Organic Crystal Engineering with 1,4-Piperazine-2,5-diones. 7. Crystal Packing of Piperazinediones Derived from 2-Amino-7-nitro-4-methoxyindan-2-carboxylic Acid

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SUPPORTING INFORMATION: X-RAY CRYSTALLOGRAPHY

General experimental.

Data were collected using a Bruker SMART 1000 diffractometer ((*S,S*)-**6**[*a*]; *rac*-**6**[*c*]; (*R,S*)-**9**; (*S,S*)-**9**)), a Nonius KappaCCD diffractometer (*rac*-**6**[*b*]) and a Bruker APEXII diffractometer (*meso*-**6**). For all data collections graphite-monochromated MoK_α radiation was used, except *meso*-**6** which was collected using synchrotron radiation (λ = 0.7749 Å) at beamline XXX of the Advanced Light Source, Berkeley, USA. Programs used: Bruker SMART ((*S,S*)-**6**[*a*]; *rac*-**6**[*c*]; (*R,S*)-**9**; (*S,S*)-**9**)), Nonius COLLECT (*rac*-**6**[*b*]) and Bruker APEXII (*meso*-**6**) for diffractometer control and data collection; Bruker SAINT ((*S,S*)-**6**[*a*]; *rac*-**6**[*c*]; (*R,S*)-**9**; (*S,S*)-**9;** *meso*-**6**)) and EvalCCD (*rac*-**6**[*b*]) for data integration and reduction; SADABS (all structures) for absorption correction; SHELXTL (all structures) for structure solution and full-matrix least-squares refinement. Molecular diagrams were produced using Mercury 1.4.1.

SMART (data collection)
Bruker (2001). SMART. Bruker AXS Inc., Madison, Wisconsin, USA.

SAINT (integration and reduction)
Bruker (2001). SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.

COLLECT (data collection)
Nonius, COLLECT, Nonius BV, Delft, The Netherlands, 1999.

EvalCCD (integration and reduction)
Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst*. **36**, 220–229.

SADABS (absorption correction)
Sheldrick, G. M. (2007). SADABS. University of Göttingen, Germany.

SHELXTL (structure solution and refinement)
Sheldrick, G. M. (2001). SHELXTL. Version 6. Bruker AXS Inc., Madison, Wisconsin, USA.

MERCURY (molecular graphics – hydrogen bonding and packing)
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst*. **39**, 453-457.

Crystallographic data for *(S,S)*-**6**[a]

Table 1. Crystal data and structure refinement for *(S,S)*-**6**[a].

Identification code	*(S,S)*-**6**[a]	
Chemical formula (moiety)	$C_{22}H_{20}N_4O_8 \cdot C_3H_7NO$	
Chemical formula (total)	$C_{25}H_{27}N_5O_9$	
Formula weight	541.52	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	orthorhombic, $P2_12_12_1$	
Unit cell parameters	a = 6.341(3) Å	α = 90°
	b = 19.275(10) Å	β = 90°
	c = 20.483(10) Å	γ = 90°
Cell volume	2503(2) Å^3	
Z	4	
Calculated density	1.437 g/cm^3	
Absorption coefficient μ	0.111 mm^{-1}	
F(000)	1136	
Crystal colour and size	colourless, 0.41 × 0.25 × 0.15 mm^3	
Reflections for cell refinement	5790 (θ range 2.2 to 25.6°)	
Data collection method	Bruker SMART 1000 CCD diffractometer thin-slice ω scans	
θ range for data collection	1.5 to 25.1°	
Index ranges	h −7 to 7, k −22 to 23, l −24 to 24	
Completeness to θ = 25.1°	87.4 %	
Reflections collected	12513	
Independent reflections	2258 (R_{int} = 0.0673)	
Reflections with $F^2>2\sigma$	1806	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.9559 and 0.9835	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.1834, 8.8568	
Data / restraints / parameters	2258 / 87 / 370	
Final R indices [$F^2>2\sigma$]	R1 = 0.1083, wR2 = 0.2743	
R indices (all data)	R1 = 0.1280, wR2 = 0.2989	
Goodness-of-fit on F^2	1.062	
Absolute structure parameter	0(10)	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.68 and −0.55 e Å^{-3}	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for *(S,S)*-**6**[a]. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1)	0.3715(10)	–0.0813(4)	0.3042(3)	0.0324(15)
O(2)	–0.3335(10)	–0.0956(3)	0.1642(3)	0.0286(15)
O(3)	–0.0276(12)	–0.1376(3)	0.5019(3)	0.0346(15)
O(4)	–0.0262(12)	–0.0722(4)	0.5876(3)	0.0378(16)
O(5)	–0.0292(11)	0.1534(3)	0.3699(3)	0.0287(14)
O(6)	0.0281(14)	–0.1182(4)	–0.1161(3)	0.0453(19)
O(7)	0.0490(12)	–0.1697(3)	–0.0228(3)	0.0361(16)
O(8)	0.0181(11)	0.1378(3)	0.0710(3)	0.0262(13)
N(1)	–0.1779(11)	–0.0836(4)	0.2621(4)	0.0241(16)
N(2)	0.2093(11)	–0.0844(4)	0.2064(4)	0.0243(16)
N(3)	–0.0276(13)	–0.0797(4)	0.5272(4)	0.0310(17)
N(4)	0.0337(12)	–0.1159(4)	–0.0565(4)	0.0283(16)
C(1)	0.2089(13)	–0.0754(5)	0.2707(4)	0.0228(18)
C(2)	–0.0002(13)	–0.0569(4)	0.3033(4)	0.0214(17)
C(3)	–0.1740(14)	–0.0822(5)	0.1970(5)	0.0258(19)
C(4)	0.0359(13)	–0.0637(4)	0.1625(4)	0.0186(16)
C(5)	–0.0136(17)	–0.0859(4)	0.3732(4)	0.0264(19)
C(6)	–0.0206(13)	–0.0249(4)	0.4167(4)	0.0253(18)
C(7)	–0.0258(13)	–0.0194(4)	0.4856(3)	0.0219(17)
C(8)	–0.0381(14)	0.0451(5)	0.5171(5)	0.031(2)
C(9)	–0.0355(15)	0.1037(5)	0.4786(5)	0.033(2)
C(10)	–0.0294(13)	0.1007(5)	0.4118(5)	0.0277(19)
C(11)	–0.0185(14)	0.0356(4)	0.3817(4)	0.0229(17)
C(12)	–0.0102(17)	0.0232(4)	0.3114(4)	0.029(2)
C(13)	–0.043(2)	0.2226(4)	0.3967(5)	0.039(2)
C(14)	0.0511(14)	–0.1017(4)	0.0964(4)	0.0237(18)
C(15)	0.0385(12)	–0.0469(4)	0.0446(4)	0.0192(17)
C(16)	0.0369(15)	–0.0504(4)	–0.0245(4)	0.0243(18)
C(17)	0.0265(14)	0.0090(5)	–0.0609(4)	0.0273(19)
C(18)	0.0217(14)	0.0738(5)	–0.0336(5)	0.032(2)
C(19)	0.0238(13)	0.0776(4)	0.0360(4)	0.0233(17)
C(20)	0.0318(13)	0.0184(4)	0.0733(4)	0.0197(16)
C(21)	0.0351(15)	0.0151(4)	0.1480(4)	0.0225(17)
C(22)	0.020(2)	0.2024(5)	0.0342(5)	0.040(2)
O(9)	0.402(6)	0.2939(18)	0.135(2)	0.089(13)
C(23)	0.522(5)	0.247(2)	0.1503(14)	0.058(3)
N(5)	0.506(3)	0.2192(10)	0.2094(10)	0.037(6)
C(24)	0.278(3)	0.2087(15)	0.2260(15)	0.058(3)
C(25)	0.603(4)	0.1517(13)	0.2228(15)	0.058(3)
O(9')	0.357(3)	0.2889(9)	0.1314(10)	0.033(5)
C(23')	0.482(5)	0.2450(18)	0.1487(13)	0.058(3)
N(5')	0.465(4)	0.2098(14)	0.2022(11)	0.055(8)
C(24')	0.328(4)	0.2320(14)	0.2526(12)	0.058(3)
C(25')	0.651(4)	0.1733(14)	0.2240(13)	0.058(3)

Table 3. Bond lengths [Å] and angles [°] for *(S,S)*-**6**[a].

O(1)–C(1)	1.244(11)	O(2)–C(3)	1.242(12)
O(3)–N(3)	1.229(10)	O(4)–N(3)	1.247(10)
O(5)–C(10)	1.331(11)	O(5)–C(13)	1.445(9)
O(6)–N(4)	1.221(10)	O(7)–N(4)	1.250(11)
O(8)–C(19)	1.365(10)	O(8)–C(22)	1.457(10)
N(1)–H(1)	0.8800	N(1)–C(2)	1.499(11)
N(1)–C(3)	1.333(12)	N(2)–H(2)	0.8800
N(2)–C(1)	1.328(11)	N(2)–C(4)	1.477(10)
N(3)–C(7)	1.442(12)	N(4)–C(16)	1.423(11)
C(1)–C(2)	1.527(12)	C(2)–C(5)	1.539(11)
C(2)–C(12)	1.553(10)	C(3)–C(4)	1.550(12)
C(4)–C(14)	1.543(10)	C(4)–C(21)	1.547(11)
C(5)–H(5A)	0.9900	C(5)–H(5B)	0.9900
C(5)–C(6)	1.476(11)	C(6)–C(7)	1.415(11)
C(6)–C(11)	1.369(12)	C(7)–C(8)	1.404(12)
C(8)–H(8)	0.9500	C(8)–C(9)	1.378(14)
C(9)–H(9)	0.9500	C(9)–C(10)	1.371(13)
C(10)–C(11)	1.399(12)	C(11)–C(12)	1.461(11)
C(12)–H(12A)	0.9900	C(12)–H(12B)	0.9900
C(13)–H(13A)	0.9800	C(13)–H(13B)	0.9800
C(13)–H(13C)	0.9800	C(14)–H(14A)	0.9900
C(14)–H(14B)	0.9900	C(14)–C(15)	1.500(12)
C(15)–C(16)	1.417(11)	C(15)–C(20)	1.389(11)
C(16)–C(17)	1.368(12)	C(17)–H(17)	0.9500
C(17)–C(18)	1.369(14)	C(18)–H(18)	0.9500
C(18)–C(19)	1.426(13)	C(19)–C(20)	1.375(11)
C(20)–C(21)	1.533(10)	C(21)–H(21A)	0.9900
C(21)–H(21B)	0.9900	C(22)–H(22A)	0.9800
C(22)–H(22B)	0.9800	C(22)–H(22C)	0.9800
O(9)–C(23)	1.224(19)	C(23)–H(23)	0.9500
C(23)–N(5)	1.325(17)	N(5)–C(24)	1.496(18)
N(5)–C(25)	1.465(18)	C(24)–H(24A)	0.9800
C(24)–H(24B)	0.9800	C(24)–H(24C)	0.9800
C(25)–H(25A)	0.9800	C(25)–H(25B)	0.9800
C(25)–H(25C)	0.9800	O(9')–C(23')	1.214(17)
C(23')–H(23')	0.9500	C(23')–N(5')	1.294(17)
N(5')–C(24')	1.414(17)	N(5')–C(25')	1.444(17)
C(24')–H(24D)	0.9800	C(24')–H(24E)	0.9800
C(24')–H(24F)	0.9800	C(25')–H(25D)	0.9800
C(25')–H(25E)	0.9800	C(25')–H(25F)	0.9800

C(10)–O(5)–C(13)	117.3(7)	C(19)–O(8)–C(22)	117.0(6)
H(1)–N(1)–C(2)	118.6	H(1)–N(1)–C(3)	118.6
C(2)–N(1)–C(3)	122.9(7)	H(2)–N(2)–C(1)	117.7
H(2)–N(2)–C(4)	117.7	C(1)–N(2)–C(4)	124.6(7)
O(3)–N(3)–O(4)	121.6(8)	O(3)–N(3)–C(7)	118.9(7)
O(4)–N(3)–C(7)	119.5(7)	O(6)–N(4)–O(7)	121.6(8)
O(6)–N(4)–C(16)	119.5(8)	O(7)–N(4)–C(16)	118.7(7)

