-10060(4)	867(4)	43.8(12)
C(10)	-2027(7)	-10600(5)	1560(5)	59.9(14)
C(11)	-1336(7)	-10304(6)	2812(5)	71.9(17)
C(12)	-2115(7)	-9491(6)	3366(5)	70.6(17)
C(13)	-3542(7)	-8969(5)	2697(5)	61.1(14)
C(14)	-4215(6)	-9234(4)	1442(4)	46.9(12)
C(15)	-7170(7)	-9656(5)	-3217(5)	68.7(16)
C(16)	-7942(7)	-9634(8)	-2200(6)	119(3)
C(17)	-8010(7)	-10654(7)	-4163(6)	104(2)
C(18)	-7399(9)	-8407(6)	-3894(6)	118(3)
C(19)	-4495(8)	-10359(6)	-4513(5)	89(2)
O(20)	-2645(6)	-8317(4)	-3850(4)	109.7(16)
C(21)	-3060(7)	-6521(5)	-2125(5)	70.8(15)
C(22)	-1363(6)	-8355(5)	-1081(4)	64.6(15)
C(23)	-667(6)	-7717(5)	187(5)	60.5(15)
C(24)	912(6)	-8265(6)	945(5)	82.3(18)
C(25)	1601(8)	-7681(8)	2218(6)	111(2)
H(2A)	-5316	-10918	-2598	80
H(6A)	-3850	-8050	-372	80
H(6B)	-5195	-7776	-1617	80
H(10A)	-1520	-11184	1157	80
H(11A)	-330	-10662	3278	80
H(12A)	-1644	-9275	4232	80
H(13A)	-4091	-8429	3107	80
H(14A)	-5200	-8857	958	80
H(16A)	-7766	-10424	-1763	80
H(16B)	-7479	-8966	-1626	80
H(16C)	-9063	-9491	-2559	80
H(17A)	-7545	-10689	-4825	80
H(17B)	-7931	-11467	-3774	80
H(17C)	-9108	-10419	-4500	80
H(18A)	-6913	-8435	-4544	80
H(18B)	-8518	-8262	-4256	80
H(18C)	-6935	-7737	-3323	80
H(19A)	-3793	-10000	-4920	80

H(19B)	-4184	-11212	-4278	80
H(19C)	-5563	-10346	-5075	80
H(21A)	-4115	-6283	-2621	80
H(21B)	-2777	-6085	-1339	80
H(21C)	-2326	-6303	-2561	80
H(22A)	-645	-8207	-1550	80
H(22B)	-1382	-9246	-940	80
H(23A)	-1405	-7811	647	80
H(23B)	-544	-6834	60	80
H(24A)	1646	-8163	482	80
H(24B)	784	-9152	1053	80
H(25A)	2603	-8062	2655	80
H(25B)	1750	-6797	2113	80
H(25C)	880	-7795	2690	80

Table 90: Bond lengths [Å], bond angles and torsion angles [°] for (2*S*,5*R*)-17.

N(1)-C(7)	1.359(6)	N(1)-C(6)	1.438(6)
N(1)-C(2)	1.445(5)	C(2)-N(3)	1.458(6)
C(2)-C(15)	1.571(7)	N(3)-C(4)	1.360(6)
N(3)-C(19)	1.469(6)	C(4)-O(20)	1.239(6)
C(4)-C(5)	1.512(7)	C(5)-C(6)	1.520(6)
C(5)-C(21)	1.531(7)	C(5)-C(22)	1.532(7)
C(7)-O(8)	1.226(6)	C(7)-C(9)	1.488(6)
C(9)-C(10)	1.376(6)	C(9)-C(14)	1.393(6)
C(10)-C(11)	1.385(7)	C(11)-C(12)	1.373(7)
C(12)-C(13)	1.370(7)	C(13)-C(14)	1.380(7)
C(15)-C(18)	1.510(8)	C(15)-C(16)	1.510(7)
C(15)-C(17)	1.521(8)	C(22)-C(23)	1.525(7)
C(23)-C(24)	1.508(6)	C(24)-C(25)	1.504(8)
C(7)-N(1)-C(6)	125.9(4)	C(7)-N(1)-C(2)	117.6(4)
C(6)-N(1)-C(2)	115.0(4)	N(1)-C(2)-N(3)	108.9(4)
N(1)-C(2)-C(15)	113.8(4)	N(3)-C(2)-C(15)	114.6(4)
C(4)-N(3)-C(2)	124.7(4)	C(4)-N(3)-C(19)	118.0(4)
C(2)-N(3)-C(19)	117.3(4)	O(20)-C(4)-N(3)	120.0(5)
O(20)-C(4)-C(5)	119.5(5)	N(3)-C(4)-C(5)	120.3(4)
C(4)-C(5)-C(6)	111.2(4)	C(4)-C(5)-C(21)	108.7(4)
C(6)-C(5)-C(21)	109.3(4)	C(4)-C(5)-C(22)	106.2(4)
C(6)-C(5)-C(22)	110.9(4)	C(21)-C(5)-C(22)	110.4(4)
N(1)-C(6)-C(5)	111.6(4)	O(8)-C(7)-N(1)	122.0(4)
O(8)-C(7)-C(9)	118.7(4)	N(1)-C(7)-C(9)	119.4(4)
C(10)-C(9)-C(14)	119.6(4)	C(10)-C(9)-C(7)	118.0(4)

