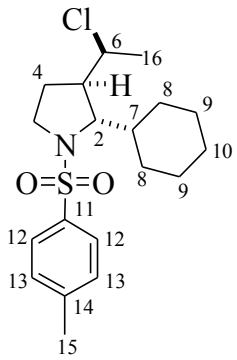
APPENDIX: X-ray Data

X-Ray data for (2*S*,3*R*)-3-((*S*)-1-chloroethyl)-2-cyclohexyl-1-tosylpyrrolidine and (2*R*,3*S*)-3-((*R*)-1-chloroethyl)-2-cyclohexyl-1-tosylpyrrolidine (119d).



$C_{19}H_{28}ClNO_2S$
Mol. Wt.: 369.95

Table 1. Crystal data and structure refinement details.

Identification code	**src1366**	
Empirical formula	C19 H28 Cl N O2 S	
Formula weight	369.93	
Temperature	120(2) K	
Wavelength	0.71073 A	
Crystal system	orthorhombic	
space group	P 21 21 21	
Unit cell dimensions	a = 9.5925(3) A	α = 90 deg.
	b = 12.9908(3) A	β = 90 deg.
	c = 15.0216(4) A	γ = 90 deg.
Volume	1871.91(9) A^3	
Z	4	
Calculated density	1.313 Mg/m^3	
Absorption coefficient	0.327 mm^-1	
F(000)	792	
Crystal size	0.52 x 0.42 x 0.08 mm	
Theta range for data collection	2.97 to 27.50 deg.	
Limiting indices	-10<=h<=12, -16<=k<=16, -19<=l<=19	
Reflections collected	16779	
unique	4283 [R(int) = 0.0484]	
Completeness to theta = 27.50	99.8 %	
Absorption correction	None	
Max. and min. transmission	0.9743 and 0.8483	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4283 / 0 / 217	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0381, wR2 = 0.0849	
R indices (all data)	R1 = 0.0521, wR2 = 0.0909	
Absolute structure parameter	0.25(6)	

Largest diff. peak and hole	0.233 and -0.377 e.A^-3

Diffractometer: *Bruker-Nonius APEX II* CCD camera (ϕ scans and ω scans to fill *asymmetric unit*). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: Sheldrick, G. M. SADABS 2007/2 - Bruker Nonius area detector scaling and absorption correction. **Structure solution**: *Sir2004* (Burla, M.C., Caliandro, R., Carrozzini, B., Cascarano, G., De Caro, L., Giacovazzo, C. & Polidori, G. (2004). J. Appl. Cryst. 37, 258). **Structure refinement**: *SHELXL97* (Sheldrick, G. M. (1997). University of Göttingen, Germany). **Graphics:** *PLATON/PLUTON* (Spek, A. L. (1990). Acta Cryst. A46, C34).

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
S(1)	7499(1)	4916(1)	6844(1)	16(1)	1
O(1)	8793(2)	4496(1)	7149(1)	21(1)	1
O(2)	6206(2)	4487(1)	7146(1)	23(1)	1
Cl(1)	9217(1)	7605(1)	4914(1)	29(1)	1
C(1)	7508(3)	6233(1)	7127(1)	16(1)	1
C(2)	6276(2)	6791(2)	7078(1)	19(1)	1
C(3)	6298(2)	7831(2)	7281(2)	21(1)	1
C(4)	7524(3)	8314(2)	7548(1)	21(1)	1
C(5)	8735(2)	7733(2)	7601(2)	22(1)	1
C(6)	8731(2)	6701(2)	7387(1)	19(1)	1
C(7)	7525(3)	9446(2)	7779(2)	28(1)	1
N(1)	7484(2)	4822(1)	5768(1)	16(1)	1
C(8)	6153(2)	5005(2)	5302(1)	19(1)	1
C(9)	6617(2)	5175(2)	4345(2)	21(1)	1
C(10)	7996(2)	5765(2)	4445(2)	17(1)	1
C(11)	8684(2)	5269(2)	5265(1)	17(1)	1
C(12)	7685(2)	6919(1)	4545(1)	17(1)	1
C(13)	9797(2)	4458(2)	5072(2)	19(1)	1
C(14)	11117(2)	4944(2)	4696(2)	25(1)	1
C(15)	12273(3)	4151(2)	4560(2)	33(1)	1
C(16)	11776(3)	3257(2)	3983(2)	33(1)	1
C(17)	10464(3)	2776(2)	4364(2)	31(1)	1
C(18)	9311(3)	3572(2)	4478(2)	24(1)	1
C(19)	7210(2)	7413(2)	3683(2)	24(1)	1

Table 3. Bond lengths [Å] and angles [°].

S(1)-O(1)	1.4306(17)

S(1)-O(2)	1.4337(17)
S(1)-N(1)	1.6216(16)
S(1)-C(1)	1.7624(18)
Cl(1)-C(12)	1.806(2)
C(1)-C(6)	1.377(3)
C(1)-C(2)	1.389(3)
C(2)-C(3)	1.386(3)
C(3)-C(4)	1.391(3)
C(4)-C(5)	1.388(3)
C(4)-C(7)	1.511(3)
C(5)-C(6)	1.379(3)
N(1)-C(8)	1.475(3)
N(1)-C(11)	1.494(3)
C(8)-C(9)	1.521(3)
C(9)-C(10)	1.537(3)
C(10)-C(12)	1.536(3)
C(10)-C(11)	1.539(3)
C(11)-C(13)	1.528(3)
C(12)-C(19)	1.515(3)
C(13)-C(14)	1.523(3)
C(13)-C(18)	1.529(3)
C(14)-C(15)	1.528(3)
C(15)-C(16)	1.525(3)
C(16)-C(17)	1.517(3)
C(17)-C(18)	1.524(3)

O(1)-S(1)-O(2)	120.05(8)
O(1)-S(1)-N(1)	107.33(10)
O(2)-S(1)-N(1)	106.17(10)
O(1)-S(1)-C(1)	106.81(11)
O(2)-S(1)-C(1)	107.78(11)
N(1)-S(1)-C(1)	108.27(9)
C(6)-C(1)-C(2)	120.60(17)
C(6)-C(1)-S(1)	120.08(18)
C(2)-C(1)-S(1)	119.32(17)
C(3)-C(2)-C(1)	119.0(2)
C(2)-C(3)-C(4)	121.0(2)
C(5)-C(4)-C(3)	118.64(17)
C(5)-C(4)-C(7)	121.0(2)
C(3)-C(4)-C(7)	120.3(2)
C(6)-C(5)-C(4)	120.8(2)
C(1)-C(6)-C(5)	119.9(2)
C(8)-N(1)-C(11)	111.39(15)
C(8)-N(1)-S(1)	117.92(15)
C(11)-N(1)-S(1)	117.91(14)
N(1)-C(8)-C(9)	102.63(17)
C(8)-C(9)-C(10)	103.39(17)

C(12)-C(10)-C(9)	109.21(17)
C(12)-C(10)-C(11)	114.45(17)
C(9)-C(10)-C(11)	103.83(17)
N(1)-C(11)-C(13)	111.45(16)
N(1)-C(11)-C(10)	103.70(17)
C(13)-C(11)-C(10)	115.93(18)
C(19)-C(12)-C(10)	112.85(17)
C(19)-C(12)-Cl(1)	107.37(14)
C(10)-C(12)-Cl(1)	110.70(14)
C(14)-C(13)-C(11)	111.36(17)
C(14)-C(13)-C(18)	110.45(19)
C(11)-C(13)-C(18)	114.61(18)
C(13)-C(14)-C(15)	111.89(19)
C(16)-C(15)-C(14)	111.3(2)
C(17)-C(16)-C(15)	111.0(2)
C(16)-C(17)-C(18)	111.42(19)
C(17)-C(18)-C(13)	110.77(19)

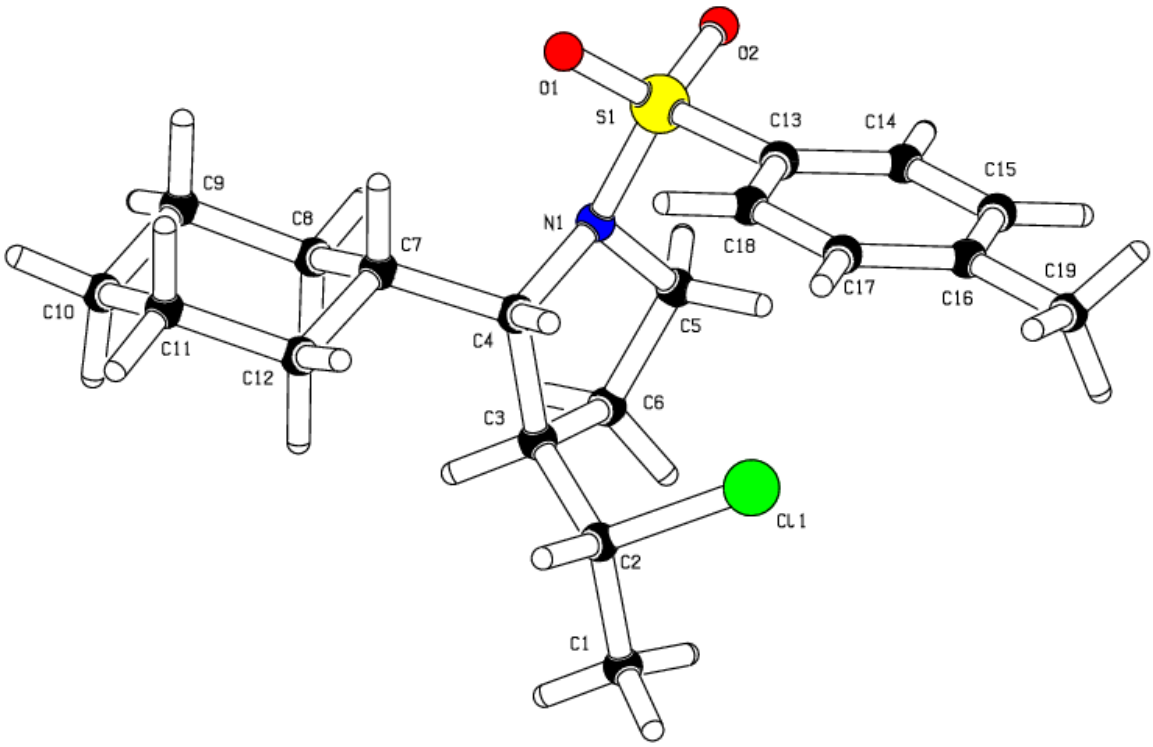
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	27(2)	18(2)	46(3)	0(2)	6(2)	5(1)
S(1)	22(1)	15(1)	12(1)	2(1)	1(1)	0(1)
O(1)	27(1)	21(1)	16(1)	3(1)	-3(1)	6(1)
O(2)	26(1)	22(1)	21(1)	4(1)	3(1)	-5(1)
Cl(1)	28(1)	23(1)	37(1)	6(1)	-7(1)	-10(1)
C(1)	20(1)	16(1)	10(1)	1(1)	1(1)	1(1)
C(2)	19(1)	22(1)	16(1)	-3(1)	-3(1)	0(1)
C(3)	22(1)	23(1)	19(1)	-1(1)	-2(1)	7(1)
C(4)	28(1)	19(1)	15(1)	-1(1)	-1(1)	0(1)
C(5)	22(1)	23(1)	21(1)	-2(1)	-2(1)	-4(1)
C(6)	20(1)	23(1)	15(1)	0(1)	2(1)	1(1)
C(7)	35(1)	19(1)	29(1)	-3(1)	-4(1)	0(1)
N(1)	21(1)	18(1)	11(1)	0(1)	0(1)	-2(1)
C(8)	20(1)	19(1)	16(1)	3(1)	-3(1)	-2(1)
C(9)	26(1)	22(1)	16(1)	-2(1)	-5(1)	-1(1)
C(10)	20(1)	18(1)	13(1)	-1(1)	-1(1)	2(1)
C(11)	20(1)	17(1)	12(1)	-1(1)	0(1)	-1(1)
C(12)	15(1)	18(1)	18(1)	1(1)	1(1)	-2(1)
C(13)	24(1)	20(1)	15(1)	-2(1)	-3(1)	6(1)
C(14)	25(1)	28(1)	24(1)	-2(1)	1(1)	5(1)
C(15)	28(1)	41(1)	29(1)	-1(1)	1(1)	9(1)
C(16)	41(1)	35(1)	24(1)	-2(1)	1(1)	21(1)
C(17)	48(2)	23(1)	22(1)	-1(1)	-3(1)	14(1)
C(18)	36(1)	18(1)	18(1)	-3(1)	-1(1)	5(1)
C(19)	30(1)	19(1)	23(1)	3(1)	-2(1)	4(1)

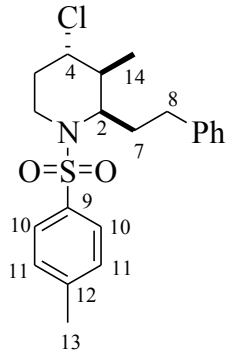
Table 5. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$Å^2 \times 10^3$].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H(2)	5431	6464	6907	23	1
H(3)	5463	8221	7238	26	1
H(5)	9578	8051	7787	26	1
H(6)	9569	6314	7418	23	1
H(7A)	8467	9656	7954	42	1
H(7B)	6880	9570	8274	42	1
H(7C)	7228	9847	7260	42	1
H(8A)	5671	5619	5541	28	1
H(8B)	5528	4401	5351	28	1
H(9A)	5922	5587	4012	32	1
H(9B)	6761	4512	4034	32	1
H(10)	8592	5649	3908	26	1
H(11)	9113	5826	5634	25	1
H(12)	6934	7008	5000	26	1
H(13)	10058	4147	5658	29	1
H(14A)	11448	5485	5109	38	1
H(14B)	10898	5275	4119	38	1
H(15A)	13083	4485	4272	49	1
H(15B)	12579	3884	5146	49	1
H(16A)	11587	3508	3373	50	1
H(16B)	12519	2729	3947	50	1
H(17A)	10679	2462	4949	47	1
H(17B)	10137	2223	3961	47	1
H(18A)	8482	3241	4747	36	1
H(18B)	9039	3845	3888	36	1
H(19A)	7076	8153	3776	36	1
H(19B)	6328	7101	3494	36	1
H(19C)	7918	7304	3223	36	1



X-Ray data for (2*R*,3*S*,4*S*)-4-chloro-3-methyl-2-phenethyl-1-tosylpiperidine and

(2*S*,3*R*,4*R*)-4-chloro-3-methyl-2-phenethyl-1-tosylpiperidine (124b).