O(1)–C(1)–N(2)	122.3(8)	O(1)–C(1)–C(2)	119.9(8)
N(2)–C(1)–C(2)	117.8(7)	N(1)–C(2)–C(1)	109.0(6)
N(1)–C(2)–C(5)	111.0(7)	N(1)–C(2)–C(12)	111.8(7)
C(1)–C(2)–C(5)	111.7(7)	C(1)–C(2)–C(12)	108.3(7)
C(5)–C(2)–C(12)	105.1(6)	O(2)–C(3)–N(1)	121.5(8)
O(2)–C(3)–C(4)	120.0(8)	N(1)–C(3)–C(4)	118.5(8)
N(2)–C(4)–C(3)	107.4(6)	N(2)–C(4)–C(14)	111.1(7)
N(2)–C(4)–C(21)	112.6(7)	C(3)–C(4)–C(14)	110.2(7)
C(3)–C(4)–C(21)	108.2(7)	C(14)–C(4)–C(21)	107.4(6)
C(2)–C(5)–H(5A)	110.6	C(2)–C(5)–H(5B)	110.6
C(2)–C(5)–C(6)	105.9(7)	H(5A)–C(5)–H(5B)	108.7
H(5A)–C(5)–C(6)	110.6	H(5B)–C(5)–C(6)	110.6
C(5)–C(6)–C(7)	131.5(8)	C(5)–C(6)–C(11)	111.2(7)
C(7)–C(6)–C(11)	117.3(7)	N(3)–C(7)–C(6)	121.9(7)
N(3)–C(7)–C(8)	116.2(7)	C(6)–C(7)–C(8)	121.8(8)
C(7)–C(8)–H(8)	121.3	C(7)–C(8)–C(9)	117.5(8)
H(8)–C(8)–C(9)	121.3	C(8)–C(9)–H(9)	118.8
C(8)–C(9)–C(10)	122.5(9)	H(9)–C(9)–C(10)	118.8
O(5)–C(10)–C(9)	127.7(8)	O(5)–C(10)–C(11)	113.6(8)
C(9)–C(10)–C(11)	118.7(9)	C(6)–C(11)–C(10)	122.1(8)
C(6)–C(11)–C(12)	112.2(7)	C(10)–C(11)–C(12)	125.6(8)
C(2)–C(12)–C(11)	105.6(7)	C(2)–C(12)–H(12A)	110.6
C(2)–C(12)–H(12B)	110.6	C(11)–C(12)–H(12A)	110.6
C(11)–C(12)–H(12B)	110.6	H(12A)–C(12)–H(12B)	108.8
O(5)–C(13)–H(13A)	109.5	O(5)–C(13)–H(13B)	109.5
O(5)–C(13)–H(13C)	109.5	H(13A)–C(13)–H(13B)	109.5
H(13A)–C(13)–H(13C)	109.5	H(13B)–C(13)–H(13C)	109.5
C(4)–C(14)–H(14A)	110.5	C(4)–C(14)–H(14B)	110.5
C(4)–C(14)–C(15)	106.4(6)	H(14A)–C(14)–H(14B)	108.6
H(14A)–C(14)–C(15)	110.5	H(14B)–C(14)–C(15)	110.5
C(14)–C(15)–C(16)	132.3(7)	C(14)–C(15)–C(20)	110.0(6)
C(16)–C(15)–C(20)	117.7(7)	N(4)–C(16)–C(15)	120.2(7)
N(4)–C(16)–C(17)	119.5(7)	C(15)–C(16)–C(17)	120.3(8)
C(16)–C(17)–H(17)	118.6	C(16)–C(17)–C(18)	122.8(8)
H(17)–C(17)–C(18)	118.6	C(17)–C(18)–H(18)	121.5
C(17)–C(18)–C(19)	117.1(8)	H(18)–C(18)–C(19)	121.5
O(8)–C(19)–C(18)	124.7(7)	O(8)–C(19)–C(20)	114.5(7)
C(18)–C(19)–C(20)	120.8(8)	C(15)–C(20)–C(19)	121.2(7)
C(15)–C(20)–C(21)	112.6(7)	C(19)–C(20)–C(21)	126.2(7)
C(4)–C(21)–C(20)	103.4(6)	C(4)–C(21)–H(21A)	111.1
C(4)–C(21)–H(21B)	111.1	C(20)–C(21)–H(21A)	111.1
C(20)–C(21)–H(21B)	111.1	H(21A)–C(21)–H(21B)	109.1
O(8)–C(22)–H(22A)	109.5	O(8)–C(22)–H(22B)	109.5
O(8)–C(22)–H(22C)	109.5	H(22A)–C(22)–H(22B)	109.5
H(22A)–C(22)–H(22C)	109.5	H(22B)–C(22)–H(22C)	109.5
O(9)–C(23)–H(23)	120.6	O(9)–C(23)–N(5)	119(3)
H(23)–C(23)–N(5)	120.6	C(23)–N(5)–C(24)	109.6(17)
C(23)–N(5)–C(25)	120(2)	C(24)–N(5)–C(25)	104.0(15)
N(5)–C(24)–H(24A)	109.5	N(5)–C(24)–H(24B)	109.5
N(5)–C(24)–H(24C)	109.5	H(24A)–C(24)–H(24B)	109.5
H(24A)–C(24)–H(24C)	109.5	H(24B)–C(24)–H(24C)	109.5

N(5)–C(25)–H(25A)	109.5	N(5)–C(25)–H(25B)	109.5
N(5)–C(25)–H(25C)	109.5	H(25A)–C(25)–H(25B)	109.5
H(25A)–C(25)–H(25C)	109.5	H(25B)–C(25)–H(25C)	109.5
O(9')–C(23')–H(23')	118.1	O(9')–C(23')–N(5')	124(2)
H(23')–C(23')–N(5')	118.1	C(23')–N(5')–C(24')	120.9(18)
C(23')–N(5')–C(25')	116.6(17)	C(24')–N(5')–C(25')	114.9(16)
N(5')–C(24')–H(24D)	109.5	N(5')–C(24')–H(24E)	109.5
N(5')–C(24')–H(24F)	109.5	H(24D)–C(24')–H(24E)	109.5
H(24D)–C(24')–H(24F)	109.5	H(24E)–C(24')–H(24F)	109.5
N(5')–C(25')–H(25D)	109.5	N(5')–C(25')–H(25E)	109.5
N(5')–C(25')–H(25F)	109.5	H(25D)–C(25')–H(25E)	109.5
H(25D)–C(25')–H(25F)	109.5	H(25E)–C(25')–H(25F)	109.5

Table 4. Anisotropic displacement parameters (Å^2) for *(S,S)*-**6**^{a}. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	0.026(3)	0.047(4)	0.024(3)	–0.003(3)	–0.004(3)	–0.008(3)
O(2)	0.020(3)	0.040(4)	0.026(3)	0.008(3)	–0.006(3)	0.004(3)
O(3)	0.036(4)	0.036(3)	0.031(3)	0.007(3)	0.002(3)	–0.001(3)
O(4)	0.036(4)	0.064(4)	0.013(3)	0.007(3)	0.005(3)	–0.005(4)
O(5)	0.038(4)	0.019(3)	0.030(3)	–0.006(2)	–0.002(3)	0.004(3)
O(6)	0.050(5)	0.054(4)	0.033(4)	–0.006(3)	–0.006(4)	–0.009(4)
O(7)	0.036(4)	0.035(3)	0.037(3)	–0.007(3)	0.003(3)	0.002(3)
O(8)	0.033(3)	0.024(3)	0.022(3)	0.003(2)	0.010(3)	0.002(3)
N(1)	0.018(3)	0.025(4)	0.029(4)	0.002(3)	0.001(3)	–0.003(3)
N(2)	0.018(3)	0.033(4)	0.023(4)	–0.003(3)	–0.002(3)	0.002(3)
N(3)	0.020(4)	0.047(4)	0.027(4)	–0.002(3)	–0.005(3)	0.008(4)
N(4)	0.014(3)	0.043(4)	0.028(4)	–0.002(3)	0.000(3)	0.000(3)
C(1)	0.021(4)	0.024(4)	0.024(4)	0.003(3)	–0.014(4)	–0.004(3)
C(2)	0.018(4)	0.017(3)	0.029(4)	–0.007(3)	0.008(4)	–0.006(3)
C(3)	0.025(4)	0.025(4)	0.028(5)	0.001(4)	0.009(4)	0.003(4)
C(4)	0.018(4)	0.027(4)	0.011(3)	0.001(3)	–0.012(3)	0.005(3)
C(5)	0.036(5)	0.026(4)	0.017(4)	–0.004(3)	0.002(4)	–0.006(4)
C(6)	0.011(4)	0.033(4)	0.032(4)	–0.009(4)	–0.007(4)	0.000(4)
C(7)	0.014(4)	0.043(5)	0.009(3)	–0.007(3)	–0.005(3)	–0.006(4)
C(8)	0.012(4)	0.043(5)	0.037(5)	–0.014(4)	0.002(4)	–0.004(4)
C(9)	0.017(4)	0.045(5)	0.038(5)	–0.011(4)	–0.002(4)	–0.005(4)
C(10)	0.012(4)	0.033(4)	0.038(5)	–0.008(4)	0.001(4)	0.008(4)
C(11)	0.016(4)	0.030(4)	0.022(4)	–0.003(3)	–0.004(3)	0.006(4)
C(12)	0.039(5)	0.022(4)	0.027(4)	0.001(3)	0.007(4)	–0.004(4)
C(13)	0.054(6)	0.013(4)	0.051(6)	–0.013(4)	0.002(6)	0.009(4)
C(14)	0.026(4)	0.026(4)	0.019(4)	–0.012(3)	–0.003(4)	0.000(4)
C(15)	0.008(3)	0.031(4)	0.019(4)	–0.007(3)	–0.001(3)	0.003(3)
C(16)	0.021(4)	0.029(4)	0.023(4)	0.005(3)	0.000(4)	0.004(4)
C(17)	0.013(4)	0.053(5)	0.017(4)	0.005(4)	–0.001(3)	–0.004(4)
C(18)	0.018(4)	0.036(4)	0.042(5)	0.005(4)	0.000(4)	–0.001(4)
C(19)	0.015(4)	0.025(4)	0.030(4)	0.003(3)	0.002(4)	–0.006(4)

C(20)	0.017(4)	0.025(4)	0.017(4)	–0.003(3)	0.000(3)	0.004(4)
C(21)	0.026(4)	0.025(4)	0.016(4)	–0.001(3)	–0.001(4)	0.003(4)
C(22)	0.046(6)	0.027(4)	0.046(5)	0.012(4)	0.009(6)	–0.008(5)
O(9)	0.089(13)	0.089(13)	0.089(13)	0.0001(11)	0.0000(11)	0.0001(11)
C(23)	0.058(3)	0.058(3)	0.058(3)	0.0000(4)	0.0000(4)	0.0001(4)
N(5)	0.038(6)	0.037(6)	0.037(6)	–0.0001(11)	0.0001(11)	0.0002(11)
C(24)	0.058(3)	0.058(3)	0.058(3)	0.0000(4)	0.0000(4)	0.0001(4)
C(25)	0.058(3)	0.058(3)	0.058(3)	0.0000(4)	0.0000(4)	0.0001(4)
O(9')	0.033(5)	0.033(5)	0.033(5)	0.0005(11)	–0.0004(11)	0.0002(11)
C(23')	0.058(3)	0.058(3)	0.058(3)	0.0000(4)	0.0000(4)	0.0001(4)
N(5')	0.055(9)	0.055(9)	0.055(9)	–0.0001(11)	0.0001(11)	0.0000(11)
C(24')	0.058(3)	0.058(3)	0.058(3)	0.0000(4)	0.0000(4)	0.0001(4)
C(25')	0.058(3)	0.058(3)	0.058(3)	0.0000(4)	0.0000(4)	0.0001(4)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for *(S,S)*-**6**[a].

	x	y	z	U
H(1)	–0.2896	–0.1009	0.2817	0.029
H(2)	0.3208	–0.1041	0.1888	0.029
H(5A)	–0.1422	–0.1145	0.3786	0.032
H(5B)	0.1112	–0.1149	0.3831	0.032
H(8)	–0.0478	0.0483	0.5633	0.037
H(9)	–0.0382	0.1479	0.4991	0.040
H(12A)	0.1163	0.0453	0.2921	0.035
H(12B)	–0.1372	0.0422	0.2897	0.035
H(13A)	–0.1816	0.2290	0.4172	0.059
H(13B)	–0.0250	0.2567	0.3617	0.059
H(13C)	0.0676	0.2290	0.4295	0.059
H(14A)	0.1862	–0.1273	0.0932	0.028
H(14B)	–0.0663	–0.1352	0.0916	0.028
H(17)	0.0223	0.0051	–0.1071	0.033
H(18)	0.0172	0.1144	–0.0598	0.038
H(21A)	–0.0912	0.0377	0.1668	0.027
H(21B)	0.1631	0.0378	0.1658	0.027
H(22A)	0.1374	0.2021	0.0033	0.060
H(22B)	0.0355	0.2416	0.0643	0.060
H(22C)	–0.1135	0.2071	0.0102	0.060
H(23)	0.6241	0.2299	0.1203	0.069
H(24A)	0.2669	0.1871	0.2691	0.086
H(24B)	0.2128	0.1785	0.1933	0.086
H(24C)	0.2060	0.2536	0.2264	0.086
H(25A)	0.5700	0.1376	0.2677	0.086
H(25B)	0.7558	0.1552	0.2175	0.086
H(25C)	0.5468	0.1171	0.1923	0.086
H(23')	0.6002	0.2361	0.1214	0.069
H(24D)	0.3253	0.1969	0.2873	0.086
H(24E)	0.1857	0.2383	0.2351	0.086

H(24F)	0.3791	0.2761	0.2705	0.086
H(25D)	0.6190	0.1486	0.2647	0.086
H(25E)	0.7647	0.2066	0.2316	0.086
H(25F)	0.6940	0.1399	0.1905	0.086

Table 6. Torsion angles [°] for *(S,S)*-**6**[a].