C(14)-C(9)-C(7)	122.3(4)	C(9)-C(10)-C(11)	121.0(5)
C(12)-C(11)-C(10)	118.8(5)	C(13)-C(12)-C(11)	121.0(5)
C(12)-C(13)-C(14)	120.5(5)	C(13)-C(14)-C(9)	119.2(5)
C(18)-C(15)-C(16)	110.4(6)	C(18)-C(15)-C(17)	107.5(5)
C(16)-C(15)-C(17)	107.6(5)	C(18)-C(15)-C(2)	112.4(5)
C(16)-C(15)-C(2)	109.4(4)	C(17)-C(15)-C(2)	109.4(5)
C(23)-C(22)-C(5)	117.0(4)	C(24)-C(23)-C(22)	112.8(4)
C(25)-C(24)-C(23)	113.9(6)		
C(7)-N(1)-C(2)-N(3)	-115.3(4)	C(6)-N(1)-C(7)-C(9)	16.1(7)
C(6)-N(1)-C(2)-N(3)	51.5(5)	C(2)-N(1)-C(7)-C(9)	-178.7(4)
C(7)-N(1)-C(2)-C(15)	115.5(5)	O(8)-C(7)-C(9)-C(10)	48.6(7)
C(6)-N(1)-C(2)-C(15)	-77.7(5)	N(1)-C(7)-C(9)-C(10)	-131.8(5)
N(1)-C(2)-N(3)-C(4)	-25.7(6)	O(8)-C(7)-C(9)-C(14)	-126.5(5)
C(15)-C(2)-N(3)-C(4)	103.1(6)	N(1)-C(7)-C(9)-C(14)	53.0(6)
N(1)-C(2)-N(3)-C(19)	156.7(4)	C(14)-C(9)-C(10)-C(11)	-2.0(7)
C(15)-C(2)-N(3)-C(19)	-74.5(6)	C(7)-C(9)-C(10)-C(11)	-177.3(5)
C(2)-N(3)-C(4)-O(20)	-174.9(5)	C(9)-C(10)-C(11)-C(12)	2.1(8)
C(19)-N(3)-C(4)-O(20)	2.7(8)	C(10)-C(11)-C(12)-C(13)	-0.5(8)
C(2)-N(3)-C(4)-C(5)	10.2(7)	C(11)-C(12)-C(13)-C(14)	-1.1(8)
C(19)-N(3)-C(4)-C(5)	-172.2(5)	C(12)-C(13)-C(14)-C(9)	1.2(7)
O(20)-C(4)-C(5)-C(6)	168.4(5)	C(10)-C(9)-C(14)-C(13)	0.3(6)
N(3)-C(4)-C(5)-C(6)	-16.7(7)	C(7)-C(9)-C(14)-C(13)	175.4(4)
O(20)-C(4)-C(5)-C(21)	48.0(7)	N(1)-C(2)-C(15)-C(18)	90.8(5)
N(3)-C(4)-C(5)-C(21)	-137.1(5)	N(3)-C(2)-C(15)-C(18)	-35.4(6)
O(20)-C(4)-C(5)-C(22)	-70.8(6)	N(1)-C(2)-C(15)-C(16)	-32.2(7)
N(3)-C(4)-C(5)-C(22)	104.1(5)	N(3)-C(2)-C(15)-C(16)	-158.5(5)
C(7)-N(1)-C(6)-C(5)	103.8(5)	N(1)-C(2)-C(15)-C(17)	-149.9(5)
C(2)-N(1)-C(6)-C(5)	-61.8(5)	N(3)-C(2)-C(15)-C(17)	83.8(6)
C(4)-C(5)-C(6)-N(1)	40.6(5)	C(4)-C(5)-C(22)-C(23)	175.2(4)
C(21)-C(5)-C(6)-N(1)	160.6(4)	C(6)-C(5)-C(22)-C(23)	-63.9(5)
C(22)-C(5)-C(6)-N(1)	-77.4(5)	C(21)-C(5)-C(22)-C(23)	57.5(5)
C(6)-N(1)-C(7)-O(8)	-164.4(5)	C(5)-C(22)-C(23)-C(24)	175.3(4)
C(2)-N(1)-C(7)-O(8)	0.8(7)	C(22)-C(23)-C(24)-C(25)	-178.2(5)

Table 91: Anisotropic displacement parameters [Å^2 x 10^3] for (2*S*,5*R*)-17.

	U11	U22	U33	U23	U13	U12
N(1)	46(2)	43(3)	34(2)	-0.7(19)	10.8(17)	-0.7(19)
C(2)	70(4)	49(3)	34(3)	1(2)	13(3)	4(3)
N(3)	89(3)	65(3)	37(2)	-15(2)	27(2)	-4(3)
C(4)	98(5)	63(4)	49(3)	4(3)	39(3)	-2(4)
C(5)	75(4)	48(3)	45(3)	1(2)	25(3)	2(3)
C(6)	58(3)	43(3)	41(3)	-2(2)	20(2)	-1(2)
C(7)	56(3)	50(4)	40(3)	2(3)	16(3)	-7(3)
O(8)	99(3)	46(2)	52(2)	2.7(17)	9(2)	-2(2)
C(9)	49(3)	40(3)	41(3)	10(2)	13(2)	-1(3)
C(10)	66(4)	61(3)	52(4)	2(3)	19(3)	2(3)
C(11)	60(4)	100(5)	47(4)	4(3)	5(3)	6(3)
C(12)	90(5)	82(4)	36(3)	-5(3)	16(3)	-17(4)
C(13)	79(4)	65(3)	45(3)	-5(3)	28(3)	-6(3)
C(14)	51(3)	49(3)	42(3)	0(2)	17(2)	-5(2)
C(15)	65(4)	76(4)	54(3)	-6(3)	3(3)	15(3)
C(16)	48(4)	202(9)	101(5)	-33(6)	16(4)	2(5)
C(17)	74(5)	123(6)	85(5)	-28(4)	-20(4)	0(4)
C(18)	109(6)	115(6)	104(6)	1(5)	-3(4)	50(5)
C(19)	127(6)	92(5)	55(3)	-24(3)	37(4)	-6(4)
O(20)	159(4)	123(4)	76(3)	-6(3)	79(3)	-26(3)
C(21)	89(4)	61(4)	63(3)	15(3)	24(3)	2(3)
C(22)	68(4)	66(4)	67(3)	0(3)	32(3)	5(3)
C(23)	66(4)	54(4)	63(4)	2(3)	23(3)	2(3)
C(24)	55(4)	96(5)	86(4)	15(4)	7(3)	-5(4)
C(25)	84(5)	153(7)	82(5)	11(4)	4(4)	-13(5)

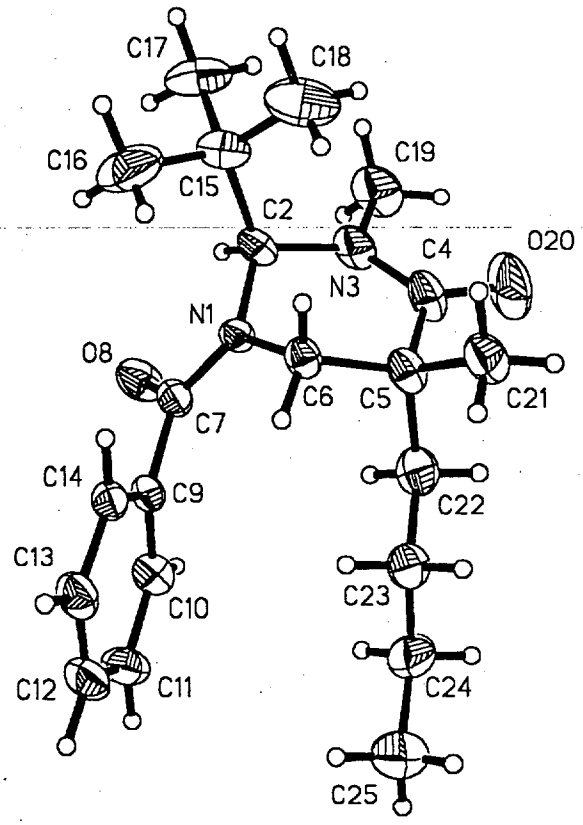

Figure 38. Thermal ellipsoid figure for compound (2*S*,5*R*)-17.

Table 92: Crystal data and data collection for compound *rac*-20.