$C_{21}H_{26}ClNO_2S$
Mol. Wt.: 391.95

Table 1. Crystal data and structure refinement details.

Identification code	**src1365**	
Empirical formula	C21 H26 Cl N O2 S	
Formula weight	391.94	
Temperature	120(2) K	
Wavelength	0.71073 A	
Crystal system	monoclinic	
space group	C 2/c	
Unit cell dimensions	a = 24.2929(8) A	alpha = 90 deg.
	b = 11.7453(3) A	beta = 105.602(2) deg.
	c = 14.3282(5) A	gamma = 90 deg.
Volume	3937.6(2) A^3	
Z	8	
Calculated density	1.322 Mg/m^3	
Absorption coefficient	0.315 mm^-1	
F(000)	1664	
Crystal size	0.40 x 0.32 x 0.18 mm	
Theta range for data collection	3.14 to 27.55 deg.	
Limiting indices	-31<=h<=26, -15<=k<=13, -18<=k<=18	
Reflections collected	22473	
unique	4529 [R(int) = 0.0566]	
Completeness to theta = 27.55	99.5 %	
Absorption correction	None	
Max. and min. transmission	0.9454 and 0.8842	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4529 / 0 / 235	
Goodness-of-fit on F^2	1.081	
Final R indices [I>2sigma(I)]	R1 = 0.0768, wR2 = 0.1804	
R indices (all data)	R1 = 0.1154, wR2 = 0.2041	
Largest diff. peak and hole	0.818 and -1.041 e.A^-3	

Diffractometer: *Bruker-Nonius APEX II* CCD camera (ϕ scans and ω scans to fill *asymmetric unit*). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: Sheldrick, G. M. SADABS 2007/2 - Bruker Nonius area detector scaling and absorption correction. **Structure solution**: *Sir2004* (Burla, M.C., Caliandro, R., Carrozzini, B., Cascarano, G., De Caro, L., Giacovazzo, C. & Polidori, G. (2004). J. Appl. Cryst. 37, 258). **Structure refinement**: *SHELXL97* (Sheldrick, G. M. (1997). University of Göttingen, Germany). **Graphics:** *PLATON/PLUTON* (Spek, A. L. (1990). Acta Cryst. A46, C34).

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
S(1)	3552(1)	8644(1)	801(1)	56(1)	1
O(1)	3006(2)	8358(3)	936(3)	86(1)	1
O(2)	3899(2)	9471(2)	1404(2)	105(2)	1
Cl(1)	3825(1)	7234(1)	-2824(1)	70(1)	1
N(1)	3443(1)	9100(2)	-297(2)	36(1)	1
C(1)	3925(1)	9538(3)	-634(2)	32(1)	1
C(2)	4119(1)	8642(3)	-1262(2)	31(1)	1
C(3)	3615(2)	8310(3)	-2092(2)	37(1)	1
C(4)	3135(2)	7845(3)	-1727(3)	43(1)	1
C(5)	2957(2)	8680(3)	-1056(3)	46(1)	1
C(6)	4640(2)	9045(4)	-1559(3)	55(1)	1
C(7)	3767(2)	10698(3)	-1121(2)	36(1)	1
C(8)	3730(2)	11609(3)	-393(3)	58(1)	1
C(9)	3432(2)	12686(3)	-836(3)	41(1)	1
C(10)	3552(2)	13221(3)	-1619(3)	45(1)	1
C(11)	3278(2)	14242(3)	-1975(3)	50(1)	1
C(12)	2873(2)	14698(3)	-1571(3)	50(1)	1
C(13)	2750(2)	14160(3)	-802(3)	53(1)	1
C(14)	3033(2)	13174(3)	-436(3)	51(1)	1
C(15)	3959(2)	7386(3)	924(2)	37(1)	1
C(16)	3692(2)	6359(3)	663(3)	37(1)	1
C(17)	4012(2)	5383(3)	741(3)	44(1)	1
C(18)	4591(2)	5405(4)	1057(4)	78(2)	1
C(19)	4846(2)	6442(6)	1299(7)	139(4)	1
C(20)	4537(2)	7426(5)	1234(5)	100(2)	1
C(21)	4928(3)	4317(6)	1130(7)	157(4)	1

Table 3. Bond lengths [Å] and angles [°].

S(1)-O(2)	1.417(4)

S(1)-O(1)	1.431(4)
S(1)-N(1)	1.614(3)
S(1)-C(15)	1.761(4)
Cl(1)-C(3)	1.802(3)
N(1)-C(5)	1.459(5)
N(1)-C(1)	1.474(4)
C(1)-C(7)	1.532(4)
C(1)-C(2)	1.538(4)
C(2)-C(3)	1.510(5)
C(2)-C(6)	1.517(5)
C(3)-C(4)	1.504(5)
C(4)-C(5)	1.515(5)
C(7)-C(8)	1.513(5)
C(8)-C(9)	1.511(5)
C(9)-C(14)	1.376(5)
C(9)-C(10)	1.384(5)
C(10)-C(11)	1.399(5)
C(11)-C(12)	1.378(6)
C(12)-C(13)	1.371(6)
C(13)-C(14)	1.377(5)
C(15)-C(20)	1.354(6)
C(15)-C(16)	1.372(5)
C(16)-C(17)	1.373(5)
C(17)-C(18)	1.357(6)
C(18)-C(19)	1.369(9)
C(18)-C(21)	1.507(7)
C(19)-C(20)	1.367(9)

O(2)-S(1)-O(1)	120.0(3)
O(2)-S(1)-N(1)	106.36(17)
O(1)-S(1)-N(1)	107.1(2)
O(2)-S(1)-C(15)	106.8(2)
O(1)-S(1)-C(15)	107.74(17)
N(1)-S(1)-C(15)	108.46(14)
C(5)-N(1)-C(1)	115.4(3)
C(5)-N(1)-S(1)	120.1(2)
C(1)-N(1)-S(1)	119.9(2)
N(1)-C(1)-C(7)	109.5(3)
N(1)-C(1)-C(2)	110.4(2)
C(7)-C(1)-C(2)	114.9(3)
C(3)-C(2)-C(6)	114.8(3)
C(3)-C(2)-C(1)	109.0(3)
C(6)-C(2)-C(1)	111.2(3)
C(4)-C(3)-C(2)	111.1(3)
C(4)-C(3)-Cl(1)	108.4(2)
C(2)-C(3)-Cl(1)	110.1(2)
C(3)-C(4)-C(5)	111.4(3)

N(1)-C(5)-C(4)	112.4(3)
C(8)-C(7)-C(1)	111.7(3)
C(9)-C(8)-C(7)	114.4(3)
C(14)-C(9)-C(10)	118.3(3)
C(14)-C(9)-C(8)	119.1(4)
C(10)-C(9)-C(8)	122.6(4)
C(9)-C(10)-C(11)	120.1(4)
C(12)-C(11)-C(10)	120.2(4)
C(13)-C(12)-C(11)	119.6(3)
C(12)-C(13)-C(14)	119.9(4)
C(9)-C(14)-C(13)	121.8(4)
C(20)-C(15)-C(16)	119.5(4)
C(20)-C(15)-S(1)	120.5(3)
C(16)-C(15)-S(1)	119.9(3)
C(15)-C(16)-C(17)	119.7(3)
C(18)-C(17)-C(16)	121.6(4)
C(17)-C(18)-C(19)	117.4(4)
C(17)-C(18)-C(21)	120.2(6)
C(19)-C(18)-C(21)	122.4(5)
C(20)-C(19)-C(18)	122.1(4)
C(15)-C(20)-C(19)	119.7(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

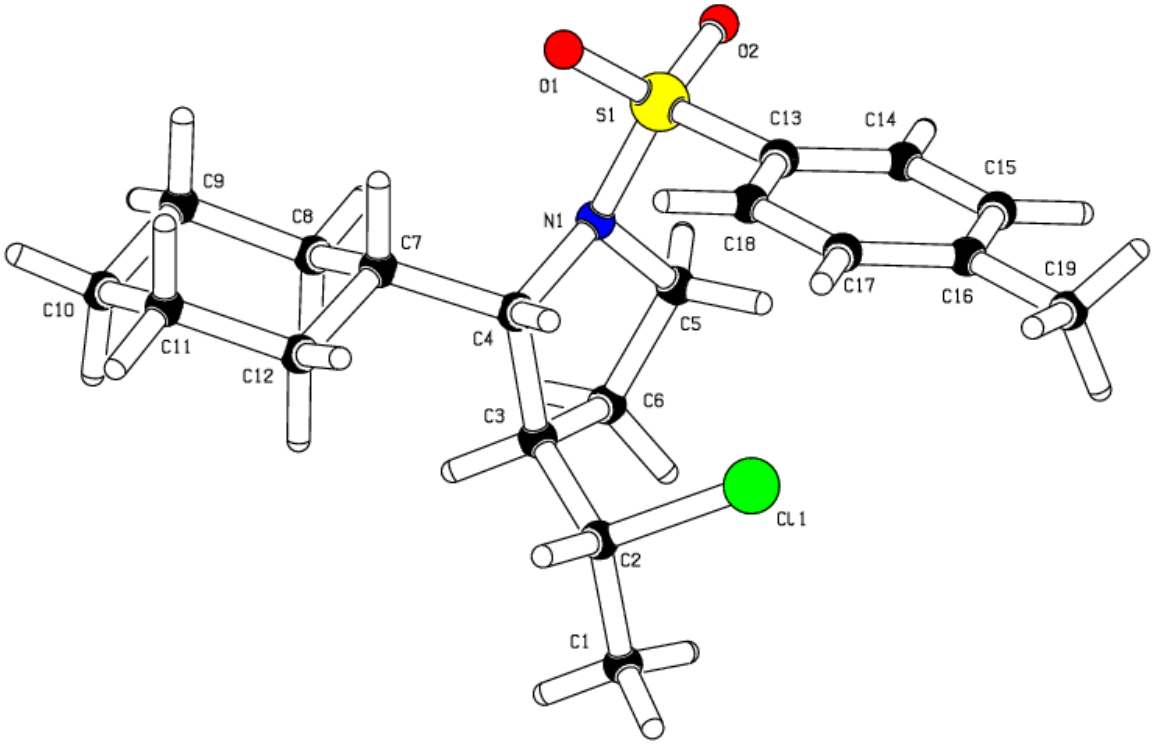
Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	112(1)	27(1)	39(1)	4(1)	42(1)	8(1)
O(1)	135(3)	55(2)	110(3)	41(2)	108(3)	43(2)
O(2)	247(5)	36(2)	32(2)	-8(1)	34(2)	-27(2)
Cl(1)	138(1)	39(1)	36(1)	0(1)	28(1)	28(1)
N(1)	47(2)	28(1)	37(1)	9(1)	21(1)	8(1)

C(1)	37(2)	26(2)	32(2)	3(1)	9(1)	-1(1)
C(2)	32(2)	28(2)	35(2)	8(1)	13(1)	6(1)
C(3)	55(2)	25(2)	30(2)	2(1)	10(2)	9(1)
C(4)	43(2)	30(2)	48(2)	6(2)	-3(2)	-5(2)
C(5)	34(2)	40(2)	67(2)	16(2)	21(2)	3(2)
C(6)	44(2)	54(2)	76(3)	22(2)	33(2)	13(2)
C(7)	46(2)	25(2)	40(2)	4(1)	16(2)	1(1)
C(8)	87(3)	29(2)	50(2)	0(2)	6(2)	15(2)
C(9)	52(2)	24(2)	43(2)	-2(1)	4(2)	1(2)
C(10)	37(2)	42(2)	50(2)	4(2)	4(2)	2(2)
C(11)	51(2)	39(2)	51(2)	10(2)	-1(2)	-13(2)
C(12)	51(2)	26(2)	58(2)	-5(2)	-10(2)	2(2)
C(13)	53(2)	40(2)	60(2)	-8(2)	6(2)	7(2)
C(14)	67(3)	34(2)	51(2)	-2(2)	14(2)	1(2)
C(15)	49(2)	35(2)	24(1)	6(1)	6(1)	-5(2)
C(16)	33(2)	34(2)	45(2)	5(1)	13(2)	1(1)
C(17)	56(2)	36(2)	44(2)	9(2)	20(2)	10(2)
C(18)	51(3)	77(3)	116(4)	70(3)	42(3)	31(2)
C(19)	30(2)	118(5)	242(9)	127(6)	-10(4)	-1(3)
C(20)	67(3)	72(3)	121(5)	57(3)	-45(3)	-33(3)
C(21)	122(5)	130(6)	268(10)	149(7)	139(7)	98(5)