C(4)–N(2)–C(1)–O(1)	−166.1(8)	C(4)–N(2)–C(1)–C(2)	13.7(13)
C(3)–N(1)–C(2)–C(1)	−38.0(10)	C(3)–N(1)–C(2)–C(5)	−161.5(8)
C(3)–N(1)–C(2)–C(12)	81.6(10)	O(1)–C(1)–C(2)–N(1)	−154.6(9)
O(1)–C(1)–C(2)–C(5)	−31.6(11)	O(1)–C(1)–C(2)–C(12)	83.6(10)
N(2)–C(1)–C(2)–N(1)	25.7(10)	N(2)–C(1)–C(2)–C(5)	148.7(8)
N(2)–C(1)–C(2)–C(12)	−96.1(9)	C(2)–N(1)–C(3)–O(2)	−169.9(8)
C(2)–N(1)–C(3)–C(4)	10.3(12)	C(1)–N(2)–C(4)–C(3)	−40.9(10)
C(1)–N(2)–C(4)–C(14)	−161.4(8)	C(1)–N(2)–C(4)–C(21)	78.0(10)
O(2)–C(3)–C(4)–N(2)	−152.3(8)	O(2)–C(3)–C(4)–C(14)	−31.2(10)
O(2)–C(3)–C(4)–C(21)	86.0(9)	N(1)–C(3)–C(4)–N(2)	27.6(10)
N(1)–C(3)–C(4)–C(14)	148.6(8)	N(1)–C(3)–C(4)–C(21)	−94.2(9)
N(1)–C(2)–C(5)–C(6)	−123.3(7)	C(1)–C(2)–C(5)–C(6)	114.8(8)
C(12)–C(2)–C(5)–C(6)	−2.4(9)	C(2)–C(5)–C(6)–C(7)	−177.4(9)
C(2)–C(5)–C(6)–C(11)	1.5(10)	C(5)–C(6)–C(7)–N(3)	−0.9(15)
C(5)–C(6)–C(7)–C(8)	−178.2(9)	C(11)–C(6)–C(7)–N(3)	−179.7(8)
C(11)–C(6)–C(7)–C(8)	2.9(13)	O(3)–N(3)–C(7)–C(6)	−1.0(13)
O(3)–N(3)–C(7)–C(8)	176.5(8)	O(4)–N(3)–C(7)–C(6)	178.0(8)
O(4)–N(3)–C(7)–C(8)	−4.5(13)	N(3)–C(7)–C(8)–C(9)	179.7(8)
C(6)–C(7)–C(8)–C(9)	−2.8(13)	C(7)–C(8)–C(9)–C(10)	2.4(14)
C(13)–O(5)–C(10)–C(9)	−2.0(14)	C(13)–O(5)–C(10)–C(11)	179.1(8)
C(8)–C(9)–C(10)–O(5)	179.1(8)	C(8)–C(9)–C(10)–C(11)	−2.1(15)
C(5)–C(6)–C(11)–C(10)	178.4(8)	C(5)–C(6)–C(11)–C(12)	0.1(11)
C(7)–C(6)–C(11)–C(10)	−2.5(13)	C(7)–C(6)–C(11)–C(12)	179.2(8)
O(5)–C(10)–C(11)–C(6)	−178.8(8)	O(5)–C(10)–C(11)–C(12)	−0.8(13)
C(9)–C(10)–C(11)–C(6)	2.2(14)	C(9)–C(10)–C(11)–C(12)	−179.8(9)
C(6)–C(11)–C(12)–C(2)	−1.6(11)	C(10)–C(11)–C(12)–C(2)	−179.8(8)
N(1)–C(2)–C(12)–C(11)	122.8(8)	C(1)–C(2)–C(12)–C(11)	−117.1(8)
C(5)–C(2)–C(12)–C(11)	2.4(10)	N(2)–C(4)–C(14)–C(15)	−128.8(7)
C(3)–C(4)–C(14)–C(15)	112.4(7)	C(21)–C(4)–C(14)–C(15)	−5.2(9)
C(4)–C(14)–C(15)–C(16)	−177.6(9)	C(4)–C(14)–C(15)–C(20)	3.9(9)
C(14)–C(15)–C(16)–N(4)	4.5(15)	C(14)–C(15)–C(16)–C(17)	−179.2(9)
C(20)–C(15)–C(16)–N(4)	−177.1(8)	C(20)–C(15)–C(16)–C(17)	−0.8(13)
O(6)–N(4)–C(16)–C(15)	178.5(8)	O(6)–N(4)–C(16)–C(17)	2.2(14)
O(7)–N(4)–C(16)–C(15)	−5.5(13)	O(7)–N(4)–C(16)–C(17)	178.1(8)
N(4)–C(16)–C(17)–C(18)	177.8(8)	C(15)–C(16)–C(17)–C(18)	1.4(14)
C(16)–C(17)–C(18)–C(19)	−1.2(14)	C(22)–O(8)–C(19)–C(18)	−2.9(13)
C(22)–O(8)–C(19)–C(20)	177.2(9)	C(17)–C(18)–C(19)–O(8)	−179.5(8)
C(17)–C(18)–C(19)–C(20)	0.5(14)	O(8)–C(19)–C(20)–C(15)	−179.9(8)
O(8)–C(19)–C(20)–C(21)	−0.1(13)	C(18)–C(19)–C(20)–C(15)	0.1(13)
C(18)–C(19)–C(20)–C(21)	179.9(9)	C(14)–C(15)–C(20)–C(19)	178.8(8)
C(14)–C(15)–C(20)–C(21)	−1.0(10)	C(16)–C(15)–C(20)–C(19)	0.0(12)

C(16)–C(15)–C(20)–C(21)	−179.8(7)	C(15)–C(20)–C(21)–C(4)	−2.2(10)
C(19)–C(20)–C(21)–C(4)	177.9(8)	N(2)–C(4)–C(21)–C(20)	127.1(7)
C(3)–C(4)–C(21)–C(20)	−114.4(7)	C(14)–C(4)–C(21)–C(20)	4.5(9)
O(9)–C(23)–N(5)–C(24)	43(5)	O(9)–C(23)–N(5)–C(25)	163(3)
O(9')–C(23')–N(5')–C(24')	−17(6)	O(9')–C(23')–N(5')–C(25')	−165(4)

Table 7. Hydrogen bonds for *(S,S)*-**6**[a] [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
N(1)–H(1)...O(1A)	0.88	2.23	2.985(10)	144
N(2)–H(2)...O(2B)	0.88	2.26	3.033(9)	147

Symmetry operations for equivalent atoms
A x−1,y,z B x+1,y,z

Crystallographic data for *rac*-**6**[b]

Table 1. Crystal data and structure refinement for *rac*-**6**[b].

Identification code	eam102	
Chemical formula (moiety)	$3C_{22}H_{20}N_4O_8 \cdot 6C_3H_7NO \cdot 2H_2O$	
Chemical formula (total)	$C_{84}H_{106}N_{18}O_{32}$	
Formula weight	1879.87	
Temperature	150(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 14.721(4) Å	α = 93.42(2)°
	b = 15.416(5) Å	β = 100.887(15)°
	c = 20.197(4) Å	γ = 94.46(2)°
Cell volume	4474(2) Å^3	
Z	2	
Calculated density	1.395 g/cm^3	
Absorption coefficient μ	0.108 mm^{-1}	
F(000)	1984	
Crystal colour and size	colourless, 0.31 × 0.26 × 0.21 mm^3	
Reflections for cell refinement	13901 (θ range 2.5 to 27.5°)	
Data collection method	Nonius KappaCCD diffractometer	
	ϕ and ω scans	
θ range for data collection	4.1 to 25.0°	
Index ranges	h −17 to 17, k −18 to 16, l −24 to 24	
Completeness to θ = 25.0°	98.7 %	
Reflections collected	70663	
Independent reflections	15554 (R_{int} = 0.0570)	
Reflections with $F^2>2\sigma$	10437	
Absorption correction	numerical	
Min. and max. transmission	0.9272 and 0.9776	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0544, 5.1175	
Data / restraints / parameters	15554 / 0 / 1266	
Final R indices [$F^2>2\sigma$]	R1 = 0.0624, wR2 = 0.1342	
R indices (all data)	R1 = 0.1046, wR2 = 0.1527	
Goodness-of-fit on F^2	1.057	
Extinction coefficient	0.0010(3)	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.52 and −0.39 e Å^{-3}	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for *rac*-**6**^{b}. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1)	0.17644(15)	0.31545(14)	0.78169(10)	0.0316(5)
O(2)	0.35896(14)	0.19567(13)	1.00803(10)	0.0277(5)
O(3)	0.31650(18)	–0.19634(15)	0.90033(17)	0.0621(8)
O(4)	0.22624(16)	–0.09485(15)	0.87971(13)	0.0449(6)
O(5)	0.61168(13)	0.12326(13)	0.91805(10)	0.0272(5)
O(6)	–0.09959(17)	0.23130(16)	0.90060(15)	0.0519(7)
O(7)	–0.20578(15)	0.32027(16)	0.89882(13)	0.0470(6)
O(8)	0.14229(14)	0.58800(12)	0.91915(11)	0.0286(5)
N(1)	0.27649(17)	0.22549(15)	0.83199(12)	0.0219(5)
N(2)	0.24956(17)	0.27749(16)	0.95826(13)	0.0220(6)
N(3)	0.30406(18)	–0.11969(16)	0.89315(13)	0.0306(6)
N(4)	–0.12441(18)	0.30552(18)	0.90173(13)	0.0314(6)
C(1)	0.2153(2)	0.28428(18)	0.83392(14)	0.0219(6)
C(2)	0.19008(19)	0.31276(18)	0.90148(14)	0.0202(6)
C(3)	0.31136(19)	0.21973(17)	0.95626(14)	0.0196(6)
C(4)	0.32392(19)	0.17968(18)	0.88770(14)	0.0201(6)
C(5)	0.42938(19)	0.18124(18)	0.88794(14)	0.0205(6)
C(6)	0.45197(19)	0.08987(17)	0.90030(13)	0.0180(6)
C(7)	0.54031(19)	0.06096(18)	0.91417(14)	0.0199(6)
C(8)	0.5500(2)	–0.02740(19)	0.92283(15)	0.0256(7)
C(9)	0.4718(2)	–0.08473(19)	0.91632(15)	0.0259(7)
C(10)	0.3841(2)	–0.05603(18)	0.90147(14)	0.0219(6)
C(11)	0.37305(19)	0.03271(18)	0.89455(13)	0.0187(6)
C(12)	0.28710(19)	0.08102(18)	0.87989(15)	0.0236(7)
C(13)	0.08537(19)	0.28246(18)	0.89982(15)	0.0216(6)
C(14)	0.03914(19)	0.36549(18)	0.90720(13)	0.0195(6)
C(15)	–0.05441(19)	0.37911(19)	0.90690(14)	0.0215(6)
C(16)	–0.0825(2)	0.4626(2)	0.91029(15)	0.0258(7)
C(17)	–0.0194(2)	0.53487(19)	0.91434(14)	0.0249(7)
C(18)	0.07374(19)	0.52254(18)	0.91579(14)	0.0212(6)
C(19)	0.10215(19)	0.43783(17)	0.91268(13)	0.0181(6)
C(20)	0.19928(19)	0.41456(17)	0.91173(15)	0.0209(6)
C(21)	0.7044(2)	0.0965(2)	0.92996(17)	0.0341(8)
C(22)	0.1149(2)	0.67581(19)	0.91691(17)	0.0333(8)
O(31)	0.31157(15)	0.16371(13)	0.70026(10)	0.0313(5)
O(32)	0.14075(14)	0.28997(13)	0.47326(10)	0.0281(5)
O(33)	–0.17319(15)	0.45988(16)	0.57046(11)	0.0408(6)
O(34)	–0.11091(15)	0.33818(15)	0.58473(12)	0.0387(6)
O(35)	0.31762(16)	–0.10873(13)	0.56229(12)	0.0390(6)
O(36)	0.44575(17)	–0.17063(13)	0.57469(12)	0.0409(6)
O(37)	0.24666(14)	0.58849(13)	0.59151(11)	0.0316(5)
O(38)	0.60263(13)	0.22224(13)	0.59532(10)	0.0282(5)
N(31)	0.22015(17)	0.26011(16)	0.64951(13)	0.0222(6)
N(32)	0.24269(16)	0.20178(15)	0.52430(13)	0.0209(5)