Identification code	ejje02	
Empirical formula	$C_{25}\ H_{24}\ N_2\ O_2$	
Formula weight	384.46	
Crystal size	0.45 x 0.35 x 0.35 mm	
Cristal color	colorless	
Crystal system	Tetragonal	
Space group	P4(3)	
Unit cell dimensions	a = 13.497(2) Å	α = 90.00 °
	b = 13.497(2) Å	β = 90.00 °
	c = 11.423(2) Å	γ = 90.00 °
Volume	2080.9(6) $Å^3$	
Z	4	
Density (calculated)	1.227 Mg/m^3	
Absorption coefficient	0.078 mm^{-1}	
F(000)	816	
Diffractometer used	Enraf-Nonius CAD4	
Radiation and wavelength	MoKα with λ=0.71073 Å	
Scan type	ω/2θ	
Temperature	293(2) K	
2θ range for data collection	4.68 to 43.96°	
Index ranges	$-14 \le h \le 1$	$-14 \le k \le 1$ $-12 \le l \le 12$
Reflections collected	4283	
Independent reflections	1981 (R_{int} = 0.0303)	
Observed reflections	1802 (F>4σ(F))	

Table 93: Solution and refinement

Solution	Direct methods
Refinement method	Full-matrix Least-Squares on F^2
Hydrogen atoms	riding model,fixed isotropic U
Weighting scheme	$w^{-1}=\sigma^2Fo^2+(0.0471P)^2+0.1090P$
	where $P=(Fo^2+2Fc^2)/3$
Data / restraints / parameters	1981 / 1 / 262
Final R indices [F>4σ(F)]	R1 = 0.0274 , wR2 = 0.0728
R indices (all data)	R1 = 0.0327 , wR2 = 0.0759
Goodness-of-Fit on F^2	1.053

Table 94: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for *rac*-20. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	6554.8(13)	2739.4(12)	1730.9(17)	43.0(4)
C(2)	6140.5(16)	2337.4(16)	641(2)	45.7(6)
N(3)	5221.5(13)	1817.7(14)	893.6(18)	51.4(5)
C(4)	5180.4(17)	1173.7(17)	1791(3)	54.0(6)
C(5)	6143.3(16)	1082.6(16)	2467(2)	47.8(6)
C(6)	6483.2(16)	2138.3(16)	2812(2)	44.2(6)
C(7)	6817.9(18)	3712.0(16)	1721(2)	51.0(6)
O(8)	6859.2(17)	4178.3(12)	797.8(17)	75.2(6)
C(9)	7043.6(18)	4229.6(16)	2845(2)	49.5(6)
C(10)	7998(2)	4530.7(19)	3074(3)	65.3(7)
C(11)	8184(2)	5139(2)	4036(3)	79.2(9)
C(12)	7419(3)	5433(2)	4731(3)	78.5(9)
C(13)	6487(3)	5119(2)	4516(3)	77.3(9)
C(14)	6294(2)	4509.3(19)	3581(2)	60.2(7)
C(15)	6881.3(16)	1747.6(15)	-83(2)	41.8(5)
C(16)	6620.2(18)	882.3(17)	-655(2)	52.1(6)
C(17)	7279(2)	409.5(19)	-1388(2)	63.2(7)
C(18)	8213(2)	799(2)	-1567(2)	63.6(7)
C(19)	8475.3(19)	1658(2)	-1007(2)	58.8(7)
C(20)	7819.6(18)	2132.7(18)	-279(2)	50.3(6)
C(21)	4336.2(19)	2066(2)	228(3)	70.7(8)
O(22)	4425.2(13)	724.8(14)	2050(2)	78.3(6)
C(23)	6045(2)	396.6(18)	3500(3)	65.0(7)
C(24)	7431.5(17)	2089.1(15)	3512(2)	45.1(6)
C(25)	8333.2(17)	1834.4(17)	3000(2)	54.1(6)
C(26)	9157(2)	1694(2)	3683(3)	70.5(8)
C(27)	9101(2)	1808(2)	4873(3)	79.6(9)
C(28)	8220(3)	2082(2)	5384(3)	80.0(9)
C(29)	7400(2)	2226(2)	4702(2)	63.5(7)
H(2A)	5962	2904	178	80
H(5A)	6635	814	1950	80
H(6A)	5979	2424	3299	80
H(10A)	8530	4314	2577	80
H(11A)	8852	5337	4205	80
H(12A)	7541	5881	5366	80
H(13A)	5955	5303	5030	80
H(14A)	5631	4289	3424	80
H(16A)	5975	605	-522	80
H(17A)	7087	-188	-1784	80
H(18A)	8678	472	-2072	80
H(19A)	9123	1934	-1129	80
H(20A)	8017	2735	102	80
H(21A)	3792	1662	482	80

H(21B)	4176	2752	346	80
H(21C)	4460	1950	-588	80
H(23A)	5848	-251	3240	80
H(23B)	6669	353	3898	80
H(23C)	5553	656	4024	80
H(25A)	8377	1768	2165	80
H(26A)	9768	1492	3325	80
H(27A)	9683	1714	5344	80
H(28A)	8184	2173	6217	80
H(29A)	6785	2417	5060	80

Table 95: Bond lengths [Å], bond angles and torsion angles [°] for *rac*-20.

N(1)-C(7)	1.360(3)	N(1)-C(2)	1.469(3)
N(1)-C(6)	1.481(3)	C(2)-N(3)	1.454(3)
C(2)-C(15)	1.522(3)	N(3)-C(4)	1.345(3)
N(3)-C(21)	1.456(3)	C(4)-O(22)	1.222(3)
C(4)-C(5)	1.517(3)	C(5)-C(23)	1.505(3)
C(5)-C(6)	1.548(3)	C(6)-C(24)	1.510(3)
C(7)-O(8)	1.229(3)	C(7)-C(9)	1.493(4)
C(9)-C(14)	1.369(4)	C(9)-C(10)	1.376(4)
C(10)-C(11)	1.395(5)	C(11)-C(12)	1.362(4)
C(12)-C(13)	1.349(4)	C(13)-C(14)	1.374(4)
C(15)-C(16)	1.384(3)	C(15)-C(20)	1.387(3)
C(16)-C(17)	1.378(4)	C(17)-C(18)	1.381(4)
C(18)-C(19)	1.370(4)	C(19)-C(20)	1.373(3)
C(24)-C(29)	1.373(4)	C(24)-C(25)	1.393(3)
C(25)-C(26)	1.371(4)	C(26)-C(27)	1.370(4)
C(27)-C(28)	1.376(5)	C(28)-C(29)	1.368(4)
C(7)-N(1)-C(2)	116.67(19)	C(7)-N(1)-C(6)	123.6(2)
C(2)-N(1)-C(6)	118.68(16)	N(3)-C(2)-N(1)	109.54(18)
N(3)-C(2)-C(15)	114.59(18)	N(1)-C(2)-C(15)	113.79(18)
C(4)-N(3)-C(2)	119.90(19)	C(4)-N(3)-C(21)	120.9(2)
C(2)-N(3)-C(21)	119.0(2)	O(22)-C(4)-N(3)	122.6(2)
O(22)-C(4)-C(5)	123.4(2)	N(3)-C(4)-C(5)	113.91(19)
C(23)-C(5)-C(4)	111.9(2)	C(23)-C(5)-C(6)	113.1(2)
C(4)-C(5)-C(6)	108.00(18)	N(1)-C(6)-C(24)	114.21(17)
N(1)-C(6)-C(5)	108.13(18)	C(24)-C(6)-C(5)	110.21(18)
O(8)-C(7)-N(1)	120.9(2)	O(8)-C(7)-C(9)	119.27(19)
N(1)-C(7)-C(9)	119.9(2)	C(14)-C(9)-C(10)	119.6(2)
C(14)-C(9)-C(7)	120.4(2)	C(10)-C(9)-C(7)	119.5(2)
C(9)-C(10)-C(11)	119.5(3)	C(12)-C(11)-C(10)	119.6(3)
C(13)-C(12)-C(11)	120.7(3)	C(12)-C(13)-C(14)	120.4(3)