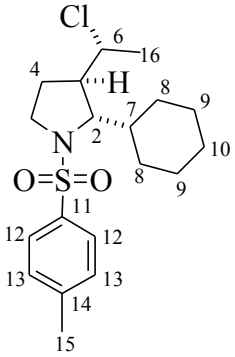
Table 5. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$Å^2 \times 10^3$].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H(1)	4252	9664	-46	48	1
H(2)	4235	7949	-851	47	1
H(3)	3477	8997	-2501	55	1
H(4A)	3258	7123	-1376	65	1
H(4B)	2803	7678	-2284	65	1
H(5A)	2759	9333	-1440	69	1
H(5B)	2684	8303	-753	69	1
H(6A)	4945	9241	-980	82	1

H(6B)	4540	9717	-1976	82	1
H(6C)	4772	8436	-1915	82	1
H(7A)	4057	10919	-1456	55	1
H(7B)	3394	10636	-1613	55	1
H(8A)	3525	11293	60	87	1
H(8B)	4122	11804	-10	87	1
H(10)	3821	12895	-1914	53	1
H(11)	3372	14621	-2498	60	1
H(12)	2681	15382	-1823	60	1
H(13)	2469	14468	-523	63	1
H(14)	2950	12820	107	62	1
H(16)	3288	6325	430	44	1
H(17)	3823	4674	569	53	1
H(19)	5251	6480	1519	167	1
H(20)	4726	8133	1406	120	1
H(21A)	5337	4486	1369	235	1
H(21B)	4852	3962	489	235	1
H(21C)	4815	3794	1579	235	1


O2
O1
S1
C13
C14
C15
C9
C8
C7
N1
C18
C19
C17
C16
C10
C11
C12
C4
C5
C6
C3
Cl1
C2
C1

X-Ray data for (2*S*,3*R*)-3-((*R*)-1-chloroethyl)-2-cyclohexyl-1-tosylpyrrolidine and (2*R*,3*S*)-3-((*S*)-1-chloroethyl)-2-cyclohexyl-1-tosylpyrrolidine (125c).



$C_{19}H_{28}ClNO_2S$
Mol. Wt.: 369.95

Table 1. Crystal data and structure refinement details.

Identification code	**2007src0763**	
Empirical formula	$C_{19}H_{28}ClNO_2S$	
Formula weight	369.93	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 15.4076(3) Å	α = 90°
	b = 12.9924(4) Å	β = 90°
	c = 9.3800(3) Å	γ = 90°
Volume	1877.70(9) Å^3	
Z	4	
Density (calculated)	1.309 Mg / m^3	
Absorption coefficient	0.326 mm^{-1}	
F(000)	792	
Crystal	Rod; Colourless	
Crystal size	0.24 × 0.10 × 0.10 mm^3	
θ range for data collection	2.99 – 28.50°	
Index ranges	$-20 \le h \le 17, -14 \le k \le 17, -12 \le l \le 12$	
Reflections collected	10624	
Independent reflections	4506 [R_{int} = 0.0506]	
Completeness to θ = 28.50°	99.3 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6519	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4506 / 1 / 220	
Goodness-of-fit on F^2	1.074	
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0699, $wR2$ = 0.1726	

R indices (all data)	$R1 = 0.0743$, $wR2 = 0.1761$
Absolute structure parameter	0.40(12)
Largest diff. peak and hole	1.193 and −0.769 e Å^{-3}

Diffractometer: *Bruker-Nonius APEX II* CCD camera (ϕ scans and ω scans to fill *asymmetric unit*). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: Sheldrick, G. M. SADABS 2007/2 - Bruker Nonius area detector scaling and absorption correction. **Structure solution**: *Sir2004* (Burla, M.C., Caliandro, R., Carrozzini, B., Cascarano, G., De Caro, L., Giacovazzo, C. & Polidori, G. (2004). J. Appl. Cryst. 37, 258). **Structure refinement**: *SHELXL97* (Sheldrick, G. M. (1997). University of Göttingen, Germany). **Graphics:** *PLATON/PLUTON* (Spek, A. L. (1990). Acta Cryst. A46, C34).

Special details:

The structure is a mixture of enantiomers with a refined ratio of 0.40(12).

All hydrogen atoms have been fixed as riding models.

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
C1	6588(3)	84(3)	4155(7)	30(1)	1
C2	5781(3)	562(3)	4821(5)	24(1)	1
C3	5669(3)	1715(3)	4487(5)	24(1)	1
C4	4831(3)	2177(3)	5167(4)	20(1)	1
C5	4717(3)	2159(4)	2553(4)	23(1)	1
C6	5647(3)	2017(4)	2915(5)	32(1)	1
C7	4989(3)	3070(3)	6201(4)	20(1)	1
C8	5506(3)	3982(3)	5568(5)	24(1)	1
C9	5584(3)	4854(3)	6652(5)	28(1)	1
C10	6019(3)	4469(4)	8020(5)	30(1)	1
C11	5533(3)	3563(4)	8666(5)	33(1)	1
C12	5428(3)	2699(3)	7578(5)	27(1)	1
C13	2898(2)	1193(2)	4013(5)	17(1)	1
C14	2667(3)	712(3)	2746(4)	25(1)	1
C15	2420(3)	−320(4)	2756(5)	29(1)	1
C16	2397(2)	−866(2)	4018(5)	21(1)	1
C17	2623(3)	−378(3)	5287(5)	26(1)	1
C18	2872(3)	648(3)	5280(5)	23(1)	1
C19	2134(3)	−1985(3)	4030(6)	29(1)	1
N1	4305(2)	2502(2)	3934(5)	17(1)	1
O1	3012(2)	2914(2)	5357(3)	23(1)	1
O2	2936(2)	2943(2)	2706(3)	23(1)	1
S1	3249(1)	2479(1)	4004(1)	16(1)	1
Cl1	4855(1)	−170(1)	4156(2)	41(1)	1

Table 3. Bond lengths [Å] and angles [°].

C1–C2	1.524(6)
C1–H1A	0.9800
C1–H1B	0.9800
C1–H1C	0.9800
C2–C3	1.540(5)
C2–Cl1	1.824(4)
C2–H2	1.0000
C3–C6	1.526(7)
C3–C4	1.560(6)
C3–H3	1.0000
C4–N1	1.474(6)
C4–C7	1.532(5)
C4–H4	1.0000
C5–C6	1.484(6)
C5–N1	1.509(6)
C5–H5A	0.9900
C5–H5B	0.9900
C6–H6A	0.9900
C6–H6B	0.9900
C7–C12	1.536(6)
C7–C8	1.546(5)
C7–H7	1.0000
C8–C9	1.527(5)
C8–H8A	0.9900
C8–H8B	0.9900
C9–C10	1.532(7)
C9–H9A	0.9900
C9–H9B	0.9900
C10–C11	1.521(7)
C10–H10A	0.9900
C10–H10B	0.9900
C11–C12	1.526(6)
C11–H11A	0.9900
C11–H11B	0.9900
C12–H12A	0.9900
C12–H12B	0.9900
C13–C18	1.384(6)
C13–C14	1.389(6)

C13–S1	1.756(3)
C14–C15	1.393(6)
C14–H14	0.9500
C15–C16	1.382(7)
C15–H15	0.9500
C16–C17	1.393(6)
C16–C19	1.509(5)
C17–C18	1.388(6)
C17–H17	0.9500
C18–H18	0.9500
C19–H19A	0.9800
C19–H19B	0.9800
C19–H19C	0.9800
N1–S1	1.629(3)
O1–S1	1.436(3)
O2–S1	1.442(3)
C2–C1–H1A	109.5
C2–C1–H1B	109.5
H1A–C1–H1B	109.5
C2–C1–H1C	109.5
H1A–C1–H1C	109.5
H1B–C1–H1C	109.5
C1–C2–C3	113.8(3)
C1–C2–Cl1	106.6(3)
C3–C2–Cl1	110.5(3)
C1–C2–H2	108.6
C3–C2–H2	108.6
Cl1–C2–H2	108.6
C6–C3–C2	116.7(4)
C6–C3–C4	106.1(3)
C2–C3–C4	112.6(3)
C6–C3–H3	107.0
C2–C3–H3	107.0
C4–C3–H3	107.0
N1–C4–C7	111.6(3)
N1–C4–C3	104.2(3)
C7–C4–C3	114.8(3)
N1–C4–H4	108.7
C7–C4–H4	108.7
C3–C4–H4	108.7

C6–C5–N1	104.2(3)
C6–C5–H5A	110.9
N1–C5–H5A	110.9
C6–C5–H5B	110.9
N1–C5–H5B	110.9
H5A–C5–H5B	108.9
C5–C6–C3	106.0(4)
C5–C6–H6A	110.5
C3–C6–H6A	110.5
C5–C6–H6B	110.5
C3–C6–H6B	110.5
H6A–C6–H6B	108.7
C4–C7–C12	111.4(3)
C4–C7–C8	114.8(3)
C12–C7–C8	109.7(3)
C4–C7–H7	106.8
C12–C7–H7	106.8
C8–C7–H7	106.8
C9–C8–C7	110.7(4)
C9–C8–H8A	109.5
C7–C8–H8A	109.5
C9–C8–H8B	109.5
C7–C8–H8B	109.5
H8A–C8–H8B	108.1
C8–C9–C10	110.5(4)
C8–C9–H9A	109.5
C10–C9–H9A	109.5
C8–C9–H9B	109.5
C10–C9–H9B	109.5
H9A–C9–H9B	108.1
C11–C10–C9	111.8(4)
C11–C10–H10A	109.3
C9–C10–H10A	109.3
C11–C10–H10B	109.3
C9–C10–H10B	109.3
H10A–C10–H10B	107.9
C10–C11–C12	110.8(4)
C10–C11–H11A	109.5
C12–C11–H11A	109.5
C10–C11–H11B	109.5

C12–C11–H11B	109.5
H11A–C11–H11B	108.1
C11–C12–C7	112.2(3)
C11–C12–H12A	109.2
C7–C12–H12A	109.2
C11–C12–H12B	109.2
C7–C12–H12B	109.2
H12A–C12–H12B	107.9
C18–C13–C14	119.9(3)
C18–C13–S1	119.9(3)
C14–C13–S1	120.2(3)
C13–C14–C15	119.8(4)
C13–C14–H14	120.1
C15–C14–H14	120.1
C16–C15–C14	120.5(4)
C16–C15–H15	119.8
C14–C15–H15	119.8
C15–C16–C17	119.5(3)
C15–C16–C19	120.5(4)
C17–C16–C19	120.0(4)
C18–C17–C16	120.2(4)
C18–C17–H17	119.9
C16–C17–H17	119.9
C13–C18–C17	120.2(4)
C13–C18–H18	119.9
C17–C18–H18	119.9
C16–C19–H19A	109.5
C16–C19–H19B	109.5
H19A–C19–H19B	109.5
C16–C19–H19C	109.5
H19A–C19–H19C	109.5
H19B–C19–H19C	109.5
C4–N1–C5	110.9(3)
C4–N1–S1	120.9(3)
C5–N1–S1	116.7(3)
O1–S1–O2	119.83(15)
O1–S1–N1	106.3(2)
O2–S1–N1	107.0(2)
O1–S1–C13	107.0(2)
O2–S1–C13	107.4(2)

N1–S1–C1	108.96(15

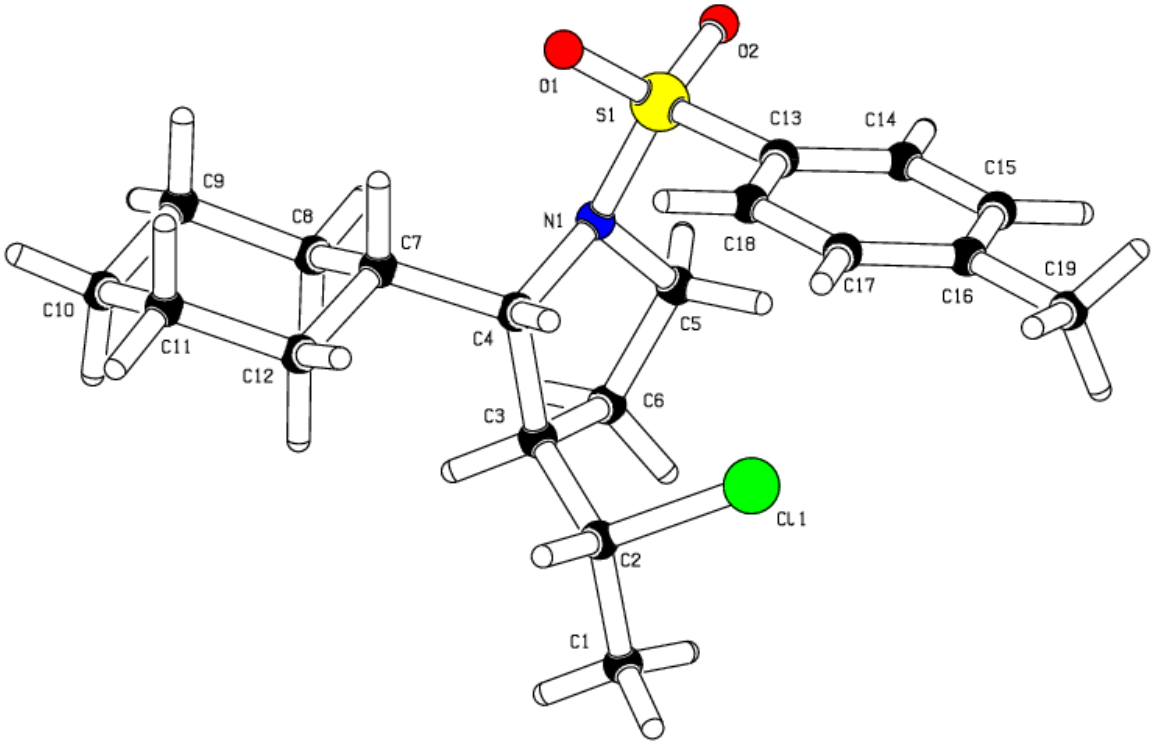
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