N(33)	–0.10499(17)	0.41738(18)	0.57846(12)	0.0265(6)
N(34)	0.40277(19)	–0.10502(15)	0.57138(12)	0.0254(6)
C(31)	0.27749(19)	0.19844(18)	0.64856(14)	0.0206(6)
C(32)	0.30579(19)	0.17223(17)	0.58178(14)	0.0192(6)
C(33)	0.18624(19)	0.26509(18)	0.52527(14)	0.0193(6)
C(34)	0.17925(18)	0.30939(17)	0.59357(13)	0.0178(6)
C(35)	0.22811(19)	0.40348(18)	0.59949(15)	0.0233(7)
C(36)	0.15044(19)	0.46157(18)	0.59123(13)	0.0191(6)
C(37)	0.1586(2)	0.55244(18)	0.58727(14)	0.0229(7)
C(38)	0.0791(2)	0.59672(19)	0.57924(14)	0.0264(7)
C(39)	–0.0062(2)	0.55158(19)	0.57646(14)	0.0242(7)
C(40)	–0.01374(19)	0.46244(18)	0.58159(13)	0.0195(6)
C(41)	0.06513(18)	0.41605(17)	0.58879(13)	0.0167(6)
C(42)	0.07529(19)	0.32045(17)	0.59566(15)	0.0206(6)
C(43)	0.30896(19)	0.07131(17)	0.57277(15)	0.0206(6)
C(44)	0.40995(19)	0.05725(17)	0.57824(13)	0.0174(6)
C(45)	0.4553(2)	–0.01964(18)	0.57806(13)	0.0202(6)
C(46)	0.5508(2)	–0.01670(19)	0.58329(13)	0.0225(7)
C(47)	0.6032(2)	0.06275(19)	0.58906(14)	0.0237(7)
C(48)	0.55990(19)	0.13996(19)	0.58964(13)	0.0211(6)
C(49)	0.46358(18)	0.13566(17)	0.58463(13)	0.0171(6)
C(50)	0.40748(19)	0.21276(18)	0.58445(15)	0.0224(6)
C(51)	0.2604(3)	0.6814(2)	0.58645(19)	0.0465(10)
C(52)	0.7014(2)	0.2319(2)	0.59910(19)	0.0409(9)
O(61)	0.12146(13)	0.29387(13)	0.16720(10)	0.0247(5)
O(62)	0.28193(14)	0.15433(13)	0.39124(10)	0.0284(5)
O(63)	0.67162(16)	0.16382(16)	0.26573(15)	0.0526(7)
O(64)	0.56633(15)	0.25138(15)	0.27150(13)	0.0441(6)
O(65)	0.24155(15)	0.57875(14)	0.27555(13)	0.0437(6)
O(66)	0.14578(16)	0.67618(13)	0.25175(11)	0.0360(6)
O(67)	0.32635(14)	–0.10815(12)	0.24296(10)	0.0258(5)
O(68)	–0.13692(13)	0.35191(13)	0.25390(10)	0.0250(5)
N(61)	0.22086(16)	0.20207(15)	0.21643(12)	0.0205(5)
N(62)	0.20242(17)	0.26082(16)	0.34348(13)	0.0225(6)
N(63)	0.59090(17)	0.17739(17)	0.26711(13)	0.0287(6)
N(64)	0.16227(18)	0.60110(15)	0.26363(12)	0.0246(6)
C(61)	0.16520(19)	0.26505(17)	0.21899(14)	0.0189(6)
C(62)	0.15324(19)	0.30503(18)	0.28743(13)	0.0190(6)
C(63)	0.25229(19)	0.19306(18)	0.34075(14)	0.0209(6)
C(64)	0.27852(18)	0.16545(18)	0.27327(14)	0.0195(6)
C(65)	0.27079(19)	0.06382(17)	0.26138(15)	0.0213(6)
C(66)	0.36675(18)	0.04203(17)	0.25707(13)	0.0167(6)
C(67)	0.3949(2)	–0.04232(18)	0.24957(13)	0.0198(6)
C(68)	0.4885(2)	–0.05272(19)	0.25097(14)	0.0231(7)
C(69)	0.5513(2)	0.01982(19)	0.25705(14)	0.0241(7)
C(70)	0.52257(19)	0.10315(18)	0.26253(14)	0.0206(6)
C(71)	0.42932(19)	0.11502(17)	0.26437(13)	0.0179(6)
C(72)	0.38354(19)	0.19661(18)	0.27689(15)	0.0223(6)
C(73)	0.18708(19)	0.40422(18)	0.29257(15)	0.0218(6)
C(74)	0.09931(19)	0.44874(17)	0.27410(13)	0.0178(6)

C(75)	0.08483(19)	0.53616(18)	0.26300(13)	0.0187(6)
C(76)	–0.0042(2)	0.56306(18)	0.25030(13)	0.0212(6)
C(77)	–0.0805(2)	0.50380(18)	0.24726(14)	0.0214(6)
C(78)	–0.06815(19)	0.41621(18)	0.25693(13)	0.0184(6)
C(79)	0.02194(19)	0.39067(17)	0.27114(13)	0.0170(6)
C(80)	0.04718(18)	0.30125(17)	0.28782(14)	0.0198(6)
C(81)	0.3506(2)	–0.19594(19)	0.23252(16)	0.0329(8)
C(82)	–0.2310(2)	0.3734(2)	0.23397(17)	0.0330(8)
O(91)	0.3647(2)	0.3785(2)	0.4876(2)	0.0891(11)
N(91)	0.4242(3)	0.4719(3)	0.42135(19)	0.0737(12)
C(91)	0.3716(3)	0.4497(3)	0.4665(2)	0.0696(13)
C(92)	0.4283(5)	0.5607(4)	0.4009(3)	0.119(2)
C(93)	0.4741(5)	0.4100(4)	0.3917(4)	0.130(3)
O(92)	–0.06546(16)	0.91709(16)	0.71056(13)	0.0441(6)
N(92)	0.0495(2)	0.89192(19)	0.65331(17)	0.0472(8)
C(94)	–0.0380(2)	0.8991(2)	0.65861(19)	0.0357(8)
C(95)	0.1222(3)	0.9048(4)	0.7118(3)	0.097(2)
C(96)	0.0739(4)	0.8703(3)	0.5881(3)	0.092(2)
O(93)	0.3860(2)	0.4101(2)	0.18041(18)	0.0860(11)
N(93)	0.4847(3)	0.5291(2)	0.22374(19)	0.0606(9)
C(97)	0.4011(3)	0.4886(4)	0.1948(2)	0.0689(13)
C(98)	0.4988(6)	0.6234(3)	0.2380(3)	0.129(3)
C(99)	0.5664(3)	0.4813(3)	0.2384(3)	0.0788(15)
O(94)	0.11028(18)	0.08231(18)	0.98043(13)	0.0566(7)
N(94)	0.02588(19)	–0.02856(17)	0.91122(15)	0.0373(7)
C(100)	0.0889(2)	0.0043(3)	0.96362(19)	0.0424(9)
C(101)	0.0047(3)	–0.1215(2)	0.8944(2)	0.0604(12)
C(102)	–0.0290(4)	0.0284(3)	0.8692(3)	0.095(2)
O(95)	–0.0885(2)	0.91830(19)	0.41554(18)	0.0690(9)
N(95)	0.0281(3)	0.8920(2)	0.3601(2)	0.0589(10)
C(103)	–0.0581(3)	0.8970(3)	0.3654(3)	0.0704(14)
C(104)	0.0599(4)	0.8598(3)	0.3012(3)	0.0869(16)
C(105)	0.1022(4)	0.9165(4)	0.4196(3)	0.0944(18)
O(96)	0.5675(2)	0.5960(2)	1.08937(19)	0.0748(9)
N(96)	0.4587(2)	0.6182(2)	0.99893(19)	0.0545(9)
C(106)	0.5426(3)	0.6020(2)	1.0289(3)	0.0612(12)
C(107)	0.3825(3)	0.6295(3)	1.0327(3)	0.0895(17)
C(108)	0.4391(4)	0.6250(3)	0.9259(3)	0.0866(16)
O(97)	0.2285(2)	0.36400(17)	1.08054(13)	0.0381(6)
O(98)	0.2476(2)	0.12794(16)	1.09244(12)	0.0328(5)

Table 3. Bond lengths [Å] and angles [°] for *rac*-**6**[b].

O(1)–C(1)	1.244(3)	O(2)–C(3)	1.238(3)
O(3)–N(3)	1.223(3)	O(4)–N(3)	1.223(3)
O(5)–C(7)	1.355(3)	O(5)–C(21)	1.438(3)
O(6)–N(4)	1.228(3)	O(7)–N(4)	1.228(3)
O(8)–C(18)	1.360(3)	O(8)–C(22)	1.443(3)
N(1)–H(1N)	0.90(3)	N(1)–C(1)	1.330(4)
N(1)–C(4)	1.459(3)	N(2)–H(2N)	0.87(3)
N(2)–C(2)	1.465(4)	N(2)–C(3)	1.326(4)
N(3)–C(10)	1.451(4)	N(4)–C(15)	1.457(4)
C(1)–C(2)	1.529(4)	C(2)–C(13)	1.569(4)
C(2)–C(20)	1.562(4)	C(3)–C(4)	1.531(4)
C(4)–C(5)	1.550(4)	C(4)–C(12)	1.563(4)
C(5)–H(5A)	0.9900	C(5)–H(5B)	0.9900
C(5)–C(6)	1.497(4)	C(6)–C(7)	1.391(4)
C(6)–C(11)	1.384(4)	C(7)–C(8)	1.399(4)
C(8)–H(8)	0.9500	C(8)–C(9)	1.375(4)
C(9)–H(9)	0.9500	C(9)–C(10)	1.383(4)
C(10)–C(11)	1.402(4)	C(11)–C(12)	1.508(4)
C(12)–H(12A)	0.9900	C(12)–H(12B)	0.9900
C(13)–H(13A)	0.9900	C(13)–H(13B)	0.9900
C(13)–C(14)	1.508(4)	C(14)–C(15)	1.408(4)
C(14)–C(19)	1.379(4)	C(15)–C(16)	1.384(4)
C(16)–H(16)	0.9500	C(16)–C(17)	1.383(4)
C(17)–H(17)	0.9500	C(17)–C(18)	1.394(4)
C(18)–C(19)	1.403(4)	C(19)–C(20)	1.504(4)
C(20)–H(20A)	0.9900	C(20)–H(20B)	0.9900
C(21)–H(21A)	0.9800	C(21)–H(21B)	0.9800
C(21)–H(21C)	0.9800	C(22)–H(22A)	0.9800
C(22)–H(22B)	0.9800	C(22)–H(22C)	0.9800
O(31)–C(31)	1.241(3)	O(32)–C(33)	1.234(3)
O(33)–N(33)	1.232(3)	O(34)–N(33)	1.233(3)
O(35)–N(34)	1.228(3)	O(36)–N(34)	1.233(3)
O(37)–C(37)	1.356(3)	O(37)–C(51)	1.444(4)
O(38)–C(48)	1.360(3)	O(38)–C(52)	1.436(4)
N(31)–H(32N)	0.78(3)	N(31)–C(31)	1.321(4)
N(31)–C(34)	1.460(3)	N(32)–H(31N)	0.81(3)
N(32)–C(32)	1.463(4)	N(32)–C(33)	1.332(4)
N(33)–C(40)	1.452(4)	N(34)–C(45)	1.459(4)
C(31)–C(32)	1.526(4)	C(32)–C(43)	1.561(4)
C(32)–C(50)	1.567(4)	C(33)–C(34)	1.527(4)
C(34)–C(35)	1.556(4)	C(34)–C(42)	1.561(4)
C(35)–H(35A)	0.9900	C(35)–H(35B)	0.9900
C(35)–C(36)	1.497(4)	C(36)–C(37)	1.405(4)
C(36)–C(41)	1.381(4)	C(37)–C(38)	1.388(4)
C(38)–H(38)	0.9500	C(38)–C(39)	1.378(4)
C(39)–H(39)	0.9500	C(39)–C(40)	1.382(4)
C(40)–C(41)	1.399(4)	C(41)–C(42)	1.505(4)
C(42)–H(42A)	0.9900	C(42)–H(42B)	0.9900