C(9)-C(14)-C(13)	120.2(3)	C(16)-C(15)-C(20)	118.2(2)
C(16)-C(15)-C(2)	122.0(2)	C(20)-C(15)-C(2)	119.45(19)
C(17)-C(16)-C(15)	120.9(2)	C(16)-C(17)-C(18)	120.2(2)
C(19)-C(18)-C(17)	119.3(3)	C(18)-C(19)-C(20)	120.7(2)
C(19)-C(20)-C(15)	120.8(2)	C(29)-C(24)-C(25)	118.4(2)
C(29)-C(24)-C(6)	119.5(2)	C(25)-C(24)-C(6)	121.9(2)
C(26)-C(25)-C(24)	120.3(3)	C(27)-C(26)-C(25)	120.3(3)
C(26)-C(27)-C(28)	119.9(3)	C(29)-C(28)-C(27)	119.7(3)
C(28)-C(29)-C(24)	121.3(3)		

C(7)-N(1)-C(2)-N(3)	-129.9(2)	C(14)-C(9)-C(10)-C(11)	-1.7(4)
C(6)-N(1)-C(2)-N(3)	38.6(3)	C(7)-C(9)-C(10)-C(11)	170.6(2)
C(7)-N(1)-C(2)-C(15)	100.4(2)	C(9)-C(10)-C(11)-C(12)	-0.5(4)
C(6)-N(1)-C(2)-C(15)	-91.1(2)	C(10)-C(11)-C(12)-C(13)	1.8(5)
N(1)-C(2)-N(3)-C(4)	-46.9(3)	C(11)-C(12)-C(13)-C(14)	-1.0(5)
C(15)-C(2)-N(3)-C(4)	82.4(3)	C(10)-C(9)-C(14)-C(13)	2.6(4)
N(1)-C(2)-N(3)-C(21)	128.1(2)	C(7)-C(9)-C(14)-C(13)	-169.7(2)
C(15)-C(2)-N(3)-C(21)	-102.7(2)	C(12)-C(13)-C(14)-C(9)	-1.2(4)
C(2)-N(3)-C(4)-O(22)	179.2(2)	N(3)-C(2)-C(15)-C(16)	13.0(3)
C(21)-N(3)-C(4)-O(22)	4.4(4)	N(1)-C(2)-C(15)-C(16)	140.1(2)
C(2)-N(3)-C(4)-C(5)	1.0(3)	N(3)-C(2)-C(15)-C(20)	-173.8(2)
C(21)-N(3)-C(4)-C(5)	-173.8(2)	N(1)-C(2)-C(15)-C(20)	-46.6(3)
O(22)-C(4)-C(5)-C(23)	-1.3(3)	C(20)-C(15)-C(16)-C(17)	0.8(3)
N(3)-C(4)-C(5)-C(23)	176.9(2)	C(2)-C(15)-C(16)-C(17)	174.2(2)
O(22)-C(4)-C(5)-C(6)	-126.5(2)	C(15)-C(16)-C(17)-C(18)	-0.4(4)
N(3)-C(4)-C(5)-C(6)	51.7(3)	C(16)-C(17)-C(18)-C(19)	0.1(4)
C(7)-N(1)-C(6)-C(24)	-58.2(3)	C(17)-C(18)-C(19)-C(20)	-0.3(4)
C(2)-N(1)-C(6)-C(24)	134.2(2)	C(18)-C(19)-C(20)-C(15)	0.8(4)
C(7)-N(1)-C(6)-C(5)	178.8(2)	C(16)-C(15)-C(20)-C(19)	-1.1(3)
C(2)-N(1)-C(6)-C(5)	11.2(2)	C(2)-C(15)-C(20)-C(19)	-174.6(2)
C(23)-C(5)-C(6)-N(1)	179.9(2)	N(1)-C(6)-C(24)-C(29)	134.1(2)
C(4)-C(5)-C(6)-N(1)	-55.7(2)	C(5)-C(6)-C(24)-C(29)	-104.0(2)
C(23)-C(5)-C(6)-C(24)	54.4(3)	N(1)-C(6)-C(24)-C(25)	-50.8(3)
C(4)-C(5)-C(6)-C(24)	178.9(2)	C(5)-C(6)-C(24)-C(25)	71.1(3)
C(2)-N(1)-C(7)-O(8)	-11.6(3)	C(29)-C(24)-C(25)-C(26)	2.1(3)
C(6)-N(1)-C(7)-O(8)	-179.5(2)	C(6)-C(24)-C(25)-C(26)	-173.0(2)
C(2)-N(1)-C(7)-C(9)	167.3(2)	C(24)-C(25)-C(26)-C(27)	-0.4(4)
C(6)-N(1)-C(7)-C(9)	-0.6(3)	C(25)-C(26)-C(27)-C(28)	-1.2(5)
O(8)-C(7)-C(9)-C(14)	103.2(3)	C(26)-C(27)-C(28)-C(29)	0.9(5)
N(1)-C(7)-C(9)-C(14)	-75.8(3)	C(27)-C(28)-C(29)-C(24)	1.0(4)
O(8)-C(7)-C(9)-C(10)	-69.1(3)	C(25)-C(24)-C(29)-C(28)	-2.5(4)
N(1)-C(7)-C(9)-C(10)	112.0(3)	C(6)-C(24)-C(29)-C(28)	172.8(2)

Table 96: Anisotropic displacement parameters [Å^2 x 10^3] for *rac*-20.

	U11	U22	U33	U23	U13	U12
N(1)	46.6(10)	33.8(10)	48.5(11)	1.3(9)	0.6(9)	-1.5(8)
C(2)	44.1(13)	41.8(12)	51.3(14)	1.9(11)	-5.9(11)	-4.7(11)
N(3)	38.0(10)	51.1(11)	65.2(14)	-2.1(11)	-3.0(10)	-0.5(9)
C(4)	46.8(15)	42.1(13)	73.1(17)	-5.0(14)	5.5(13)	-5.1(12)
C(5)	45.5(13)	37.7(12)	60.1(15)	2.2(11)	6.3(12)	-3.4(10)
C(6)	45.1(13)	39.8(12)	47.8(14)	2.9(11)	8.3(11)	-1.5(10)
C(7)	61.2(15)	35.8(12)	55.9(15)	-0.3(13)	6.0(12)	-1.7(11)
O(8)	125.0(17)	41.6(10)	59.1(12)	4.1(9)	9.7(12)	-8.5(10)
C(9)	58.3(15)	34.4(12)	55.8(15)	1.8(12)	1.2(13)	-2.8(11)
C(10)	61.0(17)	49.2(15)	86(2)	2.7(15)	-2.7(15)	-5.8(13)
C(11)	77(2)	68.1(19)	92(2)	17.2(19)	-34(2)	-21.3(16)
C(12)	114(3)	62.9(18)	58.5(18)	-6.7(15)	-18.6(19)	-19.9(19)
C(13)	103(2)	63.5(18)	65(2)	-14.2(16)	10.2(18)	-8.7(17)
C(14)	61.7(16)	54.6(15)	64.3(17)	-12.1(14)	1.9(15)	-8.4(12)
C(15)	42.8(13)	39.8(13)	42.6(13)	2.5(10)	-5.3(11)	0.4(11)
C(16)	51.9(13)	45.2(14)	59.1(15)	-2.4(13)	-7.7(13)	-5.0(11)
C(17)	73.6(19)	53.8(15)	62.3(16)	-16.6(14)	-7.3(15)	6.1(14)
C(18)	63.1(17)	73.0(18)	54.7(16)	-10.2(15)	1.6(14)	8.2(14)
C(19)	50.1(14)	73.2(18)	53.1(15)	-2.2(14)	0.6(13)	-3.6(14)
C(20)	52.2(15)	50.4(14)	48.2(14)	-5.3(12)	-0.1(12)	-6.2(12)
C(21)	47.4(15)	79.8(19)	85(2)	-1.6(17)	-5.7(15)	3.7(13)
O(22)	50.0(11)	66.6(11)	118.3(18)	7.7(12)	5.7(11)	-19.6(10)
C(23)	74.5(17)	49.2(14)	71.1(18)	5.7(14)	12.4(15)	-9.9(13)
C(24)	45.4(14)	39.2(12)	50.8(15)	6.2(11)	2.4(11)	-3.5(10)
C(25)	48.7(15)	53.6(15)	59.9(16)	7.7(12)	2.5(13)	-3.8(11)
C(26)	47.9(16)	72.8(18)	91(2)	7.2(17)	-6.5(16)	-0.4(13)
C(27)	67(2)	90(2)	81(2)	16.6(18)	-25.1(18)	-9.6(18)
C(28)	84(2)	101(2)	55.0(18)	6.8(17)	-11.5(18)	-12.7(19)
C(29)	66.9(18)	70.5(18)	53.2(17)	2.7(13)	3.0(14)	-9.0(15)