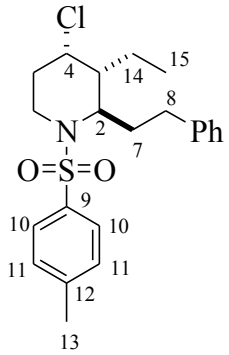
Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	27(2)	18(2)	46(3)	0(2)	6(2)	5(1)
C2	21(2)	16(2)	33(2)	−1(2)	−2(2)	1(1)
C3	24(2)	18(2)	29(2)	1(2)	0(2)	0(1)
C4	25(2)	17(2)	18(2)	−1(1)	1(2)	−1(2)
C5	22(2)	31(2)	16(2)	1(2)	5(2)	5(2)
C6	29(2)	31(2)	36(3)	−3(2)	7(2)	5(2)
C7	23(2)	16(2)	21(2)	−4(1)	3(2)	−3(1)
C8	27(2)	13(2)	31(2)	−2(2)	−1(2)	0(1)
C9	21(2)	19(2)	43(3)	−10(2)	2(2)	−5(2)
C10	28(2)	31(2)	30(2)	−10(2)	−3(2)	−2(2)
C11	34(2)	33(2)	31(3)	−6(2)	−3(2)	−6(2)
C12	30(2)	22(2)	27(2)	1(2)	−4(2)	−2(2)
C13	15(1)	15(1)	22(2)	2(2)	2(2)	0(1)
C14	38(3)	21(2)	15(2)	1(2)	−2(2)	−6(2)
C15	49(3)	20(2)	19(2)	−6(2)	−4(2)	−13(2)
C16	19(2)	17(1)	27(2)	−4(2)	−4(2)	−2(1)
C17	33(2)	20(2)	23(2)	1(2)	1(2)	−9(2)
C18	27(2)	23(2)	18(2)	−2(2)	0(2)	−7(2)
C19	34(2)	20(2)	32(2)	4(2)	4(2)	−5(1)
N1	10(1)	18(1)	22(1)	−2(1)	−6(2)	0(1)
O1	25(2)	21(2)	24(2)	−7(1)	4(1)	0(1)
O2	19(1)	19(2)	32(2)	6(1)	−4(1)	4(1)
S1	16(1)	13(1)	20(1)	−2(1)	0(1)	1(1)
Cl1	30(1)	19(1)	74(1)	−12(1)	2(1)	−4(1)

Table 5. Hydrogen coordinates [$\times 10^4$] and isotropic displacement parameters [$Å^2 \times 10^3$].

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H1A	6527	78	3115	46	1
H1B	6657	−623	4503	46	1
H1C	7099	490	4420	46	1
H2	5813	473	5878	28	1
H3	6174	2081	4925	28	1
H4	4516	1618	5683	24	1
H5A	4457	1506	2216	28	1
H5B	4645	2689	1804	28	1
H6A	5973	2664	2758	38	1
H6B	5907	1469	2320	38	1
H7	4406	3343	6476	24	1
H8A	6093	3746	5289	28	1
H8B	5208	4238	4702	28	1
H9A	5000	5125	6878	33	1
H9B	5932	5421	6239	33	1
H10A	6623	4258	7804	36	1
H10B	6043	5037	8722	36	1
H11A	4954	3793	8993	39	1
H11B	5856	3302	9505	39	1
H12A	5076	2140	8004	32	1
H12B	6006	2413	7345	32	1
H14	2678	1085	1875	30	1
H15	2265	−649	1888	35	1
H17	2607	−749	6160	31	1
H18	3025	979	6148	27	1
H19A	1576	−2064	3539	43	1
H19B	2077	−2222	5017	43	1
H19C	2576	−2395	3540	43	1


O2
O1
S1
C13
C14
C15
C9
C8
C7
N1
C18
C19
C17
C16
C10
C11
C12
C4
C5
C6
C3
Cl1
C2
C1

X-Ray data for (2*R*,3*R*,4*S*)-4-chloro-3-ethyl-2-phenethyl-1-tosylpiperidine and (2*S*,3*S*,4*R*)-4-chloro-3-ethyl-2-phenethyl-1-tosylpiperidine (129b).



$C_{22}H_{28}ClNO_2S$
Mol. Wt.: 405.98

Table 1. Crystal data and structure refinement.

Identification code	**2007src1052**	
Empirical formula	$C_{22}H_{28}ClNO_2S$	
Formula weight	405.96	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 8.9411(3) Å	α = 90°
	b = 11.0719(3) Å	β = 99.810(2)°
	c = 10.9373(4) Å	γ = 90°
Volume	1066.91(6) Å^3	
Z	2	
Density (calculated)	1.264 Mg / m^3	
Absorption coefficient	0.293 mm^{-1}	
F(000)	432	
Crystal	Block; Colourless	
Crystal size	0.60 × 0.50 × 0.30 mm^3	
θ range for data collection	3.23 – 27.47°	
Index ranges	$-10 \le h \le 11$, $-13 \le k \le 14$, $-14 \le l \le 14$	
Reflections collected	13213	
Independent reflections	4663 [R_{int} = 0.0367]	
Completeness to θ = 27.47°	99.5 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9171 and 0.8436	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4663 / 1 / 247	
Goodness-of-fit on F^2	1.121	
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0404, $wR2$ = 0.1043	
R indices (all data)	$R1$ = 0.0470, $wR2$ = 0.1078	

Absolute structure parameter	0.44(6)
Largest diff. peak and hole	0.587 and −0.522 e Å^{-3}

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit* sphere). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography,* part A, pp. 307−326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: *SADABS Version 2.10.* (G. M. Sheldrick (2003)) Bruker AXS Inc., Madison, Wisconsin, USA. S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467−473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** *ORTEP3 for Windows* (L. J. Farrugia, J. Appl. Crystallogr. 1997, 30, 565).

Special details:

The crystal was a mixture of enantiomers (~ 44% seen as flack parameter)

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [$Å^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
S1	11359(1)	–42(1)	6658(1)	27(1)	1
Cl1	5156(1)	1320(1)	3817(1)	39(1)	1
C1	7071(3)	1502(2)	4660(2)	27(1)	1
C2	8190(3)	904(2)	3958(2)	32(1)	1
C3	9800(3)	1101(2)	4653(2)	29(1)	1
N1	9857(2)	648(2)	5937(2)	22(1)	1
C4	8837(2)	1256(2)	6673(2)	20(1)	1
C5	7190(2)	1053(2)	5999(2)	21(1)	1
C6	6678(3)	–254(2)	6126(2)	26(1)	1
C7	6453(3)	–562(2)	7444(2)	29(1)	1
C8	9243(2)	2595(2)	6922(2)	20(1)	1
C9	8632(3)	3074(2)	8048(2)	35(1)	1
C10	9169(3)	4336(2)	8386(2)	23(1)	1
C11	10540(3)	4544(2)	9176(2)	28(1)	1
C12	11083(3)	5697(2)	9420(2)	32(1)	1
C13	10264(4)	6687(2)	8887(2)	37(1)	1
C14	8887(3)	6497(2)	8116(2)	37(1)	1
C15	8351(3)	5333(2)	7876(2)	32(1)	1
C16	12541(2)	1069(2)	7481(2)	24(1)	1
C17	13274(2)	1890(2)	6821(2)	26(1)	1
C18	14099(3)	2832(2)	7452(2)	28(1)	1
C19	14234(3)	2941(2)	8740(2)	30(1)	1
C20	13511(3)	2088(3)	9375(2)	32(1)	1
C22	15119(3)	3964(3)	9432(3)	49(1)	1
C21	12652(3)	1166(2)	8762(2)	27(1)	1
O1	12130(2)	–540(2)	5718(2)	42(1)	1
O2	10872(2)	–818(2)	7561(2)	39(1)	1

Table 3. Bond lengths [Å] and angles [°].

S1–O2	1.4321(19)
S1–O1	1.4414(19)
S1–N1	1.6271(19)
S1–C16	1.765(2)
Cl1–C1	1.812(2)
C1–C2	1.514(4)
C1–C5	1.533(3)
C1–H1	1.0000
C2–C3	1.525(3)
C2–H2A	0.9900
C2–H2B	0.9900
C3–N1	1.484(3)
C3–H3A	0.9900
C3–H3B	0.9900
N1–C4	1.477(3)
C4–C8	1.539(3)
C4–C5	1.547(3)
C4–H4	1.0000
C5–C6	1.531(3)
C5–H5	1.0000
C6–C7	1.528(3)
C6–H6A	0.9900
C6–H6B	0.9900
C7–H7A	0.9800
C7–H7B	0.9800
C7–H7C	0.9800
C8–C9	1.525(3)
C8–H8A	0.9900
C8–H8B	0.9900
C9–C10	1.504(3)
C9–H9A	0.9900
C9–H9B	0.9900
C10–C15	1.387(3)
C10–C11	1.394(3)
C11–C12	1.376(4)
C11–H11	0.9500
C12–C13	1.390(4)
C12–H12	0.9500

C13–C14	1.384(4)
C13–H13	0.9500
C14–C15	1.384(4)
C14–H14	0.9500
C15–H15	0.9500
C16–C17	1.392(3)
C16–C21	1.392(3)
C17–C18	1.391(3)
C17–H17	0.9500
C18–C19	1.399(3)
C18–H18	0.9500
C19–C20	1.396(4)
C19–C22	1.508(3)
C20–C21	1.380(4)
C20–H20	0.9500
C22–H22A	0.9800
C22–H22B	0.9800
C22–H22C	0.9800
C21–H21	0.9500
O2–S1–O1	120.08(12)
O2–S1–N1	107.05(11)
O1–S1–N1	106.82(11)
O2–S1–C16	107.00(11)
O1–S1–C16	108.23(11)
N1–S1–C16	107.02(10)
C2–C1–C5	113.48(19)
C2–C1–Cl1	110.01(15)
C5–C1–Cl1	110.86(16)
C2–C1–H1	107.4
C5–C1–H1	107.4
Cl1–C1–H1	107.4
C1–C2–C3	109.51(18)
C1–C2–H2A	109.8
C3–C2–H2A	109.8
C1–C2–H2B	109.8
C3–C2–H2B	109.8
H2A–C2–H2B	108.2
N1–C3–C2	107.55(19)
N1–C3–H3A	110.2
C2–C3–H3A	110.2

N1–C3–H3B	110.2
C2–C3–H3B	110.2
H3A–C3–H3B	108.5
C4–N1–C3	115.86(18)
C4–N1–S1	119.03(14)
C3–N1–S1	120.65(16)
N1–C4–C8	112.75(18)
N1–C4–C5	107.47(16)
C8–C4–C5	113.64(17)
N1–C4–H4	107.6
C8–C4–H4	107.6
C5–C4–H4	107.6
C6–C5–C1	114.85(18)
C6–C5–C4	111.67(18)
C1–C5–C4	108.26(18)
C6–C5–H5	107.2
C1–C5–H5	107.2
C4–C5–H5	107.2
C7–C6–C5	112.73(19)
C7–C6–H6A	109.0
C5–C6–H6A	109.0
C7–C6–H6B	109.0
C5–C6–H6B	109.0
H6A–C6–H6B	107.8
C6–C7–H7A	109.5
C6–C7–H7B	109.5
H7A–C7–H7B	109.5
C6–C7–H7C	109.5
H7A–C7–H7C	109.5
H7B–C7–H7C	109.5
C9–C8–C4	111.80(18)
C9–C8–H8A	109.3
C4–C8–H8A	109.3
C9–C8–H8B	109.3
C4–C8–H8B	109.3
H8A–C8–H8B	107.9
C10–C9–C8	112.2(2)
C10–C9–H9A	109.2
C8–C9–H9A	109.2
C10–C9–H9B	109.2