C(43)–H(43A)	0.9900	C(43)–H(43B)	0.9900
C(43)–C(44)	1.503(4)	C(44)–C(45)	1.405(4)
C(44)–C(49)	1.377(4)	C(45)–C(46)	1.387(4)
C(46)–H(46)	0.9500	C(46)–C(47)	1.382(4)
C(47)–H(47)	0.9500	C(47)–C(48)	1.394(4)
C(48)–C(49)	1.398(4)	C(49)–C(50)	1.499(4)
C(50)–H(50A)	0.9900	C(50)–H(50B)	0.9900
C(51)–H(51A)	0.9800	C(51)–H(51B)	0.9800
C(51)–H(51C)	0.9800	C(52)–H(52A)	0.9800
C(52)–H(52B)	0.9800	C(52)–H(52C)	0.9800
O(61)–C(61)	1.246(3)	O(62)–C(63)	1.238(3)
O(63)–N(63)	1.228(3)	O(64)–N(63)	1.226(3)
O(65)–N(64)	1.227(3)	O(66)–N(64)	1.229(3)
O(67)–C(67)	1.357(3)	O(67)–C(81)	1.440(3)
O(68)–C(78)	1.351(3)	O(68)–C(82)	1.438(3)
N(61)–H(61N)	0.92(3)	N(61)–C(61)	1.323(4)
N(61)–C(64)	1.463(3)	N(62)–H(62N)	0.79(3)
N(62)–C(62)	1.459(4)	N(62)–C(63)	1.327(4)
N(63)–C(70)	1.450(4)	N(64)–C(75)	1.455(4)
C(61)–C(62)	1.526(4)	C(62)–C(73)	1.562(4)
C(62)–C(80)	1.559(4)	C(63)–C(64)	1.531(4)
C(64)–C(65)	1.563(4)	C(64)–C(72)	1.570(4)
C(65)–H(65A)	0.9900	C(65)–H(65B)	0.9900
C(65)–C(66)	1.494(4)	C(66)–C(67)	1.404(4)
C(66)–C(71)	1.380(4)	C(67)–C(68)	1.395(4)
C(68)–H(68)	0.9500	C(68)–C(69)	1.378(4)
C(69)–H(69)	0.9500	C(69)–C(70)	1.388(4)
C(70)–C(71)	1.406(4)	C(71)–C(72)	1.503(4)
C(72)–H(72A)	0.9900	C(72)–H(72B)	0.9900
C(73)–H(73A)	0.9900	C(73)–H(73B)	0.9900
C(73)–C(74)	1.505(4)	C(74)–C(75)	1.405(4)
C(74)–C(79)	1.383(4)	C(75)–C(76)	1.388(4)
C(76)–H(76)	0.9500	C(76)–C(77)	1.380(4)
C(77)–H(77)	0.9500	C(77)–C(78)	1.397(4)
C(78)–C(79)	1.395(4)	C(79)–C(80)	1.497(4)
C(80)–H(80A)	0.9900	C(80)–H(80B)	0.9900
C(81)–H(81A)	0.9800	C(81)–H(81B)	0.9800
C(81)–H(81C)	0.9800	C(82)–H(82A)	0.9800
C(82)–H(82B)	0.9800	C(82)–H(82C)	0.9800
O(91)–C(91)	1.205(5)	N(91)–C(91)	1.346(6)
N(91)–C(92)	1.454(6)	N(91)–C(93)	1.419(7)
C(91)–H(91)	0.9500	C(92)–H(92A)	0.9800
C(92)–H(92B)	0.9800	C(92)–H(92C)	0.9800
C(93)–H(93A)	0.9800	C(93)–H(93B)	0.9800
C(93)–H(93C)	0.9800	O(92)–C(94)	1.218(4)
N(92)–C(94)	1.325(4)	N(92)–C(95)	1.429(6)
N(92)–C(96)	1.457(5)	C(94)–H(94)	0.9500
C(95)–H(95A)	0.9800	C(95)–H(95B)	0.9800
C(95)–H(95C)	0.9800	C(96)–H(96A)	0.9800
C(96)–H(96B)	0.9800	C(96)–H(96C)	0.9800
O(93)–C(97)	1.220(6)	N(93)–C(97)	1.346(6)

N(93)–C(98)	1.456(6)	N(93)–C(99)	1.452(6)
C(97)–H(97)	0.9500	C(98)–H(98A)	0.9800
C(98)–H(98B)	0.9800	C(98)–H(98C)	0.9800
C(99)–H(99A)	0.9800	C(99)–H(99B)	0.9800
C(99)–H(99C)	0.9800	O(94)–C(100)	1.230(4)
N(94)–C(100)	1.315(4)	N(94)–C(101)	1.449(4)
N(94)–C(102)	1.444(5)	C(100)–H(100)	0.9500
C(101)–H(10A)	0.9800	C(101)–H(10B)	0.9800
C(101)–H(10C)	0.9800	C(102)–H(10D)	0.9800
C(102)–H(10E)	0.9800	C(102)–H(10F)	0.9800
O(95)–C(103)	1.220(6)	N(95)–C(103)	1.301(5)
N(95)–C(104)	1.433(6)	N(95)–C(105)	1.472(6)
C(103)–H(103)	0.9500	C(104)–H(10G)	0.9800
C(104)–H(10H)	0.9800	C(104)–H(10I)	0.9800
C(105)–H(10J)	0.9800	C(105)–H(10K)	0.9800
C(105)–H(10L)	0.9800	O(96)–C(106)	1.218(5)
N(96)–C(106)	1.318(5)	N(96)–C(107)	1.435(6)
N(96)–C(108)	1.460(6)	C(106)–H(106)	0.9500
C(107)–H(10M)	0.9800	C(107)–H(10N)	0.9800
C(107)–H(10O)	0.9800	C(108)–H(10P)	0.9800
C(108)–H(10Q)	0.9800	C(108)–H(10R)	0.9800
O(97)–H(1O)	0.90(5)	O(97)–H(2O)	0.82(5)
O(98)–H(3O)	0.85(4)	O(98)–H(4O)	0.80(4)

C(7)–O(5)–C(21)	117.8(2)	C(18)–O(8)–C(22)	117.0(2)
H(1N)–N(1)–C(1)	115.4(19)	H(1N)–N(1)–C(4)	116.5(19)
C(1)–N(1)–C(4)	128.1(2)	H(2N)–N(2)–C(2)	117(2)
H(2N)–N(2)–C(3)	115(2)	C(2)–N(2)–C(3)	128.3(3)
O(3)–N(3)–O(4)	122.1(3)	O(3)–N(3)–C(10)	119.0(3)
O(4)–N(3)–C(10)	118.9(2)	O(6)–N(4)–O(7)	122.7(3)
O(6)–N(4)–C(15)	118.7(3)	O(7)–N(4)–C(15)	118.6(3)
O(1)–C(1)–N(1)	121.5(3)	O(1)–C(1)–C(2)	118.9(2)
N(1)–C(1)–C(2)	119.5(2)	N(2)–C(2)–C(1)	111.6(2)
N(2)–C(2)–C(13)	110.3(2)	N(2)–C(2)–C(20)	109.5(2)
C(1)–C(2)–C(13)	109.4(2)	C(1)–C(2)–C(20)	109.8(2)
C(13)–C(2)–C(20)	106.2(2)	O(2)–C(3)–N(2)	122.5(3)
O(2)–C(3)–C(4)	118.2(2)	N(2)–C(3)–C(4)	119.3(2)
N(1)–C(4)–C(3)	111.6(2)	N(1)–C(4)–C(5)	111.4(2)
N(1)–C(4)–C(12)	110.6(2)	C(3)–C(4)–C(5)	108.4(2)
C(3)–C(4)–C(12)	109.1(2)	C(5)–C(4)–C(12)	105.5(2)
C(4)–C(5)–H(5A)	110.9	C(4)–C(5)–H(5B)	110.9
C(4)–C(5)–C(6)	104.5(2)	H(5A)–C(5)–H(5B)	108.9
H(5A)–C(5)–C(6)	110.9	H(5B)–C(5)–C(6)	110.9
C(5)–C(6)–C(7)	126.4(2)	C(5)–C(6)–C(11)	112.3(2)
C(7)–C(6)–C(11)	121.3(2)	O(5)–C(7)–C(6)	115.5(2)
O(5)–C(7)–C(8)	124.9(3)	C(6)–C(7)–C(8)	119.6(3)
C(7)–C(8)–H(8)	120.3	C(7)–C(8)–C(9)	119.4(3)
H(8)–C(8)–C(9)	120.3	C(8)–C(9)–H(9)	119.6
C(8)–C(9)–C(10)	120.8(3)	H(9)–C(9)–C(10)	119.6
N(3)–C(10)–C(9)	118.6(3)	N(3)–C(10)–C(11)	120.9(3)
C(9)–C(10)–C(11)	120.5(3)	C(6)–C(11)–C(10)	118.3(3)

C(6)–C(11)–C(12)	110.3(2)	C(10)–C(11)–C(12)	131.4(3)
C(4)–C(12)–C(11)	104.9(2)	C(4)–C(12)–H(12A)	110.8
C(4)–C(12)–H(12B)	110.8	C(11)–C(12)–H(12A)	110.8
C(11)–C(12)–H(12B)	110.8	H(12A)–C(12)–H(12B)	108.8
C(2)–C(13)–H(13A)	110.7	C(2)–C(13)–H(13B)	110.7
C(2)–C(13)–C(14)	105.2(2)	H(13A)–C(13)–H(13B)	108.8
H(13A)–C(13)–C(14)	110.7	H(13B)–C(13)–C(14)	110.7
C(13)–C(14)–C(15)	130.9(3)	C(13)–C(14)–C(19)	111.1(2)
C(15)–C(14)–C(19)	118.0(3)	N(4)–C(15)–C(14)	120.8(3)
N(4)–C(15)–C(16)	118.3(3)	C(14)–C(15)–C(16)	120.9(3)
C(15)–C(16)–H(16)	119.6	C(15)–C(16)–C(17)	120.8(3)
H(16)–C(16)–C(17)	119.6	C(16)–C(17)–H(17)	120.5
C(16)–C(17)–C(18)	118.9(3)	H(17)–C(17)–C(18)	120.5
O(8)–C(18)–C(17)	124.6(3)	O(8)–C(18)–C(19)	115.3(2)
C(17)–C(18)–C(19)	120.1(3)	C(14)–C(19)–C(18)	121.2(3)
C(14)–C(19)–C(20)	112.8(2)	C(18)–C(19)–C(20)	126.0(2)
C(2)–C(20)–C(19)	104.6(2)	C(2)–C(20)–H(20A)	110.8
C(2)–C(20)–H(20B)	110.8	C(19)–C(20)–H(20A)	110.8
C(19)–C(20)–H(20B)	110.8	H(20A)–C(20)–H(20B)	108.9
O(5)–C(21)–H(21A)	109.5	O(5)–C(21)–H(21B)	109.5
O(5)–C(21)–H(21C)	109.5	H(21A)–C(21)–H(21B)	109.5
H(21A)–C(21)–H(21C)	109.5	H(21B)–C(21)–H(21C)	109.5
O(8)–C(22)–H(22A)	109.5	O(8)–C(22)–H(22B)	109.5
O(8)–C(22)–H(22C)	109.5	H(22A)–C(22)–H(22B)	109.5
H(22A)–C(22)–H(22C)	109.5	H(22B)–C(22)–H(22C)	109.5
C(37)–O(37)–C(51)	117.8(3)	C(48)–O(38)–C(52)	117.9(2)
H(32N)–N(31)–C(31)	117(2)	H(32N)–N(31)–C(34)	115(2)
C(31)–N(31)–C(34)	128.0(3)	H(31N)–N(32)–C(32)	115(2)
H(31N)–N(32)–C(33)	116(2)	C(32)–N(32)–C(33)	127.4(3)
O(33)–N(33)–O(34)	122.6(3)	O(33)–N(33)–C(40)	118.8(3)
O(34)–N(33)–C(40)	118.6(2)	O(35)–N(34)–O(36)	122.6(3)
O(35)–N(34)–C(45)	118.8(2)	O(36)–N(34)–C(45)	118.6(3)
O(31)–C(31)–N(31)	122.4(3)	O(31)–C(31)–C(32)	119.1(2)
N(31)–C(31)–C(32)	118.4(2)	N(32)–C(32)–C(31)	111.4(2)
N(32)–C(32)–C(43)	110.0(2)	N(32)–C(32)–C(50)	110.3(2)
C(31)–C(32)–C(43)	110.7(2)	C(31)–C(32)–C(50)	108.4(2)
C(43)–C(32)–C(50)	105.9(2)	O(32)–C(33)–N(32)	122.6(3)
O(32)–C(33)–C(34)	119.0(2)	N(32)–C(33)–C(34)	118.4(2)
N(31)–C(34)–C(33)	111.6(2)	N(31)–C(34)–C(35)	111.1(2)
N(31)–C(34)–C(42)	110.3(2)	C(33)–C(34)–C(35)	108.3(2)
C(33)–C(34)–C(42)	109.6(2)	C(35)–C(34)–C(42)	105.8(2)
C(34)–C(35)–H(35A)	110.8	C(34)–C(35)–H(35B)	110.8
C(34)–C(35)–C(36)	104.7(2)	H(35A)–C(35)–H(35B)	108.9
H(35A)–C(35)–C(36)	110.8	H(35B)–C(35)–C(36)	110.8
C(35)–C(36)–C(37)	126.5(3)	C(35)–C(36)–C(41)	112.3(2)
C(37)–C(36)–C(41)	121.1(3)	O(37)–C(37)–C(36)	114.6(3)
O(37)–C(37)–C(38)	126.1(3)	C(36)–C(37)–C(38)	119.3(3)
C(37)–C(38)–H(38)	120.1	C(37)–C(38)–C(39)	119.8(3)
H(38)–C(38)–C(39)	120.1	C(38)–C(39)–H(39)	119.7
C(38)–C(39)–C(40)	120.7(3)	H(39)–C(39)–C(40)	119.7
N(33)–C(40)–C(39)	118.9(2)	N(33)–C(40)–C(41)	120.5(2)