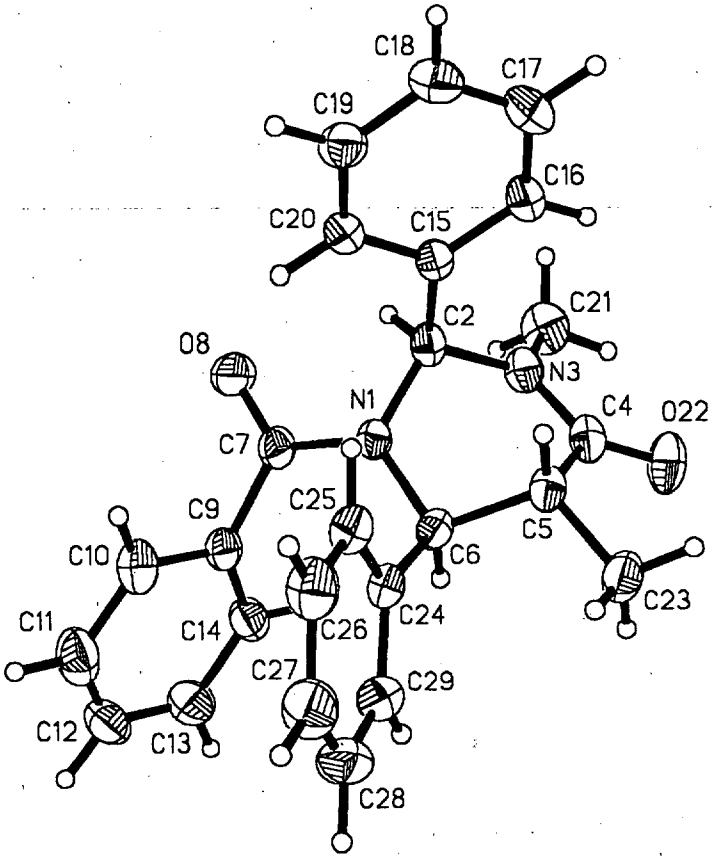

Figure 39. Thermal ellipsoid figure for compound *rac*-20.

Compound *rac*-**18**.

CSD REFCODE = **JOPZET** ; SPACE GRP. IS PBCA

Unit cell:

a =	20.712 Å	α =	90.00°
b =	15.076 Å	β =	90.00°
c =	10.807 Å	γ =	90.00°

Table 97: Atomic coordinates for *rac*-18.

Atom	x	y	z
N(1)	0.4572(1)	0.0908(1)	0.2002(2)
C(2)	0.3982(1)	0.0376(2)	0.1831(3)
N(3)	0.3511(1)	0.0887(2)	0.1106(2)
C(4)	0.3456(1)	0.1774(2)	0.1178(3)
C(5)	0.3837(1)	0.2216(2)	0.2199(3)
C(6)	0.4534(1)	0.1870(2)	0.2283(3)
C(7)	0.5135(1)	0.0513(2)	0.1657(3)
O(8)	0.5175(1)	-0.0277(1)	0.1382(2)
C(9)	0.5740(1)	0.1061(2)	0.1632(3)
C(10)	0.6198(2)	0.0960(2)	0.2549(3)
C(11)	0.6777(2)	0.1406(3)	0.2475(4)
C(12)	0.6908(2)	0.1941(3)	0.1480(5)
C(13)	0.6463(2)	0.2039(2)	0.0556(4)
C(14)	0.5878(2)	0.1605(2)	0.0639(3)
C(15)	0.3713(1)	-0.0085(2)	0.3009(3)
C(16)	0.4254(2)	-0.0652(3)	0.3568(5)
C(17)	0.3164(2)	-0.0703(3)	0.2610(4)
C(18)	0.3447(2)	0.0532(3)	0.3991(4)
C(19)	0.3207(2)	0.0451(3)	0.0048(4)
O(20)	0.3112(1)	0.2193(1)	0.0470(2)
C(21)	0.3825(2)	0.3222(2)	0.2057(5)
C(22)	0.4831(2)	0.2108(3)	0.3525(4)
H(2A)	0.411(1)	-0.012(1)	0.131(2)
H(5A)	0.361(1)	0.204(1)	0.302(2)
H(6A)	0.478(1)	0.215(1)	0.164(2)
H(10A)	0.611(1)	0.053(2)	0.318(2)
H(11A)	0.707(2)	0.130(2)	0.316(3)
H(12A)	0.730(1)	0.224(2)	0.147(3)
H(13A)	0.653(1)	0.244(2)	-0.020(3)
H(14A)	0.557(1)	0.167(2)	0.004(3)
H(16A)	0.459(1)	-0.023(2)	0.392(3)

H(16B)	0.443(2)	-0.113(3)	0.298(3)
H(16C)	0.408(1)	-0.101(2)	0.424(3)
H(17A)	0.331(1)	-0.116(2)	0.194(3)
H(17B)	0.277(1)	-0.038(2)	0.227(3)
H(17C)	0.306(2)	-0.107(2)	0.330(3)
H(18A)	0.378(1)	0.096(2)	0.434(3)
H(18B)	0.328(1)	0.015(2)	0.467(3)
H(18C)	0.308(1)	0.092(2)	0.370(3)
H(19A)	0.319(1)	-0.016(2)	0.010(3)
H(19B)	0.340(2)	0.056(3)	-0.061(4)
H(19C)	0.276(2)	0.060(3)	0.002(4)
H(21A)	0.403(2)	0.355(2)	0.273(3)
H(21B)	0.336(1)	0.342(2)	0.194(3)
H(21C)	0.406(2)	0.339(3)	0.136(3)
H(22A)	0.533(2)	0.208(2)	0.355(3)
H(22B)	0.466(2)	0.172(2)	0.416(3)
H(22C)	0.481(2)	0.275(2)	0.371(3)

Table 98: Bond lengths [Å], bond angles and torsion angles [°] for *rac*-19.