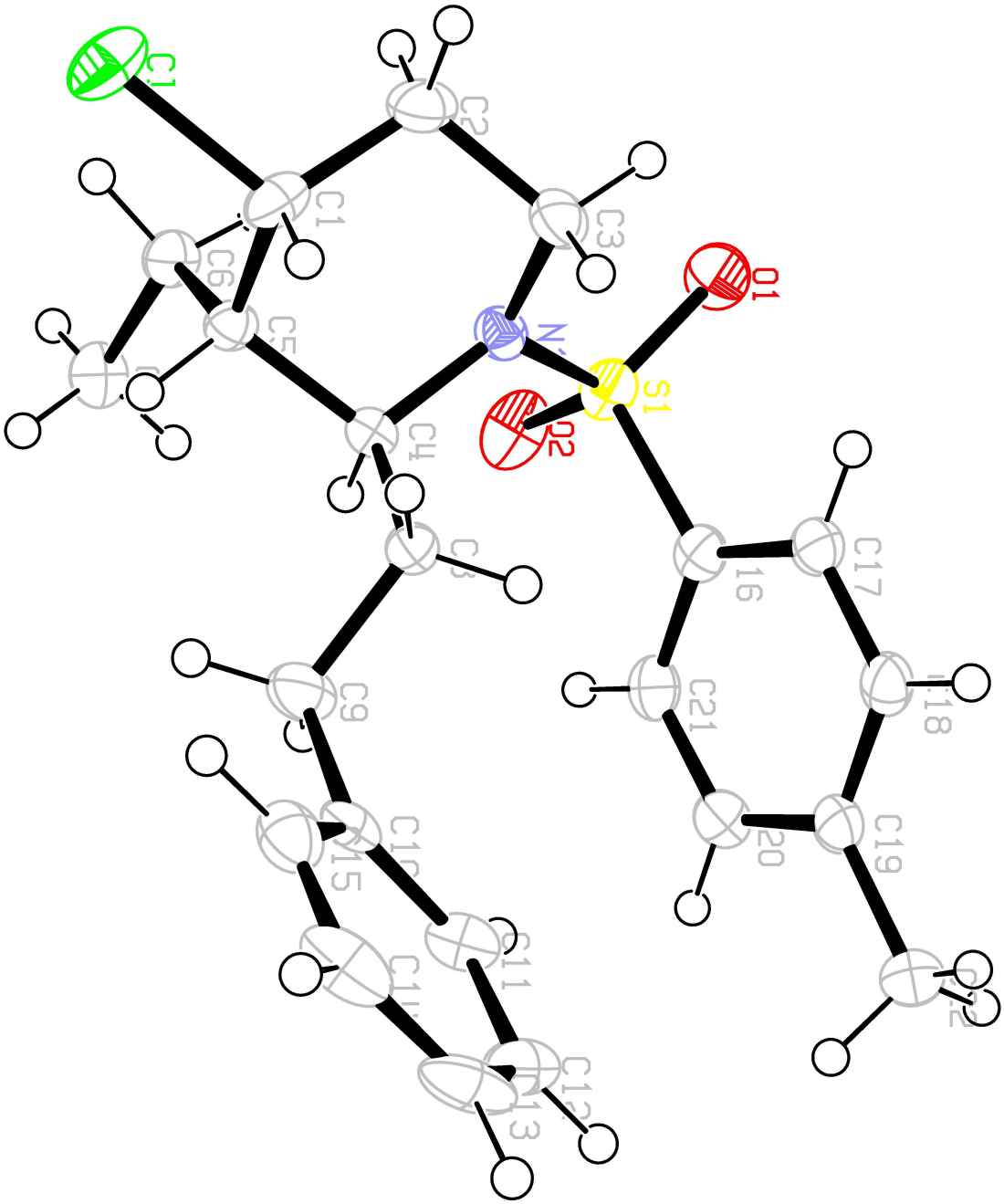
C8–C9–H9B	109.2
H9A–C9–H9B	107.9
C15–C10–C11	117.8(2)
C15–C10–C9	121.1(2)
C11–C10–C9	121.1(2)
C12–C11–C10	121.1(2)
C12–C11–H11	119.4
C10–C11–H11	119.4
C11–C12–C13	120.5(2)
C11–C12–H12	119.8
C13–C12–H12	119.8
C14–C13–C12	119.1(2)
C14–C13–H13	120.5
C12–C13–H13	120.5
C13–C14–C15	120.0(2)
C13–C14–H14	120.0
C15–C14–H14	120.0
C14–C15–C10	121.5(2)
C14–C15–H15	119.2
C10–C15–H15	119.2
C17–C16–C21	120.8(2)
C17–C16–S1	118.99(17)
C21–C16–S1	120.10(18)
C16–C17–C18	119.3(2)
C16–C17–H17	120.3
C18–C17–H17	120.3
C17–C18–C19	120.8(2)
C17–C18–H18	119.6
C19–C18–H18	119.6
C20–C19–C18	118.4(2)
C20–C19–C22	120.4(2)
C18–C19–C22	121.2(2)
C21–C20–C19	121.7(2)
C21–C20–H20	119.2
C19–C20–H20	119.2
C19–C22–H22A	109.5
C19–C22–H22B	109.5
H22A–C22–H22B	109.5
C19–C22–H22C	109.5
H22A–C22–H22C	109.5

H22B–C22–H22C	109.5
C20–C21–C16	119.0(2)
C20–C21–H21	120.5
C16–C21–H21	120.5

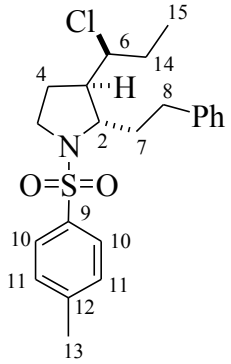
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	26(1)	14(1)	41(1)	−4(1)	4(1)	2(1)
Cl1	33(1)	43(1)	36(1)	6(1)	−11(1)	−5(1)
C1	27(1)	28(1)	23(1)	4(1)	−4(1)	−6(1)
C2	40(1)	37(1)	19(1)	−2(1)	5(1)	−10(1)
C3	32(1)	31(1)	25(1)	−1(1)	12(1)	−5(1)
N1	24(1)	20(1)	24(1)	−1(1)	7(1)	1(1)
C4	23(1)	18(1)	19(1)	1(1)	5(1)	1(1)
C5	23(1)	19(1)	21(1)	−2(1)	4(1)	−3(1)
C6	29(1)	23(1)	26(1)	2(1)	7(1)	−8(1)
C7	31(1)	23(1)	33(1)	8(1)	8(1)	−1(1)
C8	21(1)	17(1)	21(1)	0(1)	4(1)	−1(1)
C9	46(2)	30(1)	32(1)	−8(1)	19(1)	−14(1)
C10	31(1)	21(1)	19(1)	−2(1)	12(1)	1(1)
C11	39(1)	22(1)	22(1)	1(1)	3(1)	7(1)
C12	41(2)	30(1)	25(1)	−6(1)	5(1)	−5(1)
C13	74(2)	16(1)	26(1)	−3(1)	22(1)	−4(1)
C14	59(2)	28(1)	28(1)	8(1)	17(1)	19(1)
C15	30(1)	42(2)	24(1)	3(1)	7(1)	6(1)
C16	20(1)	20(1)	32(1)	−1(1)	3(1)	6(1)
C17	21(1)	27(1)	30(1)	−4(1)	5(1)	3(1)
C18	24(1)	22(1)	40(1)	−5(1)	11(1)	−1(1)
C19	23(1)	32(1)	39(1)	−11(1)	12(1)	−2(1)
C20	29(1)	40(1)	28(1)	−4(1)	7(1)	0(1)
C22	41(2)	55(2)	54(2)	−32(2)	20(1)	−20(1)
C21	23(1)	27(1)	32(1)	6(1)	6(1)	4(1)
O1	33(1)	32(1)	61(1)	−24(1)	11(1)	6(1)
O2	38(1)	20(1)	56(1)	14(1)	1(1)	−4(1)


Cl1
C2
C1
C3
C6
O1
C5
N1
S1
O2
C4
C8
C16
C17
C9
C21
C18
C10
C15
C20
C19
C11
C14
C12
C13

X-Ray data for (2*S*,3*R*)-3-((*S*)-1-chloropropyl)-2-phenethyl-1-tosylpyrrolidine and (2*R*,3*S*)-3-((*R*)-1-chloropropyl)-2-phenethyl-1-tosylpyrrolidine (130b).



$C_{22}H_{28}ClNO_2S$
Mol. Wt.: 405.98

Table 1. Crystal data and structure refinement.

Identification code	**2007src1051**	
Empirical formula	$C_{22}H_{28}ClNO_2S$	
Formula weight	405.96	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 14.7643(7) Å	α = 90°
	b = 13.3490(6) Å	β = 90°
	c = 10.3953(3) Å	γ = 90°
Volume	2048.80(15) Å^3	
Z	4	
Density (calculated)	1.316 Mg / m^3	
Absorption coefficient	0.306 mm^{-1}	
F(000)	864	
Crystal	Block; Colourless	
Crystal size	0.20 × 0.20 × 0.01 mm^3	
θ range for data collection	3.05 – 27.48°	
Index ranges	$-17 \le h \le 19, -17 \le k \le 17, -13 \le l \le 13$	
Reflections collected	16800	
Independent reflections	4515 [R_{int} = 0.0836]	
Completeness to θ = 27.48°	99.6 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9970 and 0.9414	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4515 / 1 / 246	
Goodness-of-fit on F^2	1.052	
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0504, $wR2$ = 0.1017	

R indices (all data)	$R1 = 0.0832$, $wR2 = 0.1143$
Absolute structure parameter	0.10(8)
Largest diff. peak and hole	0.271 and −0.398 e Å^{-3}

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit* sphere). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307–326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: *SADABS Version 2.10.* (G. M. Sheldrick (2003)) Bruker AXS Inc., Madison, Wisconsin, USA. S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467–473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** *ORTEP3 for Windows* (L. J. Farrugia, J. Appl. Crystallogr. 1997, 30, 565).

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [Å$^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
S1	8051(1)	2344(1)	8686(1)	23(1)	1
Cl1	10046(1)	−382(1)	9938(1)	40(1)	1
O1	7819(2)	2773(2)	9910(2)	29(1)	1
O2	7715(2)	2790(2)	7521(2)	30(1)	1
C16	7683(2)	1084(2)	8732(3)	23(1)	1
N1	9145(2)	2358(2)	8570(3)	21(1)	1
C18	7336(2)	−455(3)	7643(4)	33(1)	1
C7	11983(2)	−246(2)	8600(4)	33(1)	1
C20	7152(2)	−332(3)	9920(4)	34(1)	1
C2	10507(2)	1428(2)	8876(3)	22(1)	1
C21	7441(2)	645(2)	9893(3)	29(1)	1
C9	10617(2)	2431(2)	11629(3)	26(1)	1
C17	7632(2)	528(2)	7590(3)	29(1)	1
C10	10710(2)	3197(2)	12701(3)	24(1)	1
C19	7090(2)	−900(2)	8799(4)	33(1)	1
C5	10327(2)	331(2)	8512(3)	25(1)	1
C22	6733(3)	−1958(3)	8835(5)	48(1)	1
C11	10998(2)	2882(3)	13917(3)	31(1)	1
C14	10620(2)	4881(3)	13535(4)	36(1)	1
C12	11095(2)	3555(3)	14915(3)	34(1)	1
C6	11111(2)	−193(3)	7831(3)	31(1)	1
C8	10027(2)	2779(2)	10503(3)	26(1)	1
C4	9582(2)	2283(3)	7294(3)	27(1)	1
C13	10908(2)	4559(3)	14735(3)	36(1)	1
C1	9723(2)	1934(2)	9609(3)	23(1)	1
C15	10539(2)	4214(2)	12527(3)	30(1)	1
C3	10565(2)	2085(2)	7649(3)	28(1)	1

Table 3. Bond lengths [Å] and angles [°].

S1–O1	1.436(2)
S1–O2	1.438(2)
S1–N1	1.619(2)
S1–C16	1.768(3)
Cl1–C5	1.810(3)
C16–C21	1.388(5)
C16–C17	1.402(5)
N1–C4	1.478(4)
N1–C1	1.488(4)
C18–C17	1.384(5)
C18–C19	1.389(5)
C18–H18	0.9500
C7–C6	1.517(5)
C7–H7A	0.9800
C7–H7B	0.9800
C7–H7C	0.9800
C20–C21	1.373(5)
C20–C19	1.393(5)
C20–H20	0.9500
C2–C5	1.536(4)
C2–C1	1.542(4)
C2–C3	1.550(4)
C2–H2	1.0000
C21–H21	0.9500
C9–C10	1.518(4)
C9–C8	1.531(4)
C9–H9A	0.9900
C9–H9B	0.9900
C17–H17	0.9500
C10–C15	1.393(5)
C10–C11	1.399(4)
C19–C22	1.508(5)
C5–C6	1.526(4)
C5–H5	1.0000
C22–H22A	0.9800
C22–H22B	0.9800
C22–H22C	0.9800
C11–C12	1.379(4)

C11–H11	0.9500
C14–C15	1.380(5)
C14–C13	1.386(5)
C14–H14	0.9500
C12–C13	1.381(5)
C12–H12	0.9500
C6–H6A	0.9900
C6–H6B	0.9900
C8–C1	1.529(4)
C8–H8A	0.9900
C8–H8B	0.9900
C4–C3	1.521(4)
C4–H4A	0.9900
C4–H4B	0.9900
C13–H13	0.9500
C1–H1	1.0000
C15–H15	0.9500
C3–H3A	0.9900
C3–H3B	0.9900
O1–S1–O2	119.91(12)
O1–S1–N1	107.41(14)
O2–S1–N1	106.04(14)
O1–S1–C16	106.38(15)
O2–S1–C16	108.08(15)
N1–S1–C16	108.65(13)
C21–C16–C17	119.9(3)
C21–C16–S1	120.3(3)
C17–C16–S1	119.8(2)
C4–N1–C1	112.0(2)
C4–N1–S1	120.1(2)
C1–N1–S1	120.9(2)
C17–C18–C19	121.5(3)
C17–C18–H18	119.3
C19–C18–H18	119.3
C6–C7–H7A	109.5
C6–C7–H7B	109.5
H7A–C7–H7B	109.5
C6–C7–H7C	109.5
H7A–C7–H7C	109.5
H7B–C7–H7C	109.5