C(39)–C(40)–C(41)	120.6(3)	C(36)–C(41)–C(40)	118.4(2)
C(36)–C(41)–C(42)	110.8(2)	C(40)–C(41)–C(42)	130.7(2)
C(34)–C(42)–C(41)	105.1(2)	C(34)–C(42)–H(42A)	110.7
C(34)–C(42)–H(42B)	110.7	C(41)–C(42)–H(42A)	110.7
C(41)–C(42)–H(42B)	110.7	H(42A)–C(42)–H(42B)	108.8
C(32)–C(43)–H(43A)	110.7	C(32)–C(43)–H(43B)	110.7
C(32)–C(43)–C(44)	105.5(2)	H(43A)–C(43)–H(43B)	108.8
H(43A)–C(43)–C(44)	110.7	H(43B)–C(43)–C(44)	110.7
C(43)–C(44)–C(45)	131.2(2)	C(43)–C(44)–C(49)	111.0(2)
C(45)–C(44)–C(49)	117.8(2)	N(34)–C(45)–C(44)	120.8(2)
N(34)–C(45)–C(46)	118.1(2)	C(44)–C(45)–C(46)	121.1(3)
C(45)–C(46)–H(46)	119.9	C(45)–C(46)–C(47)	120.1(3)
H(46)–C(46)–C(47)	119.9	C(46)–C(47)–H(47)	120.1
C(46)–C(47)–C(48)	119.8(3)	H(47)–C(47)–C(48)	120.1
O(38)–C(48)–C(47)	126.1(3)	O(38)–C(48)–C(49)	114.7(2)
C(47)–C(48)–C(49)	119.2(3)	C(44)–C(49)–C(48)	121.9(3)
C(44)–C(49)–C(50)	112.8(2)	C(48)–C(49)–C(50)	125.3(2)
C(32)–C(50)–C(49)	104.5(2)	C(32)–C(50)–H(50A)	110.9
C(32)–C(50)–H(50B)	110.9	C(49)–C(50)–H(50A)	110.9
C(49)–C(50)–H(50B)	110.9	H(50A)–C(50)–H(50B)	108.9
O(37)–C(51)–H(51A)	109.5	O(37)–C(51)–H(51B)	109.5
O(37)–C(51)–H(51C)	109.5	H(51A)–C(51)–H(51B)	109.5
H(51A)–C(51)–H(51C)	109.5	H(51B)–C(51)–H(51C)	109.5
O(38)–C(52)–H(52A)	109.5	O(38)–C(52)–H(52B)	109.5
O(38)–C(52)–H(52C)	109.5	H(52A)–C(52)–H(52B)	109.5
H(52A)–C(52)–H(52C)	109.5	H(52B)–C(52)–H(52C)	109.5
C(67)–O(67)–C(81)	117.7(2)	C(78)–O(68)–C(82)	117.7(2)
H(61N)–N(61)–C(61)	117.1(19)	H(61N)–N(61)–C(64)	115.0(19)
C(61)–N(61)–C(64)	127.6(2)	H(62N)–N(62)–C(62)	115(2)
H(62N)–N(62)–C(63)	116(2)	C(62)–N(62)–C(63)	128.2(3)
O(63)–N(63)–O(64)	122.1(3)	O(63)–N(63)–C(70)	118.6(3)
O(64)–N(63)–C(70)	119.3(2)	O(65)–N(64)–O(66)	122.5(2)
O(65)–N(64)–C(75)	118.8(2)	O(66)–N(64)–C(75)	118.8(2)
O(61)–C(61)–N(61)	122.5(3)	O(61)–C(61)–C(62)	117.8(2)
N(61)–C(61)–C(62)	119.7(2)	N(62)–C(62)–C(61)	112.1(2)
N(62)–C(62)–C(73)	111.7(2)	N(62)–C(62)–C(80)	111.2(2)
C(61)–C(62)–C(73)	108.1(2)	C(61)–C(62)–C(80)	108.0(2)
C(73)–C(62)–C(80)	105.4(2)	O(62)–C(63)–N(62)	122.5(3)
O(62)–C(63)–C(64)	119.0(2)	N(62)–C(63)–C(64)	118.4(2)
N(61)–C(64)–C(63)	111.8(2)	N(61)–C(64)–C(65)	109.8(2)
N(61)–C(64)–C(72)	110.0(2)	C(63)–C(64)–C(65)	110.8(2)
C(63)–C(64)–C(72)	108.5(2)	C(65)–C(64)–C(72)	105.8(2)
C(64)–C(65)–H(65A)	110.7	C(64)–C(65)–H(65B)	110.7
C(64)–C(65)–C(66)	105.0(2)	H(65A)–C(65)–H(65B)	108.8
H(65A)–C(65)–C(66)	110.7	H(65B)–C(65)–C(66)	110.7
C(65)–C(66)–C(67)	125.8(2)	C(65)–C(66)–C(71)	112.7(2)
C(67)–C(66)–C(71)	121.4(3)	O(67)–C(67)–C(66)	115.3(2)
O(67)–C(67)–C(68)	125.4(2)	C(66)–C(67)–C(68)	119.3(3)
C(67)–C(68)–H(68)	120.2	C(67)–C(68)–C(69)	119.6(3)
H(68)–C(68)–C(69)	120.2	C(68)–C(69)–H(69)	119.6
C(68)–C(69)–C(70)	120.8(3)	H(69)–C(69)–C(70)	119.6

N(63)–C(70)–C(69)	118.6(3)	N(63)–C(70)–C(71)	120.9(3)
C(69)–C(70)–C(71)	120.5(3)	C(66)–C(71)–C(70)	118.2(2)
C(66)–C(71)–C(72)	111.1(2)	C(70)–C(71)–C(72)	130.5(2)
C(64)–C(72)–C(71)	105.3(2)	C(64)–C(72)–H(72A)	110.7
C(64)–C(72)–H(72B)	110.7	C(71)–C(72)–H(72A)	110.7
C(71)–C(72)–H(72B)	110.7	H(72A)–C(72)–H(72B)	108.8
C(62)–C(73)–H(73A)	110.9	C(62)–C(73)–H(73B)	110.9
C(62)–C(73)–C(74)	104.4(2)	H(73A)–C(73)–H(73B)	108.9
H(73A)–C(73)–C(74)	110.9	H(73B)–C(73)–C(74)	110.9
C(73)–C(74)–C(75)	131.5(2)	C(73)–C(74)–C(79)	110.8(2)
C(75)–C(74)–C(79)	117.7(2)	N(64)–C(75)–C(74)	121.3(2)
N(64)–C(75)–C(76)	117.9(2)	C(74)–C(75)–C(76)	120.9(3)
C(75)–C(76)–H(76)	119.8	C(75)–C(76)–C(77)	120.4(3)
H(76)–C(76)–C(77)	119.8	C(76)–C(77)–H(77)	120.0
C(76)–C(77)–C(78)	119.9(3)	H(77)–C(77)–C(78)	120.0
O(68)–C(78)–C(77)	125.5(2)	O(68)–C(78)–C(79)	115.5(2)
C(77)–C(78)–C(79)	118.9(3)	C(74)–C(79)–C(78)	122.2(2)
C(74)–C(79)–C(80)	112.3(2)	C(78)–C(79)–C(80)	125.5(2)
C(62)–C(80)–C(79)	103.9(2)	C(62)–C(80)–H(80A)	111.0
C(62)–C(80)–H(80B)	111.0	C(79)–C(80)–H(80A)	111.0
C(79)–C(80)–H(80B)	111.0	H(80A)–C(80)–H(80B)	109.0
O(67)–C(81)–H(81A)	109.5	O(67)–C(81)–H(81B)	109.5
O(67)–C(81)–H(81C)	109.5	H(81A)–C(81)–H(81B)	109.5
H(81A)–C(81)–H(81C)	109.5	H(81B)–C(81)–H(81C)	109.5
O(68)–C(82)–H(82A)	109.5	O(68)–C(82)–H(82B)	109.5
O(68)–C(82)–H(82C)	109.5	H(82A)–C(82)–H(82B)	109.5
H(82A)–C(82)–H(82C)	109.5	H(82B)–C(82)–H(82C)	109.5
C(91)–N(91)–C(92)	119.5(5)	C(91)–N(91)–C(93)	121.6(5)
C(92)–N(91)–C(93)	118.9(5)	O(91)–C(91)–N(91)	124.7(5)
O(91)–C(91)–H(91)	117.7	N(91)–C(91)–H(91)	117.7
N(91)–C(92)–H(92A)	109.5	N(91)–C(92)–H(92B)	109.5
N(91)–C(92)–H(92C)	109.5	H(92A)–C(92)–H(92B)	109.5
H(92A)–C(92)–H(92C)	109.5	H(92B)–C(92)–H(92C)	109.5
N(91)–C(93)–H(93A)	109.5	N(91)–C(93)–H(93B)	109.5
N(91)–C(93)–H(93C)	109.5	H(93A)–C(93)–H(93B)	109.5
H(93A)–C(93)–H(93C)	109.5	H(93B)–C(93)–H(93C)	109.5
C(94)–N(92)–C(95)	120.6(4)	C(94)–N(92)–C(96)	121.0(4)
C(95)–N(92)–C(96)	118.4(4)	O(92)–C(94)–N(92)	126.0(4)
O(92)–C(94)–H(94)	117.0	N(92)–C(94)–H(94)	117.0
N(92)–C(95)–H(95A)	109.5	N(92)–C(95)–H(95B)	109.5
N(92)–C(95)–H(95C)	109.5	H(95A)–C(95)–H(95B)	109.5
H(95A)–C(95)–H(95C)	109.5	H(95B)–C(95)–H(95C)	109.5
N(92)–C(96)–H(96A)	109.5	N(92)–C(96)–H(96B)	109.5
N(92)–C(96)–H(96C)	109.5	H(96A)–C(96)–H(96B)	109.5
H(96A)–C(96)–H(96C)	109.5	H(96B)–C(96)–H(96C)	109.5
C(97)–N(93)–C(98)	121.8(5)	C(97)–N(93)–C(99)	121.4(4)
C(98)–N(93)–C(99)	116.7(5)	O(93)–C(97)–N(93)	124.4(4)
O(93)–C(97)–H(97)	117.8	N(93)–C(97)–H(97)	117.8
N(93)–C(98)–H(98A)	109.5	N(93)–C(98)–H(98B)	109.5
N(93)–C(98)–H(98C)	109.5	H(98A)–C(98)–H(98B)	109.5
H(98A)–C(98)–H(98C)	109.5	H(98B)–C(98)–H(98C)	109.5