N(1)-C(2)	1.473(3)	C(7)-O(8)	1.230(3)
N(1)-C(6)	1.484(3)	C(7)-C(9)	1.501(3)
N(1)-C(7)	1.361(3)	C(9)-C(10)	1.380(5)
C(2)-N(3)	1.469(4)	C(9)-C(14)	1.381(4)
C(2)-C(15)	1.554(4)	C(10)-C(11)	1.377(6)
N(3)-C(4)	1.344(4)	C(11)-C(12)	1.371(7)
N(3)-C(19)	1.461(5)	C(12)-C(13)	1.367(6)
C(4)-C(5)	1.511(4)	C(13)-C(14)	1.380(6)
C(4)-O(20)	1.222(3)	C(15)-C(16)	1.533(5)
C(5)-C(6)	1.538(3)	C(15)-C(17)	1.532(5)
C(5)-C(21)	1.525(4)	C(15)-C(18)	1.515(5)
C(6)-C(22)	1.519(5)		
C(2)-N(1)-C(6)	120.9(4)	N(1)-C(7)-O(8)	123.2(4)
C(2)-N(1)-C(7)	116.0(4)	N(1)-C(7)-C(9)	118.6(4)
C(6)-N(1)-C(7)	121.9(4)	O(8)-C(7)-C(9)	118.2(4)
N(1)-C(2)-N(3)	109.4(4)	C(7)-C(9)-C(10)	120.0(5)
N(1)-C(2)-C(15)	116.0(4)	C(7)-C(9)-C(14)	120.9(5)
N(3)-C(2)-C(15)	115.7(4)	C(10)-C(9)-C(14)	118.8(5)
C(2)-N(3)-C(4)	123.2(4)	C(9)-C(10)-C(11)	120.2(6)
C(2)-N(3)-C(19)	117.9(5)	C(10)-C(11)-C(12)	120.3(7)
C(4)-N(3)-C(19)	117.1(5)	C(11)-C(12)-C(13)	120.2(7)
N(3)-C(4)-C(5)	115.9(4)	C(12)-C(13)-C(14)	119.6(6)
N(3)-C(4)-O(20)	121.8(5)	C(9)-C(14)-C(13)	120.9(6)

C(5)-C(4)-O(20)	122.3(4)	C(2)-C(15)-C(16)	108.1(5)
C(4)-C(5)-C(6)	112.6(4)	C(2)-C(15)-C(17)	107.9(4)
C(4)-C(5)-C(21)	110.9(5)	C(2)-C(15)-C(18)	115.5(5)
C(6)-C(5)-C(21)	111.0(4)	C(16)-C(15)-C(17)	108.3(5)
N(1)-C(6)-C(5)	111.7(4)	C(16)-C(15)-C(18)	109.4(5)
N(1)-C(6)-C(22)	113.0(4)	C(17)-C(15)-C(18)	107.5(5)
C(5)-C(6)-C(22)	110.6(5)		
C(4)-N(3)-C(2)-N(1)	-33.3(4)	C(14)-C(13)-C(12)-C(11)	0.8(7)
C(4)-C(5)-C(6)-N(1)	-36.0(4)	C(15)-C(2)-N(1)-C(6)	-91.9(4)
C(5)-C(4)-N(3)-C(2)	-9.2(4)	C(15)-C(2)-N(1)-C(7)	100.3(5)
C(5)-C(6)-N(1)-C(2)	-7.1(4)	C(15)-C(2)-N(3)-C(4)	99.9(5)
C(6)-N(1)-C(2)-N(3)	41.2(4)	C(16)-C(15)-C(2)-N(1)	-55.2(4)
C(6)-C(5)-C(4)-N(3)	45.6(4)	C(16)-C(15)-C(2)-N(3)	174.7(5)
C(7)-N(1)-C(2)-N(3)	-126.7(4)	C(17)-C(15)-C(2)-N(1)	-172.1(5)
C(7)-N(1)-C(6)-C(5)	160.0(5)	C(17)-C(15)-C(2)-N(3)	57.8(4)
O(8)-C(7)-N(1)-C(2)	-9.9(4)	C(18)-C(15)-C(2)-N(1)	67.6(5)
O(8)-C(7)-N(1)-C(6)	-177.7(6)	C(18)-C(15)-C(2)-N(3)	-62.5(5)
C(9)-C(7)-N(1)-C(2)	171.2(6)	C(19)-N(3)-C(2)-N(1)	130.8(5)
C(9)-C(7)-N(1)-C(6)	3.5(4)	C(19)-N(3)-C(2)-C(15)	-96.0(5)
C(10)-C(9)-C(7)-N(1)	105.3(5)	C(19)-N(3)-C(4)-C(5)	-173.4(6)
C(10)-C(9)-C(7)-O(8)	-73.6(5)	O(20)-C(4)-N(3)-C(2)	171.8(6)
C(11)-C(10)-C(9)-C(7)	174.6(7)	O(20)-C(4)-N(3)-C(19)	7.5(5)
C(12)-C(11)-C(10)-C(9)	-1.2(7)	O(20)-C(4)-C(5)-C(6)	-135.3(6)
C(12)-C(13)-C(14)-C(9)	-1.1(6)	C(21)-C(5)-C(4)-N(3)	170.7(5)
C(13)-C(12)-C(11)-C(10)	0.3(7)	C(21)-C(5)-C(4)-O(20)	-10.3(5)
C(13)-C(14)-C(9)-C(7)	-173.4(7)	C(21)-C(5)-C(6)-N(1)	-161.0(5)
C(13)-C(14)-C(9)-C(10)	0.3(6)	C(22)-C(6)-N(1)-C(2)	118.3(5)
C(14)-C(9)-C(7)-N(1)	-81.2(5)	C(22)-C(6)-N(1)-C(7)	-74.6(5)
C(14)-C(9)-C(7)-O(8)	100.0(5)	C(22)-C(6)-C(5)-C(4)	-162.7(5)
C(14)-C(9)-C(10)-C(11)	0.9(6)	C(22)-C(6)-C(5)-C(21)	72.3(5)

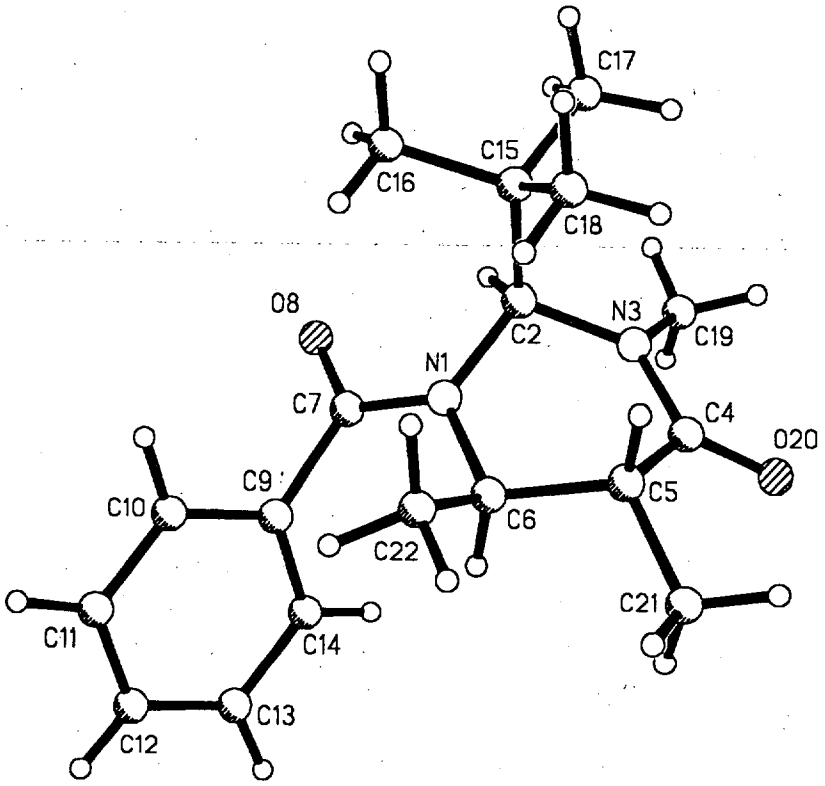

Figure 40. Structure and solid-state conformation of *rac*-18.