C21–C20–C19	121.3(3)
C21–C20–H20	119.3
C19–C20–H20	119.3
C5–C2–C1	114.2(2)
C5–C2–C3	110.3(2)
C1–C2–C3	101.5(2)
C5–C2–H2	110.2
C1–C2–H2	110.2
C3–C2–H2	110.2
C20–C21–C16	119.9(3)
C20–C21–H21	120.0
C16–C21–H21	120.0
C10–C9–C8	114.1(3)
C10–C9–H9A	108.7
C8–C9–H9A	108.7
C10–C9–H9B	108.7
C8–C9–H9B	108.7
H9A–C9–H9B	107.6
C18–C17–C16	119.0(3)
C18–C17–H17	120.5
C16–C17–H17	120.5
C15–C10–C11	117.7(3)
C15–C10–C9	123.0(3)
C11–C10–C9	119.2(3)
C18–C19–C20	118.3(3)
C18–C19–C22	120.9(4)
C20–C19–C22	120.8(4)
C6–C5–C2	114.9(3)
C6–C5–Cl1	108.2(2)
C2–C5–Cl1	109.9(2)
C6–C5–H5	107.9
C2–C5–H5	107.9
Cl1–C5–H5	107.9
C19–C22–H22A	109.5
C19–C22–H22B	109.5
H22A–C22–H22B	109.5
C19–C22–H22C	109.5
H22A–C22–H22C	109.5
H22B–C22–H22C	109.5
C12–C11–C10	121.1(3)

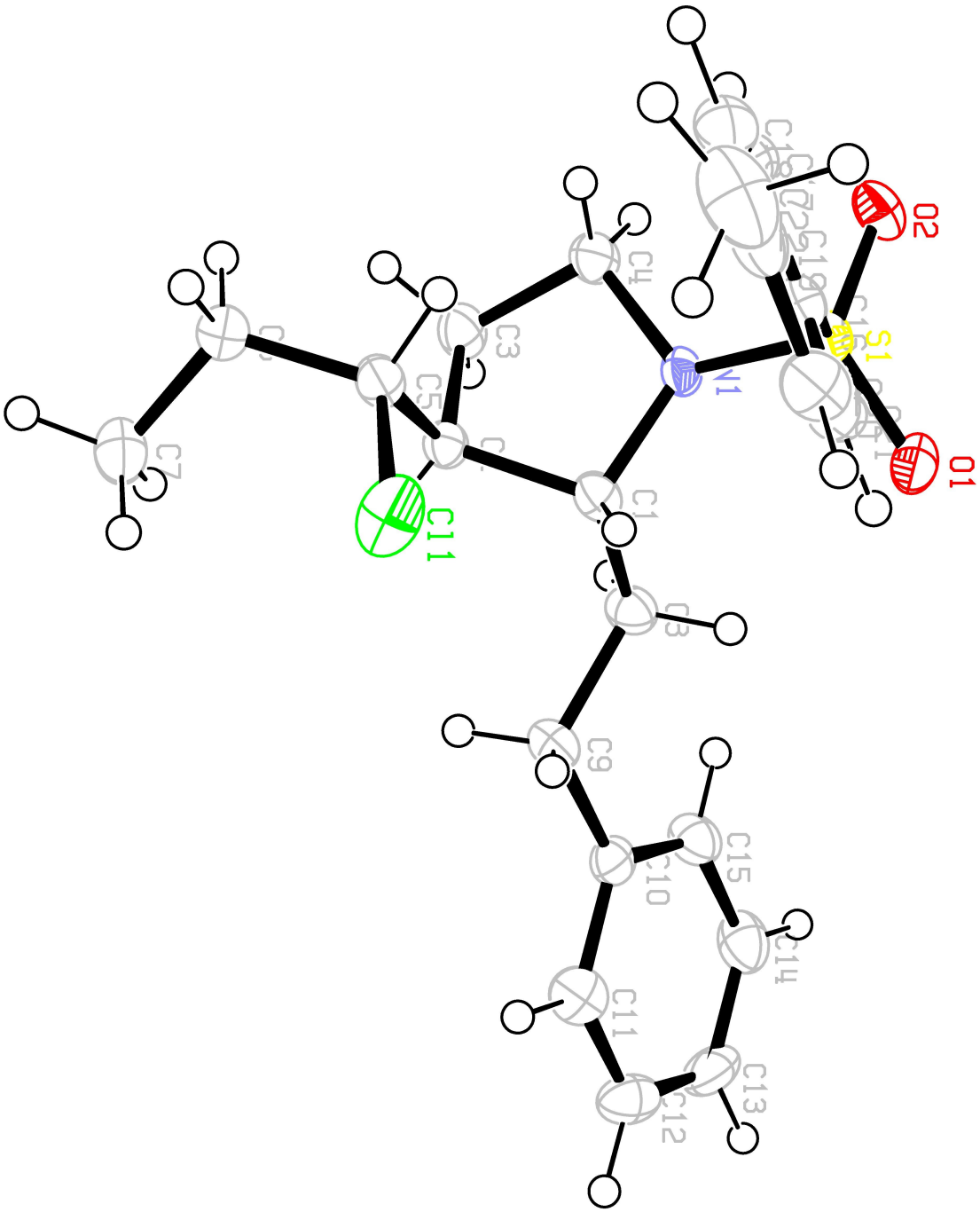
C12–C11–H11	119.5
C10–C11–H11	119.5
C15–C14–C13	120.6(3)
C15–C14–H14	119.7
C13–C14–H14	119.7
C11–C12–C13	120.6(3)
C11–C12–H12	119.7
C13–C12–H12	119.7
C7–C6–C5	114.9(3)
C7–C6–H6A	108.6
C5–C6–H6A	108.6
C7–C6–H6B	108.6
C5–C6–H6B	108.6
H6A–C6–H6B	107.5
C1–C8–C9	114.1(3)
C1–C8–H8A	108.7
C9–C8–H8A	108.7
C1–C8–H8B	108.7
C9–C8–H8B	108.7
H8A–C8–H8B	107.6
N1–C4–C3	102.2(2)
N1–C4–H4A	111.3
C3–C4–H4A	111.3
N1–C4–H4B	111.3
C3–C4–H4B	111.3
H4A–C4–H4B	109.2
C12–C13–C14	119.0(3)
C12–C13–H13	120.5
C14–C13–H13	120.5
N1–C1–C8	109.2(2)
N1–C1–C2	103.8(2)
C8–C1–C2	113.7(3)
N1–C1–H1	110.0
C8–C1–H1	110.0
C2–C1–H1	110.0
C14–C15–C10	121.0(3)
C14–C15–H15	119.5
C10–C15–H15	119.5
C4–C3–C2	104.2(3)
C4–C3–H3A	110.9

C2–C3–H3A	110.9
C4–C3–H3B	110.9
C2–C3–H3B	110.9
H3A–C3–H3B	108.9

Symmetry transformations used to generate equivalent atoms:

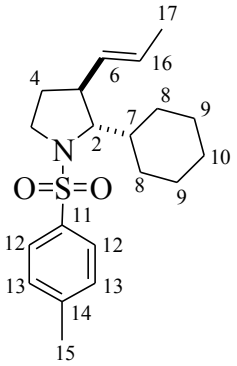
Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	17(1)	24(1)	28(1)	0(1)	−1(1)	2(1)
Cl1	48(1)	25(1)	47(1)	5(1)	16(1)	0(1)
O1	23(1)	30(1)	34(1)	−5(1)	5(1)	3(1)
O2	25(1)	31(1)	34(1)	8(1)	−6(1)	4(1)
C16	14(1)	26(2)	28(1)	1(2)	−3(2)	1(1)
N1	15(1)	25(1)	23(1)	1(1)	1(1)	1(1)
C18	29(2)	31(2)	39(2)	−11(2)	−8(2)	−1(2)
C7	29(2)	30(2)	42(2)	−2(2)	0(2)	5(1)
C20	30(2)	38(2)	35(2)	9(2)	1(2)	−5(2)
C2	17(2)	26(2)	21(2)	1(1)	1(1)	0(1)
C21	25(2)	38(2)	25(2)	3(2)	0(2)	−2(2)
C9	26(2)	26(2)	28(2)	2(1)	−5(1)	2(2)
C17	24(2)	33(2)	29(2)	−3(1)	0(1)	−3(2)
C10	17(2)	29(2)	26(2)	−4(1)	0(1)	−2(1)
C19	20(2)	30(2)	48(2)	6(2)	−2(2)	−1(1)
C5	23(2)	26(2)	27(2)	0(1)	−2(1)	3(1)
C22	34(2)	31(2)	78(3)	4(2)	−10(2)	−6(2)
C11	28(2)	31(2)	34(2)	6(1)	2(2)	−7(1)
C14	33(2)	29(2)	47(2)	−7(2)	−6(2)	4(2)
C12	32(2)	44(2)	24(2)	2(2)	2(2)	−11(2)
C6	29(2)	34(2)	29(2)	−5(1)	−2(1)	6(2)
C8	29(2)	23(2)	26(2)	0(1)	−5(1)	2(1)
C4	20(2)	38(2)	25(2)	2(1)	2(1)	−2(2)
C13	36(2)	48(2)	25(2)	−14(2)	4(2)	−3(2)
C1	19(2)	25(2)	25(2)	2(1)	−2(1)	−1(1)
C15	29(2)	29(2)	33(2)	−2(2)	−7(2)	0(2)
C3	21(2)	32(2)	30(2)	4(1)	3(1)	0(1)



X-Ray data for (2*S*,3*S*,*E*)-2-cyclohexyl-3-(prop-1-enyl)-1-tosylpyrrolidine and

(2*R*,3*R*,*E*)-2-cyclohexyl-3-(prop-1-enyl)-1-tosylpyrrolidine (131c).



$C_{20}H_{29}NO_2S$
Mol. Wt.: 347.51

Table 1. Crystal data and structure refinement.

Identification code	**2007src1050**	
Empirical formula	$C_{20}H_{29}NO_2S$	
Formula weight	347.50	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*P*21/*c*	
Unit cell dimensions	a = 7.7257(2) Å	α = 90°
	b = 21.1223(7) Å	β = 96.654(2)°
	c = 11.5315(2) Å	γ = 90°
Volume	1869.09(9) Å^3	
Z	4	
Density (calculated)	1.235 Mg / m^3	
Absorption coefficient	0.185 mm^{-1}	
F(000)	752	
Crystal	Block; Colourless	
Crystal size	0.26 × 0.06 × 0.02 mm^3	
θ range for data collection	3.17 – 27.48°	
Index ranges	$-10 \le h \le 10, -27 \le k \le 27, -11 \le l \le 14$	
Reflections collected	20906	
Independent reflections	4239 [R_{int} = 0.0585]	
Completeness to θ = 27.48°	99.3 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.9963 and 0.9535	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4239 / 0 / 218	
Goodness-of-fit on F^2	0.965	
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0678, *wR2* = 0.1531	
R indices (all data)	*R1* = 0.0950, *wR2* = 0.1737	

Largest diff. peak and hole	0.680 and −0.369 e Å^{-3}

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit* sphere). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography*, part A, pp. 307−326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: *SADABS Version 2.10.* (G. M. Sheldrick (2003)) Bruker AXS Inc., Madison, Wisconsin, USA. S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467−473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** *ORTEP3 for Windows* (L. J. Farrugia, J. Appl. Crystallogr. 1997, 30, 565).

Table 2. Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [Å^2 × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
S1	3421(1)	3096(1)	3734(1)	28(1)	1
O1	2761(3)	3313(1)	4774(2)	32(1)	1
O2	2662(3)	3312(1)	2606(2)	34(1)	1
N1	5468(3)	3287(1)	3844(2)	31(1)	1
C1	6572(3)	3244(1)	4997(2)	28(1)	1
C2	8261(4)	2920(2)	4682(3)	35(1)	1
C3	8349(4)	3108(2)	3407(3)	39(1)	1
C4	6453(4)	3112(2)	2861(2)	36(1)	1
C5	8153(4)	2217(2)	4819(3)	35(1)	1
C6	9248(4)	1867(2)	5494(3)	36(1)	1
C7	9104(5)	1165(2)	5625(3)	44(1)	1
C8	6758(4)	3893(2)	5586(2)	31(1)	1
C9	7581(4)	4405(2)	4890(3)	37(1)	1
C10	7602(5)	5043(2)	5502(3)	44(1)	1
C11	8579(5)	5001(2)	6728(3)	45(1)	1
C12	7808(5)	4486(2)	7437(3)	49(1)	1
C13	7744(4)	3848(2)	6817(3)	38(1)	1
C14	3291(4)	2261(1)	3715(2)	28(1)	1
C15	3516(4)	1929(2)	4764(2)	31(1)	1
C16	3476(4)	1274(2)	4747(3)	35(1)	1
C17	3213(4)	937(2)	3698(3)	35(1)	1
C18	2998(4)	1280(2)	2665(3)	37(1)	1
C19	3039(4)	1933(2)	2658(2)	33(1)	1
C20	3098(5)	228(2)	3687(3)	49(1)	1

Table 3. Bond lengths [Å] and angles [°].