N(93)–C(99)–H(99A)	109.5	N(93)–C(99)–H(99B)	109.5
N(93)–C(99)–H(99C)	109.5	H(99A)–C(99)–H(99B)	109.5
H(99A)–C(99)–H(99C)	109.5	H(99B)–C(99)–H(99C)	109.5
C(100)–N(94)–C(101)	123.0(3)	C(100)–N(94)–C(102)	120.1(3)
C(101)–N(94)–C(102)	116.8(3)	O(94)–C(100)–N(94)	126.1(4)
O(94)–C(100)–H(100)	117.0	N(94)–C(100)–H(100)	117.0
N(94)–C(101)–H(10A)	109.5	N(94)–C(101)–H(10B)	109.5
N(94)–C(101)–H(10C)	109.5	H(10A)–C(101)–H(10B)	109.5
H(10A)–C(101)–H(10C)	109.5	H(10B)–C(101)–H(10C)	109.5
N(94)–C(102)–H(10D)	109.5	N(94)–C(102)–H(10E)	109.5
N(94)–C(102)–H(10F)	109.5	H(10D)–C(102)–H(10E)	109.5
H(10D)–C(102)–H(10F)	109.5	H(10E)–C(102)–H(10F)	109.5
C(103)–N(95)–C(104)	126.1(5)	C(103)–N(95)–C(105)	119.3(4)
C(104)–N(95)–C(105)	114.6(4)	O(95)–C(103)–N(95)	128.3(5)
O(95)–C(103)–H(103)	115.8	N(95)–C(103)–H(103)	115.8
N(95)–C(104)–H(10G)	109.5	N(95)–C(104)–H(10H)	109.5
N(95)–C(104)–H(10I)	109.5	H(10G)–C(104)–H(10H)	109.5
H(10G)–C(104)–H(10I)	109.5	H(10H)–C(104)–H(10I)	109.5
N(95)–C(105)–H(10J)	109.5	N(95)–C(105)–H(10K)	109.5
N(95)–C(105)–H(10L)	109.5	H(10J)–C(105)–H(10K)	109.5
H(10J)–C(105)–H(10L)	109.5	H(10K)–C(105)–H(10L)	109.5
C(106)–N(96)–C(107)	124.9(5)	C(106)–N(96)–C(108)	119.3(4)
C(107)–N(96)–C(108)	115.8(4)	O(96)–C(106)–N(96)	125.2(5)
O(96)–C(106)–H(106)	117.4	N(96)–C(106)–H(106)	117.4
N(96)–C(107)–H(10M)	109.5	N(96)–C(107)–H(10N)	109.5
N(96)–C(107)–H(10O)	109.5	H(10M)–C(107)–H(10N)	109.5
H(10M)–C(107)–H(10O)	109.5	H(10N)–C(107)–H(10O)	109.5
N(96)–C(108)–H(10P)	109.5	N(96)–C(108)–H(10Q)	109.5
N(96)–C(108)–H(10R)	109.5	H(10P)–C(108)–H(10Q)	109.5
H(10P)–C(108)–H(10R)	109.5	H(10Q)–C(108)–H(10R)	109.5
H(1O)–O(97)–H(2O)	102(4)	H(3O)–O(98)–H(4O)	106(4)

Table 4. Anisotropic displacement parameters ($Å^2$) for *rac*-**6**[b]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	0.0400(13)	0.0366(13)	0.0211(12)	0.0082(9)	0.0036(10)	0.0227(10)
O(2)	0.0291(12)	0.0350(12)	0.0206(11)	0.0080(9)	0.0021(9)	0.0150(10)
O(3)	0.0468(16)	0.0199(14)	0.119(3)	0.0170(14)	0.0118(16)	0.0012(12)
O(4)	0.0255(14)	0.0327(13)	0.0750(19)	0.0019(12)	0.0072(12)	0.0005(11)
O(5)	0.0168(11)	0.0274(11)	0.0382(13)	0.0080(9)	0.0048(9)	0.0040(9)
O(6)	0.0361(15)	0.0297(14)	0.092(2)	0.0075(13)	0.0187(14)	
–0.0020(12)						
O(7)	0.0197(13)	0.0565(16)	0.0655(18)	–0.0024(13)	0.0137(11)	0.0001(11)
O(8)	0.0308(12)	0.0170(11)	0.0374(13)	0.0012(9)	0.0045(10)	0.0046(9)
N(1)	0.0270(14)	0.0270(14)	0.0147(13)	0.0061(10)	0.0056(10)	0.0141(11)
N(2)	0.0254(14)	0.0260(14)	0.0170(14)	0.0035(11)	0.0060(11)	0.0106(11)
N(3)	0.0291(16)	0.0236(15)	0.0398(17)	0.0028(12)	0.0088(12)	0.0006(12)
N(4)	0.0243(16)	0.0374(17)	0.0324(16)	0.0008(12)	0.0072(12)	0.0001(13)

C(1)	0.0228(16)	0.0210(15)	0.0226(16)	0.0042(12)	0.0034(12)	0.0070(13)
C(2)	0.0217(15)	0.0194(15)	0.0210(15)	0.0041(12)	0.0040(12)	0.0087(12)
C(3)	0.0197(15)	0.0189(15)	0.0223(16)	0.0067(12)	0.0057(12)	0.0066(12)
C(4)	0.0226(16)	0.0185(15)	0.0216(15)	0.0035(12)	0.0060(12)	0.0109(12)
C(5)	0.0207(15)	0.0203(15)	0.0221(16)	0.0038(12)	0.0060(12)	0.0063(12)
C(6)	0.0218(16)	0.0191(15)	0.0147(14)	0.0026(11)	0.0053(11)	0.0064(12)
C(7)	0.0196(15)	0.0249(16)	0.0173(15)	0.0056(12)	0.0057(12)	0.0059(13)
C(8)	0.0217(16)	0.0288(17)	0.0284(17)	0.0079(13)	0.0046(13)	0.0122(13)
C(9)	0.0314(18)	0.0190(15)	0.0295(17)	0.0062(13)	0.0067(13)	0.0110(14)
C(10)	0.0259(17)	0.0183(15)	0.0233(16)	0.0046(12)	0.0080(12)	0.0032(13)
C(11)	0.0189(15)	0.0232(15)	0.0157(15)	0.0029(11)	0.0055(11)	0.0058(12)
C(12)	0.0172(15)	0.0249(16)	0.0301(17)	0.0028(13)	0.0057(12)	0.0081(12)
C(13)	0.0202(15)	0.0186(15)	0.0259(16)	0.0017(12)	0.0035(12)	0.0029(12)
C(14)	0.0238(16)	0.0211(15)	0.0140(14)	0.0013(11)	0.0028(11)	0.0069(12)
C(15)	0.0196(16)	0.0274(17)	0.0181(15)	0.0013(12)	0.0054(12)	0.0016(13)
C(16)	0.0186(16)	0.0359(18)	0.0238(17)	0.0003(13)	0.0044(12)	0.0090(14)
C(17)	0.0289(18)	0.0235(16)	0.0239(16)	0.0004(13)	0.0053(13)	0.0135(14)
C(18)	0.0231(16)	0.0227(16)	0.0172(15)	0.0016(12)	0.0020(12)	0.0035(13)
C(19)	0.0203(15)	0.0198(15)	0.0151(15)	0.0034(11)	0.0035(11)	0.0058(12)
C(20)	0.0200(15)	0.0191(15)	0.0244(16)	0.0031(12)	0.0041(12)	0.0064(12)
C(21)	0.0158(16)	0.044(2)	0.042(2)	0.0084(16)	0.0026(14)	0.0046(14)
C(22)	0.048(2)	0.0162(16)	0.038(2)	0.0030(13)	0.0101(16)	0.0074(14)
O(31)	0.0403(13)	0.0347(12)	0.0213(12)	0.0074(9)	0.0038(10)	0.0204(10)
O(32)	0.0319(12)	0.0354(12)	0.0195(11)	0.0066(9)	0.0044(9)	0.0163(10)
O(33)	0.0227(12)	0.0622(16)	0.0388(14)	–0.0007(12)	0.0037(10)	0.0215(12)
O(34)	0.0241(12)	0.0373(14)	0.0566(16)	0.0086(11)	0.0118(11)	0.0016(10)
O(35)	0.0320(14)	0.0233(12)	0.0625(17)	0.0015(11)	0.0126(11)	0.0011(10)
O(36)	0.0527(15)	0.0191(12)	0.0509(16)	0.0042(10)	0.0053(12)	0.0147(11)
O(37)	0.0337(13)	0.0200(11)	0.0382(13)	0.0042(9)	0.0033(10)	–0.0083(9)
O(38)	0.0172(11)	0.0307(12)	0.0359(13)	–0.0003(9)	0.0063(9)	–0.0036(9)
N(31)	0.0279(15)	0.0249(14)	0.0157(14)	0.0003(11)	0.0063(11)	0.0108(11)
N(32)	0.0248(14)	0.0234(14)	0.0159(14)	–0.0007(11)	0.0059(11)	0.0079(11)
N(33)	0.0193(14)	0.0429(17)	0.0184(14)	–0.0011(11)	0.0045(10)	0.0103(12)
N(34)	0.0376(17)	0.0191(14)	0.0201(14)	0.0035(10)	0.0047(11)	0.0066(12)
C(31)	0.0182(15)	0.0218(15)	0.0219(16)	0.0021(12)	0.0026(12)	0.0056(12)
C(32)	0.0168(15)	0.0190(15)	0.0222(16)	0.0032(12)	0.0021(12)	0.0065(12)
C(33)	0.0179(15)	0.0202(15)	0.0210(16)	0.0039(12)	0.0050(12)	0.0039(12)
C(34)	0.0191(15)	0.0170(14)	0.0186(15)	0.0047(11)	0.0036(11)	0.0077(12)
C(35)	0.0171(15)	0.0232(16)	0.0288(17)	0.0008(13)	0.0031(12)	0.0009(12)
C(36)	0.0225(16)	0.0207(15)	0.0148(14)	0.0020(11)	0.0043(11)	0.0058(12)
C(37)	0.0309(18)	0.0212(16)	0.0159(15)	0.0004(12)	0.0038(12)	
–0.0006(13)						
C(38)	0.045(2)	0.0162(15)	0.0188(16)	0.0018(12)	0.0062(14)	0.0087(14)
C(39)	0.0324(18)	0.0279(17)	0.0141(15)	0.0012(12)	0.0031(12)	0.0168(14)
C(40)	0.0203(15)	0.0273(16)	0.0122(14)	0.0011(12)	0.0039(11)	0.0093(13)
C(41)	0.0207(15)	0.0191(14)	0.0109(14)	0.0002(11)	0.0038(11)	0.0039(12)
C(42)	0.0194(15)	0.0173(15)	0.0271(16)	0.0043(12)	0.0081(12)	0.0038(12)
C(43)	0.0182(15)	0.0179(15)	0.0249(16)	0.0012(12)	0.0020(12)	0.0020(12)
C(44)	0.0190(15)	0.0200(15)	0.0138(14)	0.0027(11)	0.0032(11)	0.0051(12)
C(45)	0.0266(17)	0.0197(15)	0.0154(15)	0.0031(11)	0.0044(12)	0.0069(13)