Compound *rac*-**19**.

CSD REFCODE = **JOPZIX** ; SPACE GRP. IS P21/C

Unit cell:

a =	8.311 Å	α =	90.00°
b =	22.648 Å	β =	105.48°
c =	11.782 Å	γ =	90.00°

Table 99: Atomic coordinates for *rac*-19.

Atom	x	y	z
N(1)	0.4595(3)	0.0861(1)	0.7393(2)
C(2)	0.5803(3)	0.0611(1)	0.8427(3)
N(3)	0.6554(3)	0.1103(1)	0.9210(2)
C(4)	0.6874(4)	0.1636(1)	0.8814(3)
C(5)	0.6525(4)	0.1718(1)	0.7481(3)
C(6)	0.5048(4)	0.1363(1)	0.6730(2)
C(7)	0.3003(4)	0.0655(1)	0.7150(3)
O(8)	0.2607(3)	0.0234(1)	0.7674(2)
C(9)	0.1694(4)	0.0940(1)	0.6170(3)
C(10)	0.1095(4)	0.0636(2)	0.5114(3)
C(11)	-0.0175(5)	0.0860(2)	0.4228(4)
C(12)	-0.0901(5)	0.1383(2)	0.4368(4)
C(13)	-0.0336(5)	0.1698(2)	0.5400(5)
C(14)	0.0975(4)	0.1473(2)	0.6316(3)
C(15)	0.7053(4)	0.0151(1)	0.8183(3)
C(16)	0.6123(5)	-0.0266(2)	0.7202(3)
C(17)	0.7711(5)	-0.0218(2)	0.9317(3)
C(18)	0.8565(4)	0.0417(2)	0.7866(3)
C(19)	0.6891(6)	0.1021(2)	1.0480(3)
O(20)	0.7490(3)	0.2034(1)	0.9498(2)
C(21)	0.6360(5)	0.2379(2)	0.7131(3)
C(22)	0.4707(5)	0.2657(1)	0.7079(3)
C(23)	0.3608(6)	0.2836(2)	0.6018(3)
C(24)	0.2060(7)	0.3062(2)	0.5962(4)
C(25)	0.1556(7)	0.3125(2)	0.6966(5)
C(26)	0.2608(7)	0.2968(2)	0.8023(4)
C(27)	0.4149(6)	0.2731(2)	0.8082(3)
C(28)	0.5355(5)	0.1176(2)	0.5565(3)
H(2A)	0.5080(5)	0.0390(2)	0.887(4)
H(5A)	0.7540(5)	0.1590(2)	0.733(4)
H(6A)	0.4100(5)	0.1640(2)	0.660(3)
H(10A)	0.1650(5)	0.0260(2)	0.512(4)

H(11A)	-0.0630(5)	0.0630(2)	0.346(4)
H(12A)	-0.1870(5)	0.1590(2)	0.383(4)
H(13A)	-0.0760(5)	0.2080(2)	0.562(4)
H(14A)	0.1330(5)	0.1700(2)	0.706(3)
H(16A)	0.5651	-0.0018	0.6399
H(16B)	0.5095	-0.0470	0.7453
H(16C)	0.6969	-0.0603	0.7062
H(17A)	0.6671	-0.0413	0.9568
H(17B)	0.8400	0.0064	1.0018
H(17C)	0.8521	-0.0563	0.9157
H(18A)	0.8150	0.0679	0.7076
H(18B)	0.9368	0.0067	0.7719
H(18C)	0.9247	0.0694	0.8580
H(19A)	0.802(6)	0.095(2)	1.083(4)
H(19B)	0.647(5)	0.062(2)	1.067(3)
H(19C)	0.635(5)	0.138(2)	1.080(3)
H(21A)	0.657(5)	0.244(2)	0.636(4)
H(21B)	0.736(5)	0.260(2)	0.772(4)
H(23A)	0.412(5)	0.274(2)	0.535(4)
H(24A)	0.138(5)	0.315(2)	0.519(4)
H(25A)	0.040(5)	0.323(2)	0.697(4)
H(26A)	0.213(5)	0.298(2)	0.881(4)
H(27A)	0.500(5)	0.262(2)	0.881(4)
H(28A)	0.633(6)	0.085(2)	0.572(4)
H(28B)	0.552(5)	0.153(2)	0.510(4)
H(28C)	0.447(6)	0.104(2)	0.506(4)

Table 100: Bond lengths [Å], bond angles and torsion angles [°] for *rac*-19.

N(1)-C(2)	1.470(4)	C(9)-C(14)	1.378(5)
N(1)-C(6)	1.484(3)	C(10)-C(11)	1.369(5)
N(1)-C(7)	1.359(3)	C(11)-C(12)	1.359(6)
C(2)-N(3)	1.475(4)	C(12)-C(13)	1.380(7)
C(2)-C(15)	1.551(3)	C(13)-C(14)	1.409(6)
N(3)-C(4)	1.346(3)	C(15)-C(16)	1.532(5)
N(3)-C(19)	1.459(4)	C(15)-C(17)	1.547(5)
C(4)-C(5)	1.530(5)	C(15)-C(18)	1.527(4)
C(4)-O(20)	1.226(4)	C(21)-C(22)	1.498(5)
C(5)-C(6)	1.535(4)	C(22)-C(23)	1.397(5)
C(5)-C(21)	1.549(5)	C(22)-C(27)	1.390(5)
C(6)-C(28)	1.522(4)	C(23)-C(24)	1.370(6)
C(7)-O(8)	1.228(3)	C(24)-C(25)	1.364(7)
C(7)-C(9)	1.504(4)	C(25)-C(26)	1.364(7)
C(9)-C(10)	1.393(5)	C(26)-C(27)	1.373(6)