S1–O1	1.432(2)
S1–O2	1.439(2)
S1–N1	1.623(2)
S1–C14	1.765(3)
N1–C4	1.483(4)
N1–C1	1.497(3)
C1–C8	1.531(4)
C1–C2	1.553(4)
C1–H1	0.9800
C2–C5	1.496(5)
C2–C3	1.533(4)
C2–H2	0.9800
C3–C4	1.526(4)
C3–H3A	0.9700
C3–H3B	0.9700
C4–H4A	0.9700
C4–H4B	0.9700
C5–C6	1.310(4)
C5–H5	0.9300
C6–C7	1.494(5)
C6–H6	0.9300
C7–H7A	0.9600
C7–H7B	0.9600
C7–H7C	0.9600
C8–C9	1.529(4)
C8–C13	1.534(4)
C8–H8	0.9800
C9–C10	1.519(5)
C9–H9A	0.9700
C9–H9B	0.9700
C10–C11	1.526(4)
C10–H10A	0.9700
C10–H10B	0.9700
C11–C12	1.524(5)
C11–H11A	0.9700
C11–H11B	0.9700
C12–C13	1.523(5)
C12–H12A	0.9700

C12–H12B	0.9700
C13–H13A	0.9700
C13–H13B	0.9700
C14–C15	1.391(4)
C14–C19	1.397(4)
C15–C16	1.383(4)
C15–H15	0.9300
C16–C17	1.398(4)
C16–H16	0.9300
C17–C18	1.389(4)
C17–C20	1.499(5)
C18–C19	1.379(5)
C18–H18	0.9300
C19–H19	0.9300
C20–H20A	0.9667
C20–H20B	1.0140
C20–H20C	0.9623
O1–S1–O2	120.56(13)
O1–S1–N1	107.05(12)
O2–S1–N1	106.42(12)
O1–S1–C14	107.78(13)
O2–S1–C14	106.85(13)
N1–S1–C14	107.60(14)
C4–N1–C1	112.0(2)
C4–N1–S1	117.38(19)
C1–N1–S1	120.24(18)
N1–C1–C8	110.7(2)
N1–C1–C2	103.1(2)
C8–C1–C2	117.4(2)
N1–C1–H1	108.4
C8–C1–H1	108.4
C2–C1–H1	108.4
C5–C2–C3	111.6(3)
C5–C2–C1	110.7(2)
C3–C2–C1	104.0(2)
C5–C2–H2	110.1
C3–C2–H2	110.1
C1–C2–H2	110.1
C4–C3–C2	104.4(2)
C4–C3–H3A	110.9

C2–C3–H3A	110.9
C4–C3–H3B	110.9
C2–C3–H3B	110.9
H3A–C3–H3B	108.9
N1–C4–C3	103.8(2)
N1–C4–H4A	111.0
C3–C4–H4A	111.0
N1–C4–H4B	111.0
C3–C4–H4B	111.0
H4A–C4–H4B	109.0
C6–C5–C2	125.7(3)
C6–C5–H5	117.1
C2–C5–H5	117.1
C5–C6–C7	124.7(3)
C5–C6–H6	117.6
C7–C6–H6	117.6
C6–C7–H7A	109.5
C6–C7–H7B	109.5
H7A–C7–H7B	109.5
C6–C7–H7C	109.5
H7A–C7–H7C	109.5
H7B–C7–H7C	109.5
C9–C8–C1	115.1(2)
C9–C8–C13	109.7(2)
C1–C8–C13	111.5(2)
C9–C8–H8	106.7
C1–C8–H8	106.7
C13–C8–H8	106.7
C10–C9–C8	111.4(3)
C10–C9–H9A	109.3
C8–C9–H9A	109.3
C10–C9–H9B	109.3
C8–C9–H9B	109.3
H9A–C9–H9B	108.0
C9–C10–C11	111.0(3)
C9–C10–H10A	109.4
C11–C10–H10A	109.4
C9–C10–H10B	109.4
C11–C10–H10B	109.4
H10A–C10–H10B	108.0

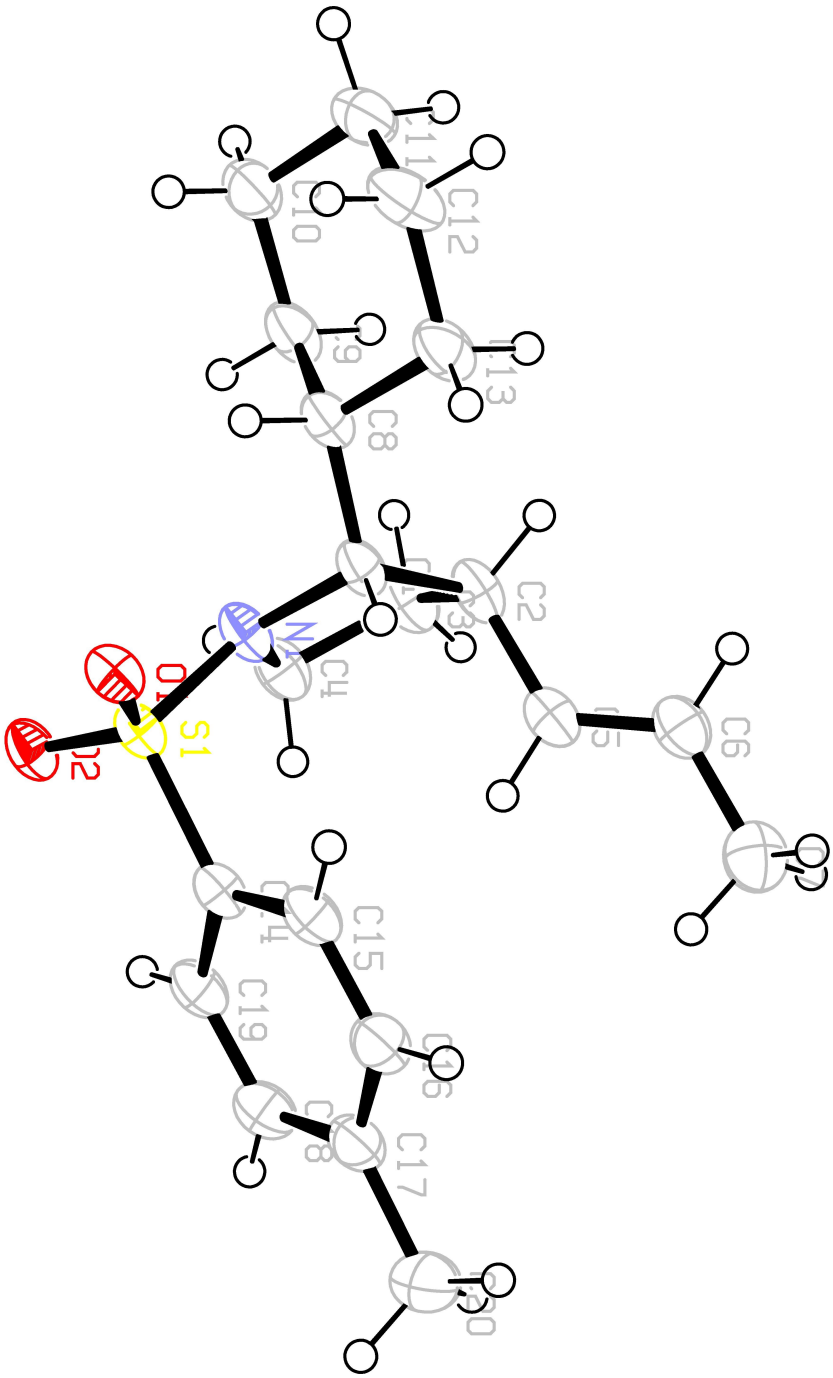
C12–C11–C10	110.8(3)
C12–C11–H11A	109.5
C10–C11–H11A	109.5
C12–C11–H11B	109.5
C10–C11–H11B	109.5
H11A–C11–H11B	108.1
C13–C12–C11	111.9(3)
C13–C12–H12A	109.2
C11–C12–H12A	109.2
C13–C12–H12B	109.2
C11–C12–H12B	109.2
H12A–C12–H12B	107.9
C12–C13–C8	111.4(3)
C12–C13–H13A	109.3
C8–C13–H13A	109.3
C12–C13–H13B	109.3
C8–C13–H13B	109.3
H13A–C13–H13B	108.0
C15–C14–C19	119.9(3)
C15–C14–S1	119.5(2)
C19–C14–S1	120.6(2)
C16–C15–C14	119.5(3)
C16–C15–H15	120.3
C14–C15–H15	120.3
C15–C16–C17	121.5(3)
C15–C16–H16	119.2
C17–C16–H16	119.2
C18–C17–C16	117.8(3)
C18–C17–C20	120.8(3)
C16–C17–C20	121.3(3)
C19–C18–C17	121.8(3)
C19–C18–H18	119.1
C17–C18–H18	119.1
C18–C19–C14	119.5(3)
C18–C19–H19	120.3
C14–C19–H19	120.3
C17–C20–H20A	111.3
C17–C20–H20B	106.0
H20A–C20–H20B	107.8
C17–C20–H20C	111.3

H20A–C20–H20C	112.1
H20B–C20–H20C	108.1

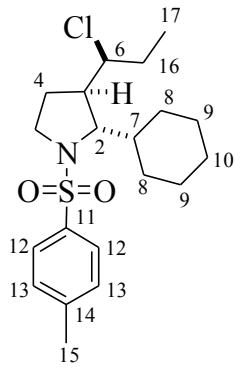
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	22(1)	37(1)	24(1)	1(1)	−1(1)	−3(1)
O1	26(1)	39(1)	30(1)	−2(1)	2(1)	−4(1)
O2	29(1)	45(1)	26(1)	4(1)	−6(1)	−2(1)
N1	24(1)	44(2)	23(1)	4(1)	−1(1)	−6(1)
C1	23(1)	38(2)	22(1)	5(1)	−2(1)	−4(1)
C2	22(1)	51(2)	31(2)	4(1)	−1(1)	−3(1)
C3	28(2)	57(2)	32(2)	3(1)	6(1)	−5(1)
C4	30(2)	51(2)	26(1)	3(1)	2(1)	−4(1)
C5	26(2)	45(2)	32(2)	−3(1)	0(1)	−2(1)
C6	33(2)	46(2)	28(1)	−2(1)	1(1)	−1(1)
C7	45(2)	51(2)	37(2)	−2(2)	5(1)	5(2)
C8	25(1)	39(2)	26(1)	4(1)	−3(1)	−6(1)
C9	31(2)	46(2)	32(2)	12(1)	−7(1)	−11(1)
C10	38(2)	41(2)	49(2)	9(2)	−11(2)	−9(2)
C11	43(2)	41(2)	49(2)	−1(2)	−10(2)	−11(2)
C12	49(2)	59(2)	35(2)	−6(2)	−7(2)	−16(2)
C13	39(2)	45(2)	27(1)	6(1)	−7(1)	−9(1)
C14	22(1)	37(2)	26(1)	0(1)	1(1)	−4(1)
C15	28(1)	43(2)	24(1)	−1(1)	1(1)	−6(1)
C16	32(2)	40(2)	33(2)	4(1)	0(1)	−5(1)
C17	27(2)	39(2)	38(2)	−2(1)	−1(1)	−5(1)
C18	35(2)	44(2)	31(2)	−6(1)	0(1)	−6(1)
C19	31(2)	45(2)	22(1)	−1(1)	−2(1)	−7(1)
C20	53(2)	40(2)	50(2)	−4(2)	−4(2)	−7(2)


C11
C10
C12
C9
C13
C8
C2
C3
N
C4
O1
S1
O2
C5
C6
C14
C15
C19
C16
C18
C17
C20

X-Ray data for (2*S*,3*R*)-3-((*S*)-1-chloropropyl)-2-cyclohexyl-1-tosylpyrrolidine and (2*R*,3*S*)-3-((*R*)-1-chloropropyl)-2-cyclohexyl-1-tosylpyrrolidine (130c).



$C_{20}H_{30}ClNO_2S$
Mol. Wt.: 383.98

Table 1. Crystal data and structure refinement.

Identification code	**2007src1053**	
Empirical formula	$C_{20}H_{30}ClNO_2S$	
Formula weight	383.96	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	*Pbca*	
Unit cell dimensions	a = 13.0538(3) Å	α = 90°
	b = 15.5288(3) Å	β = 90°
	c = 19.1088(4) Å	γ = 90°
Volume	3873.54(14) Å^3	
Z	8	
Density (calculated)	1.317 Mg / m^3	
Absorption coefficient	0.319 mm^{-1}	
F(000)	1648	
Crystal	Wedge; Colourless	
Crystal size	0.60 × 0.50 × 0.50 mm^3	
θ range for data collection	2.95 – 27.48°	
Index ranges	$-16 \le h \le 16, -20 \le k \le 19, -24 \le l \le 24$	
Reflections collected	31418	
Independent reflections	4422 [R_{int} = 0.0516]	
Completeness to θ = 27.48°	99.6 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	0.8569 and 0.8318	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4422 / 0 / 228	
Goodness-of-fit on F^2	1.025	
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0406, $wR2$ = 0.1017	

R indices (all data)	$R1 = 0.0550$, $wR2 = 0.1096$
Largest diff. peak and hole	0.875 and −0.417 e Å^{-3}

Diffractometer: *Nonius KappaCCD* area detector (ϕ scans and ω scans to fill *asymmetric unit* sphere). **Cell determination:** DirAx (Duisenberg, A.J.M.(1992). J. Appl. Cryst. 25, 92-96.) **Data collection:** Collect (Collect: Data collection software, R. Hooft, Nonius B.V., 1998). **Data reduction and cell refinement**: *Denzo* (Z. Otwinowski & W. Minor, *Methods in Enzymology* (1997) Vol. **276**: *Macromolecular Crystallography,* part A, pp. 307−326; C. W. Carter, Jr. & R. M. Sweet, Eds., Academic Press). **Absorption correction**: *SADABS Version 2.10.* (G. M. Sheldrick (2003)) Bruker AXS Inc., Madison, Wisconsin, USA. S**tructure solution**: *SHELXS97* (G. M. Sheldrick, Acta Cryst. (1990) A**46** 467−473). S**tructure refinement**: *SHELXL97* (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** *ORTEP3 for Windows* (L. J. Farrugia, J. Appl. Crystallogr. 1997, 30, 565).