C(2)-N(1)-C(6)	121.2(3)	C(7)-C(9)-C(14)	121.9(5)
C(2)-N(1)-C(7)	117.0(4)	C(10)-C(9)-C(14)	118.8(5)
C(6)-N(1)-C(7)	121.4(4)	C(9)-C(10)-C(11)	121.1(6)
N(1)-C(2)-N(3)	108.0(3)	C(10)-C(11)-C(12)	120.5(6)
N(1)-C(2)-C(15)	116.6(4)	C(11)-C(12)-C(13)	120.0(7)
N(3)-C(2)-C(15)	115.5(4)	C(12)-C(13)-C(14)	120.0(7)
C(2)-N(3)-C(4)	123.4(4)	C(9)-C(14)-C(13)	119.6(6)
C(2)-N(3)-C(19)	118.6(4)	C(2)-C(15)-C(16)	109.0(4)
C(4)-N(3)-C(19)	117.9(4)	C(2)-C(15)-C(17)	107.6(4)
N(3)-C(4)-C(5)	117.6(4)	C(2)-C(15)-C(18)	114.6(4)
N(3)-C(4)-O(20)	121.2(4)	C(16)-C(15)-C(17)	108.0(4)
C(5)-C(4)-O(20)	121.1(4)	C(16)-C(15)-C(18)	109.9(4)
C(4)-C(5)-C(6)	115.6(4)	C(17)-C(15)-C(18)	107.5(4)
C(4)-C(5)-C(21)	111.7(4)	C(5)-C(21)-C(22)	115.6(5)
C(6)-C(5)-C(21)	110.6(4)	C(21)-C(22)-C(23)	122.2(5)
N(1)-C(6)-C(5)	112.0(3)	C(21)-C(22)-C(27)	121.8(5)
N(1)-C(6)-C(28)	112.9(4)	C(23)-C(22)-C(27)	116.0(5)
C(5)-C(6)-C(28)	111.4(4)	C(22)-C(23)-C(24)	122.2(6)
N(1)-C(7)-O(8)	122.5(4)	C(23)-C(24)-C(25)	120.0(7)
N(1)-C(7)-C(9)	118.6(4)	C(24)-C(25)-C(26)	119.6(8)
O(8)-C(7)-C(9)	118.9(4)	C(25)-C(26)-C(27)	120.7(7)
C(7)-C(9)-C(10)	119.1(4)	C(22)-C(27)-C(26)	121.5(6)

C(4)-N(3)-C(2)-N(1)	-35.2(4)	C(17)-C(15)-C(2)-N(1)	-158.8(5)
C(4)-C(5)-C(6)-N(1)	-19.3(4)	C(17)-C(15)-C(2)-N(3)	72.7(4)
C(5)-C(4)-N(3)-C(2)	-3.6(4)	C(18)-C(15)-C(2)-N(1)	81.8(4)
C(5)-C(6)-N(1)-C(2)	-22.2(3)	C(18)-C(15)-C(2)-N(3)	-46.7(4)
C(6)-N(1)-C(2)-N(3)	48.9(4)	C(19)-N(3)-C(2)-N(1)	141.5(5)
C(6)-C(5)-C(4)-N(3)	32.9(4)	C(19)-N(3)-C(2)-C(15)	-85.9(5)
C(7)-N(1)-C(2)-N(3)	-124.2(4)	C(19)-N(3)-C(4)-C(5)	179.7(5)
C(7)-N(1)-C(6)-C(5)	150.6(5)	O(20)-C(4)-N(3)-C(2)	179.5(6)
O(8)-C(7)-N(1)-C(2)	-8.1(4)	O(20)-C(4)-N(3)-C(19)	2.8(5)
O(8)-C(7)-N(1)-C(6)	178.7(6)	O(20)-C(4)-C(5)-C(6)	-150.2(5)
C(9)-C(7)-N(1)-C(2)	174.3(5)	C(21)-C(5)-C(4)-N(3)	160.5(5)
C(9)-C(7)-N(1)-C(6)	1.1(4)	C(21)-C(5)-C(4)-O(20)	-22.6(4)
C(10)-C(9)-C(7)-N(1)	106.7(5)	C(21)-C(5)-C(6)-N(1)	-147.5(5)
C(10)-C(9)-C(7)-O(8)	-70.9(5)	C(22)-C(21)-C(5)-C(4)	-80.0(5)
C(11)-C(10)-C(9)-C(7)	175.5(7)	C(22)-C(21)-C(5)-C(6)	50.3(5)
C(12)-C(11)-C(10)-C(9)	-1.0(6)	C(23)-C(22)-C(21)-C(5)	-111.4(6)
C(12)-C(13)-C(14)-C(9)	0.5(6)	C(24)-C(23)-C(22)-C(21)	176.5(9)
C(13)-C(12)-C(11)-C(10)	1.3(7)	C(25)-C(24)-C(23)-C(22)	0.8(7)
C(13)-C(14)-C(9)-C(7)	-175.1(7)	C(25)-C(26)-C(27)-C(22)	1.7(7)
C(13)-C(14)-C(9)-C(10)	-0.2(6)	C(26)-C(25)-C(24)-C(23)	0.7(7)
C(14)-C(9)-C(7)-N(1)	-78.4(5)	C(26)-C(27)-C(22)-C(21)	-177.8(9)
C(14)-C(9)-C(7)-O(8)	103.9(5)	C(26)-C(27)-C(22)-C(23)	-0.2(7)
C(14)-C(9)-C(10)-C(11)	0.5(6)	C(27)-C(22)-C(21)-C(5)	66.0(6)

C(14)-C(13)-C(12)-C(11)	-1.0(7)	C(27)-C(22)-C(23)-C(24)	-1.1(6)
C(15)-C(2)-N(1)-C(6)	-83.1(4)	C(27)-C(26)-C(25)-C(24)	-1.9(8)
C(15)-C(2)-N(1)-C(7)	103.8(4)	C(28)-C(6)-N(1)-C(2)	104.5(4)
C(15)-C(2)-N(3)-C(4)	97.4(4)	C(28)-C(6)-N(1)-C(7)	-82.7(4)
C(16)-C(15)-C(2)-N(1)	-41.9(4)	C(28)-C(6)-C(5)-C(4)	-146.8(5)
C(16)-C(15)-C(2)-N(3)	-170.4(5)	C(28)-C(6)-C(5)-C(21)	85.0(5)

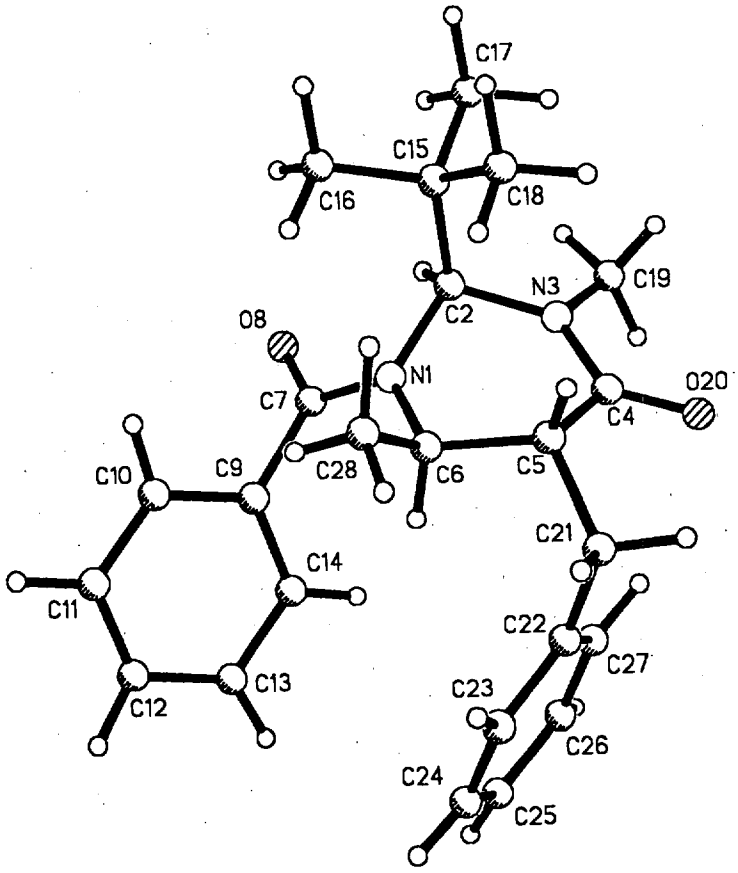

Figure 41. Structure and solid-state conformation of *rac*-19