Table 2. Atomic coordinates [$\times 10^4$], equivalent isotropic displacement parameters [Å$^2 \times 10^3$] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
S1	2799(1)	8292(1)	962(1)	16(1)	1
Cl1	625(1)	9994(1)	1954(1)	30(1)	1
O1	2918(1)	8092(1)	232(1)	22(1)	1
O2	3502(1)	7934(1)	1461(1)	23(1)	1
N1	2875(1)	9328(1)	1054(1)	16(1)	1
C16	293(1)	7602(1)	2059(1)	21(1)	1
C14	1554(1)	7948(1)	1190(1)	15(1)	1
C18	−111(1)	7447(1)	843(1)	22(1)	1
C15	1273(1)	7878(1)	1891(1)	18(1)	1
C2	2109(1)	10731(1)	1108(1)	17(1)	1
C9	1933(1)	10619(1)	−555(1)	20(1)	1
C17	−407(1)	7371(1)	1540(1)	20(1)	1
C3	2964(1)	10641(1)	1655(1)	22(1)	1
C8	2663(1)	10093(1)	−94(1)	17(1)	1
C19	859(1)	7740(1)	666(1)	19(1)	1
C6	220(1)	11102(1)	881(1)	22(1)	1
C5	1045(1)	10897(1)	1418(1)	20(1)	1
C4	3126(2)	9678(1)	1755(1)	22(1)	1
C1	2205(1)	9920(1)	636(1)	16(1)	1
C7	−797(2)	11372(1)	1197(1)	28(1)	1
C20	−1448(2)	7021(1)	1731(1)	29(1)	1
C13	3710(1)	10530(1)	−71(1)	22(1)	1
C11	3417(2)	11143(1)	−1278(1)	31(1)	1
C10	2365(2)	10723(1)	−1295(1)	26(1)	1
C12	4150(2)	10642(1)	−807(1)	28(1)	1

Table 3. Bond lengths [Å] and angles [°].

S1–O2	1.4360(13)
S1–O1	1.4376(13)
S1–N1	1.6203(15)
S1–C14	1.7654(17)
Cl1–C5	1.8212(18)
N1–C4	1.483(2)
N1–C1	1.499(2)
C16–C15	1.387(3)
C16–C17	1.396(3)
C16–H16	0.9500
C14–C19	1.390(2)
C14–C15	1.393(2)
C18–C19	1.387(3)
C18–C17	1.392(2)
C18–H18	0.9500
C15–H15	0.9500
C2–C5	1.532(2)
C2–C3	1.535(2)
C2–C1	1.554(2)
C2–H2	1.0000
C9–C10	1.531(2)
C9–C8	1.534(2)
C9–H9A	0.9900
C9–H9B	0.9900
C17–C20	1.508(3)
C3–C4	1.523(3)
C3–H3A	0.9900
C3–H3B	0.9900
C8–C13	1.527(3)
C8–C1	1.541(2)
C8–H8	1.0000
C19–H19	0.9500
C6–C7	1.518(3)
C6–C5	1.522(3)
C6–H6A	0.9900
C6–H6B	0.9900
C5–H5	1.0000
C4–H4A	0.9900

C4–H4B	0.9900
C1–H1	1.0000
C7–H7A	0.9800
C7–H7B	0.9800
C7–H7C	0.9800
C20–H20A	0.9800
C20–H20B	0.9800
C20–H20C	0.9800
C13–C12	1.529(2)
C13–H13A	0.9900
C13–H13B	0.9900
C11–C10	1.522(3)
C11–C12	1.526(3)
C11–H11A	0.9900
C11–H11B	0.9900
C10–H10A	0.9900
C10–H10B	0.9900
C12–H12A	0.9900
C12–H12B	0.9900
O2–S1–O1	119.50(8)
O2–S1–N1	105.89(8)
O1–S1–N1	108.24(7)
O2–S1–C14	107.85(8)
O1–S1–C14	105.86(8)
N1–S1–C14	109.24(8)
C4–N1–C1	112.66(13)
C4–N1–S1	118.37(11)
C1–N1–S1	121.01(11)
C15–C16–C17	121.15(16)
C15–C16–H16	119.4
C17–C16–H16	119.4
C19–C14–C15	120.10(16)
C19–C14–S1	119.62(13)
C15–C14–S1	120.28(13)
C19–C18–C17	120.96(16)
C19–C18–H18	119.5
C17–C18–H18	119.5
C16–C15–C14	119.45(16)
C16–C15–H15	120.3
C14–C15–H15	120.3

C5–C2–C3	114.30(14)
C5–C2–C1	115.71(14)
C3–C2–C1	105.27(13)
C5–C2–H2	107.0
C3–C2–H2	107.0
C1–C2–H2	107.0
C10–C9–C8	110.95(15)
C10–C9–H9A	109.4
C8–C9–H9A	109.4
C10–C9–H9B	109.4
C8–C9–H9B	109.4
H9A–C9–H9B	108.0
C18–C17–C16	118.51(17)
C18–C17–C20	120.78(17)
C16–C17–C20	120.68(16)
C4–C3–C2	105.97(14)
C4–C3–H3A	110.5
C2–C3–H3A	110.5
C4–C3–H3B	110.5
C2–C3–H3B	110.5
H3A–C3–H3B	108.7
C13–C8–C9	109.58(14)
C13–C8–C1	113.54(14)
C9–C8–C1	111.84(14)
C13–C8–H8	107.2
C9–C8–H8	107.2
C1–C8–H8	107.2
C18–C19–C14	119.80(16)
C18–C19–H19	120.1
C14–C19–H19	120.1
C7–C6–C5	114.08(15)
C7–C6–H6A	108.7
C5–C6–H6A	108.7
C7–C6–H6B	108.7
C5–C6–H6B	108.7
H6A–C6–H6B	107.6
C6–C5–C2	114.62(14)
C6–C5–Cl1	109.13(13)
C2–C5–Cl1	111.13(12)
C6–C5–H5	107.2

C2–C5–H5	107.2
Cl1–C5–H5	107.2
N1–C4–C3	102.46(14)
N1–C4–H4A	111.3
C3–C4–H4A	111.3
N1–C4–H4B	111.3
C3–C4–H4B	111.3
H4A–C4–H4B	109.2
N1–C1–C8	111.26(14)
N1–C1–C2	103.59(13)
C8–C1–C2	114.53(13)
N1–C1–H1	109.1
C8–C1–H1	109.1
C2–C1–H1	109.1
C6–C7–H7A	109.5
C6–C7–H7B	109.5
H7A–C7–H7B	109.5
C6–C7–H7C	109.5
H7A–C7–H7C	109.5
H7B–C7–H7C	109.5
C17–C20–H20A	109.5
C17–C20–H20B	109.5
H20A–C20–H20B	109.5
C17–C20–H20C	109.5
H20A–C20–H20C	109.5
H20B–C20–H20C	109.5
C8–C13–C12	111.16(15)
C8–C13–H13A	109.4
C12–C13–H13A	109.4
C8–C13–H13B	109.4
C12–C13–H13B	109.4
H13A–C13–H13B	108.0
C10–C11–C12	111.14(16)
C10–C11–H11A	109.4
C12–C11–H11A	109.4
C10–C11–H11B	109.4
C12–C11–H11B	109.4
H11A–C11–H11B	108.0
C11–C10–C9	110.96(16)
C11–C10–H10A	109.4

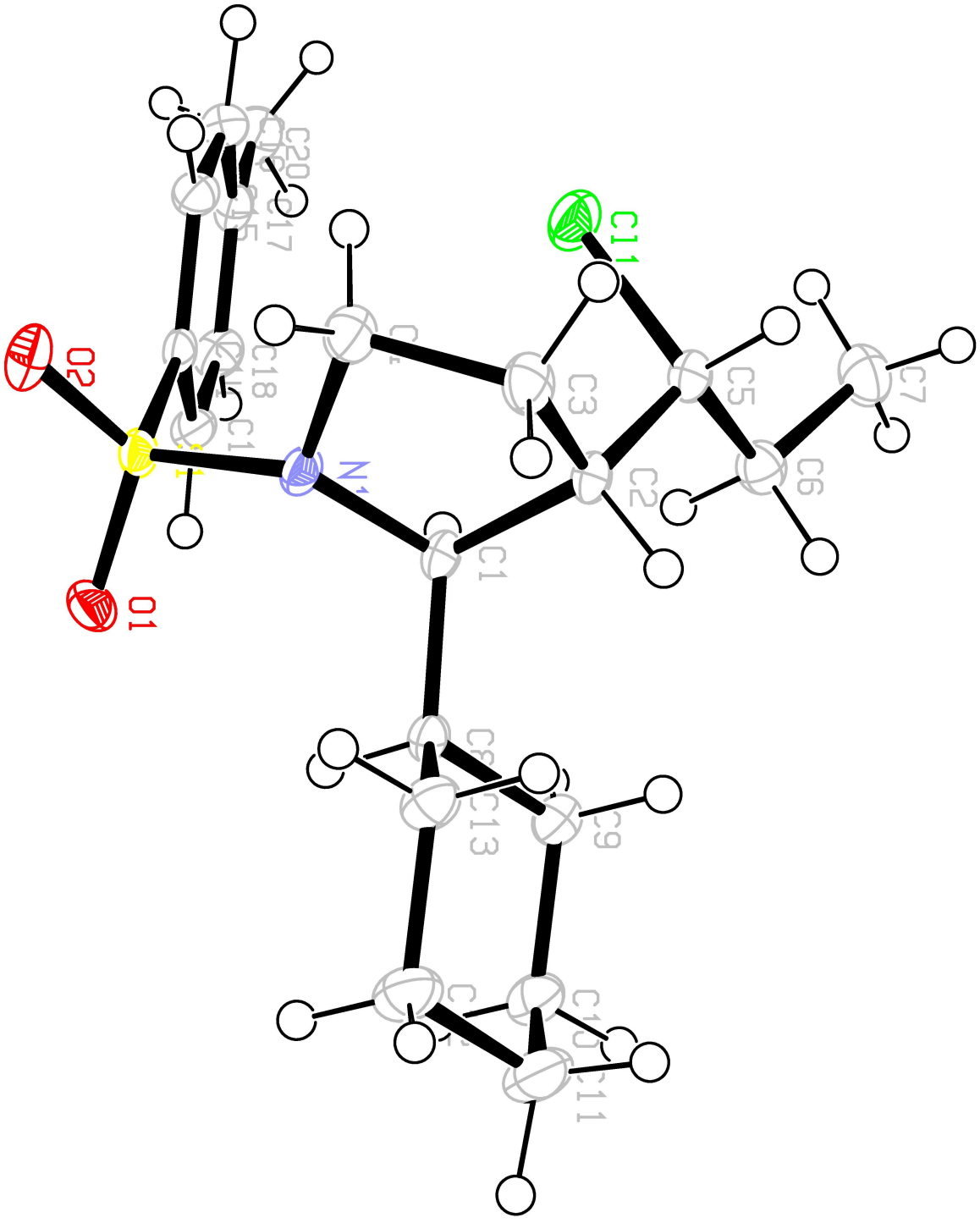
C9–C10–H10A	109.4
C11–C10–H10B	109.4
C9–C10–H10B	109.4
H10A–C10–H10B	108.0
C11–C12–C13	111.32(16)
C11–C12–H12A	109.4
C13–C12–H12A	109.4
C11–C12–H12B	109.4
C13–C12–H12B	109.4
H12A–C12–H12B	108.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S1	18(1)	10(1)	20(1)	1(1)	3(1)	1(1)
Cl1	32(1)	22(1)	36(1)	11(1)	12(1)	5(1)
O1	29(1)	16(1)	23(1)	−3(1)	9(1)	1(1)
O2	19(1)	17(1)	33(1)	5(1)	−3(1)	3(1)
N1	21(1)	11(1)	17(1)	2(1)	−1(1)	0(1)
C16	24(1)	20(1)	18(1)	2(1)	3(1)	2(1)
C14	18(1)	9(1)	19(1)	0(1)	1(1)	2(1)
C18	23(1)	21(1)	21(1)	1(1)	−6(1)	−2(1)
C15	23(1)	16(1)	16(1)	0(1)	−2(1)	−1(1)
C2	21(1)	10(1)	20(1)	0(1)	1(1)	0(1)
C9	21(1)	19(1)	20(1)	2(1)	−2(1)	0(1)
C17	19(1)	14(1)	25(1)	3(1)	1(1)	2(1)
C3	26(1)	16(1)	24(1)	−3(1)	−3(1)	−1(1)
C8	22(1)	11(1)	18(1)	0(1)	0(1)	0(1)
C19	25(1)	17(1)	15(1)	2(1)	−1(1)	1(1)
C6	22(1)	20(1)	23(1)	−1(1)	1(1)	−1(1)
C5	26(1)	13(1)	22(1)	0(1)	3(1)	0(1)
C4	28(1)	18(1)	20(1)	−2(1)	−5(1)	1(1)
C1	18(1)	10(1)	19(1)	1(1)	−1(1)	0(1)
C7	27(1)	28(1)	30(1)	−4(1)	−1(1)	7(1)
C20	23(1)	29(1)	36(1)	5(1)	2(1)	−4(1)
C13	20(1)	23(1)	23(1)	5(1)	1(1)	−2(1)

C11	34(1)	31(1)	27(1)	12(1)	4(1)	−2(1)
C10	32(1)	25(1)	20(1)	5(1)	−1(1)	2(1)
C12	25(1)	32(1)	28(1)	9(1)	5(1)	−3(1)


C20
C17
C15
C11
O2
C18
C16
C14
C3
C5
C7
C12
C2
C6
N1
C1
O1
C8
C13
C9
C10
C11