C(46)	0.0287(17)	0.0268(16)	0.0140(15)	0.0018(12)	0.0042(12)	0.0141(13)
C(47)	0.0180(15)	0.0379(19)	0.0163(15)	0.0016(13)	0.0031(12)	0.0093(14)
C(48)	0.0226(16)	0.0267(16)	0.0132(15)	0.0001(12)	0.0032(12)	
–0.0004(13)						
C(49)	0.0158(15)	0.0200(15)	0.0162(14)	0.0022(11)	0.0033(11)	0.0042(12)
C(50)	0.0184(15)	0.0175(15)	0.0312(17)	0.0020(12)	0.0046(12)	0.0014(12)
C(51)	0.055(2)	0.0275(19)	0.050(2)	0.0095(16)	–0.0034(18)	
–0.0123(17)						
C(52)	0.0186(17)	0.052(2)	0.050(2)	–0.0073(17)	0.0100(15)	
–0.0102(16)						
O(61)	0.0270(11)	0.0282(11)	0.0193(11)	0.0048(9)	0.0020(9)	0.0083(9)
O(62)	0.0311(12)	0.0340(12)	0.0228(12)	0.0074(9)	0.0044(9)	0.0177(10)
O(63)	0.0188(13)	0.0486(16)	0.092(2)	0.0030(14)	0.0174(13)	0.0014(11)
O(64)	0.0302(13)	0.0278(13)	0.0763(19)	0.0106(12)	0.0141(12)	0.0010(11)
O(65)	0.0229(13)	0.0318(13)	0.0767(19)	0.0070(12)	0.0104(12)	
–0.0004(10)						
O(66)	0.0454(14)	0.0162(12)	0.0463(15)	0.0082(10)	0.0086(11)	
–0.0002(10)						
O(67)	0.0281(12)	0.0159(10)	0.0335(12)	–0.0009(9)	0.0068(9)	0.0014(9)
O(68)	0.0167(11)	0.0273(11)	0.0301(12)	0.0060(9)	0.0013(9)	0.0022(9)
N(61)	0.0219(13)	0.0258(14)	0.0151(13)	0.0001(10)	0.0047(10)	0.0086(11)
N(62)	0.0292(15)	0.0255(14)	0.0147(14)	0.0007(11)	0.0051(11)	0.0127(11)
N(63)	0.0197(15)	0.0338(16)	0.0340(16)	0.0045(12)	0.0082(11)	0.0021(12)
N(64)	0.0286(15)	0.0199(14)	0.0246(14)	–0.0020(10)	0.0065(11)	
–0.0027(11)						
C(61)	0.0171(15)	0.0192(15)	0.0208(16)	0.0027(12)	0.0042(12)	0.0019(12)
C(62)	0.0212(15)	0.0201(15)	0.0170(15)	0.0038(11)	0.0041(12)	0.0071(12)
C(63)	0.0171(15)	0.0213(15)	0.0235(16)	0.0009(12)	0.0007(12)	0.0055(12)
C(64)	0.0150(14)	0.0208(15)	0.0230(16)	0.0008(12)	0.0029(12)	0.0065(12)
C(65)	0.0187(15)	0.0179(15)	0.0277(16)	0.0008(12)	0.0056(12)	0.0021(12)
C(66)	0.0190(15)	0.0200(15)	0.0122(14)	0.0028(11)	0.0039(11)	0.0047(12)
C(67)	0.0265(16)	0.0202(15)	0.0134(14)	0.0009(11)	0.0043(12)	0.0046(13)
C(68)	0.0288(17)	0.0222(16)	0.0203(16)	–0.0003(12)	0.0065(12)	0.0122(13)
C(69)	0.0194(16)	0.0337(18)	0.0215(16)	0.0014(13)	0.0067(12)	0.0111(14)
C(70)	0.0194(15)	0.0248(16)	0.0187(15)	0.0041(12)	0.0053(12)	0.0025(12)
C(71)	0.0200(15)	0.0186(15)	0.0150(14)	0.0030(11)	0.0024(11)	0.0030(12)
C(72)	0.0202(15)	0.0207(15)	0.0267(17)	0.0014(12)	0.0055(12)	0.0044(12)
C(73)	0.0185(15)	0.0219(15)	0.0251(16)	0.0008(12)	0.0038(12)	0.0041(12)
C(74)	0.0215(15)	0.0179(15)	0.0148(14)	0.0003(11)	0.0052(11)	0.0040(12)
C(75)	0.0218(16)	0.0210(15)	0.0142(14)	0.0014(11)	0.0059(11)	0.0019(12)
C(76)	0.0292(17)	0.0179(15)	0.0168(15)	0.0026(11)	0.0030(12)	0.0068(13)
C(77)	0.0202(16)	0.0262(16)	0.0182(15)	0.0030(12)	0.0019(12)	0.0089(13)
C(78)	0.0186(15)	0.0213(15)	0.0150(14)	0.0011(11)	0.0019(11)	0.0038(12)
C(79)	0.0216(15)	0.0177(14)	0.0130(14)	0.0014(11)	0.0043(11)	0.0063(12)
C(80)	0.0176(15)	0.0193(15)	0.0236(16)	0.0022(12)	0.0057(12)	0.0039(12)
C(81)	0.047(2)	0.0195(16)	0.0318(19)	–0.0007(13)	0.0088(15)	0.0015(15)
C(82)	0.0162(16)	0.045(2)	0.0370(19)	0.0071(15)	0.0020(13)	0.0014(14)
O(91)	0.093(3)	0.070(2)	0.125(3)	0.047(2)	0.057(2)	0.0199(19)
N(91)	0.080(3)	0.077(3)	0.058(2)	0.014(2)	0.007(2)	–0.024(2)
C(91)	0.062(3)	0.079(3)	0.073(3)	0.024(3)	0.016(2)	0.013(3)

C(92)	0.132(6)	0.096(5)	0.117(5)	0.054(4)	–0.011(4)	–0.009(4)
C(93)	0.182(7)	0.087(4)	0.139(6)	–0.024(4)	0.096(6)	–0.011(5)
O(92)	0.0384(14)	0.0475(15)	0.0500(16)	0.0012(12)	0.0185(12)	0.0046(12)
N(92)	0.0404(19)	0.0381(17)	0.073(2)	0.0192(16)	0.0286(17)	0.0102(14)
C(94)	0.035(2)	0.0260(18)	0.047(2)	0.0071(15)	0.0095(17)	0.0013(15)
C(95)	0.030(2)	0.148(5)	0.118(5)	0.064(4)	0.010(3)	0.017(3)
C(96)	0.129(5)	0.045(3)	0.130(5)	–0.008(3)	0.103(4)	0.001(3)
O(93)	0.068(2)	0.079(3)	0.096(3)	–0.008(2)	–0.0067(19)	
–0.0158(19)						
N(93)	0.065(3)	0.045(2)	0.070(2)	–0.0056(17)	0.0115(19)	0.0078(18)
C(97)	0.056(3)	0.086(4)	0.069(3)	0.009(3)	0.014(2)	0.022(3)
C(98)	0.216(8)	0.046(3)	0.128(6)	–0.018(3)	0.050(5)	0.005(4)
C(99)	0.056(3)	0.093(4)	0.079(4)	–0.005(3)	–0.005(2)	0.008(3)
O(94)	0.0560(17)	0.0628(19)	0.0444(16)	–0.0127(13)	0.0112(13)	
–0.0265(14)						
N(94)	0.0313(16)	0.0320(16)	0.0453(18)	–0.0070(13)	0.0054(13)	
–0.0044(13)						
C(100)	0.0282(19)	0.053(2)	0.047(2)	0.0042(19)	0.0129(17)	
–0.0022(18)						
C(101)	0.049(3)	0.038(2)	0.094(3)	–0.017(2)	0.025(2)	–0.0034(19)
C(102)	0.146(5)	0.057(3)	0.059(3)	–0.001(2)	–0.037(3)	0.016(3)
O(95)	0.065(2)	0.0578(19)	0.097(3)	0.0093(17)	0.0472(19)	0.0037(15)
N(95)	0.063(2)	0.0407(19)	0.087(3)	0.0216(18)	0.041(2)	0.0166(17)
C(103)	0.064(3)	0.039(2)	0.114(4)	0.022(3)	0.032(3)	–0.002(2)
C(104)	0.100(4)	0.064(3)	0.110(5)	0.006(3)	0.052(4)	0.020(3)
C(105)	0.072(4)	0.126(5)	0.093(4)	0.031(4)	0.015(3)	0.040(3)
O(96)	0.082(2)	0.060(2)	0.075(2)	–0.0017(17)	–0.0016(19)	0.0068(17)
N(96)	0.043(2)	0.0373(18)	0.078(3)	–0.0064(17)	0.0014(18)	0.0051(15)
C(106)	0.046(3)	0.028(2)	0.103(4)	–0.010(2)	0.004(3)	0.0015(18)
C(107)	0.046(3)	0.083(4)	0.141(5)	–0.013(3)	0.029(3)	0.001(3)
C(108)	0.098(4)	0.059(3)	0.101(5)	0.003(3)	0.007(3)	0.025(3)
O(97)	0.0438(16)	0.0450(15)	0.0283(14)	0.0026(11)	0.0132(13)	0.0071(13)
O(98)	0.0361(15)	0.0375(14)	0.0274(14)	0.0000(11)	0.0124(12)	0.0065(12)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for *rac*-**6**[b].

	x	y	z	U
H(1N)	0.289(2)	0.2121(19)	0.7909(16)	0.026(8)
H(2N)	0.243(2)	0.295(2)	0.9989(16)	0.027(9)
H(5A)	0.4431	0.1977	0.8440	0.025
H(5B)	0.4654	0.2231	0.9243	0.025
H(8)	0.6100	–0.0477	0.9331	0.031
H(9)	0.4782	–0.1448	0.9221	0.031
H(12A)	0.2461	0.0683	0.9124	0.028
H(12B)	0.2519	0.0643	0.8335	0.028
H(13A)	0.0573	0.2488	0.8565	0.026
H(13B)	0.0792	0.2455	0.9375	0.026
H(16)	–0.1460	0.4703	0.9098	0.031
H(17)	–0.0392	0.5920	0.9161	0.030
H(20A)	0.2416	0.4351	0.9549	0.025
H(20B)	0.2233	0.4408	0.8742	0.025
H(21A)	0.7164	0.0691	0.9730	0.051
H(21B)	0.7491	0.1475	0.9319	0.051
H(21C)	0.7109	0.0545	0.8931	0.051
H(22A)	0.0682	0.6798	0.8759	0.050
H(22B)	0.1693	0.7166	0.9166	0.050
H(22C)	0.0885	0.6906	0.9568	0.050
H(31N)	0.251(2)	0.1845(19)	0.4872(16)	0.020(8)
H(32N)	0.209(2)	0.2748(19)	0.6847(16)	0.019(9)
H(35A)	0.2698	0.4167	0.6441	0.028
H(35B)	0.2650	0.4108	0.5636	0.028
H(38)	0.0836	0.6580	0.5757	0.032
H(39)	–0.0605	0.5821	0.5710	0.029
H(42A)	0.0337	0.2847	0.5580	0.025
H(42B)	0.0602	0.3028	0.6389	0.025
H(43A)	0.2832	0.0423	0.6085	0.025
H(43B)	0.2727	0.0477	0.5281	0.025
H(46)	0.5803	–0.0694	0.5829	0.027
H(47)	0.6687	0.0647	0.5926	0.028
H(50A)	0.4112	0.2461	0.5445	0.027
H(50B)	0.4296	0.2521	0.6259	0.027
H(51A)	0.2247	0.6966	0.5433	0.070
H(51B)	0.3265	0.6986	0.5888	0.070
H(51C)	0.2392	0.7123	0.6238	0.070
H(52A)	0.7323	0.2054	0.6392	0.061
H(52B)	0.7229	0.2941	0.6022	0.061
H(52C)	0.7163	0.2029	0.5585	0.061
H(61N)	0.230(2)	0.183(2)	0.1744(17)	0.030(9)
H(62N)	0.1920(19)	0.2748(18)	0.3796(15)	0.015(8)
H(65A)	0.2495	0.0360	0.2994	0.026
H(65B)	0.2266	0.0438	0.2189	0.026
H(68)	0.5089	–0.1095	0.2478	0.028

H(69)	0.6149	0.0127	0.2575	0.029
H(72A)	0.3903	0.2378	0.2420	0.027
H(72B)	0.4114	0.2259	0.3219	0.027
H(73A)	0.2200	0.4240	0.3390	0.026
H(73B)	0.2292	0.4163	0.2607	0.026
H(76)	–0.0128	0.6226	0.2437	0.025
H(77)	–0.1413	0.5226	0.2386	0.026
H(80A)	0.0119	0.2564	0.2535	0.024
H(80B)	0.0347	0.2881	0.3328	0.024
H(81A)	0.3769	–0.2013	0.1915	0.049
H(81B)	0.2949	–0.2368	0.2275	0.049
H(81C)	0.3966	–0.2095	0.2714	0.049
H(82A)	–0.2452	0.4156	0.2680	0.049
H(82B)	–0.2736	0.3204	0.2302	0.049
H(82C)	–0.2385	0.3988	0.1901	0.049
H(91)	0.3374	0.4933	0.4829	0.084
H(92A)	0.3980	0.5974	0.4298	0.178
H(92B)	0.3964	0.5611	0.3537	0.178
H(92C)	0.4934	0.5836	0.4052	0.178
H(93A)	0.5398	0.4319	0.3989	0.196
H(93B)	0.4488	0.4008	0.3431	0.196
H(93C)	0.4682	0.3547	0.4127	0.196
H(94)	–0.0836	0.8892	0.6182	0.043
H(95A)	0.0961	0.9211	0.7515	0.145
H(95B)	0.1681	0.9515	0.7053	0.145
H(95C)	0.1523	0.8507	0.7187	0.145
H(96A)	0.0171	0.8579	0.5535	0.138
H(96B)	0.1091	0.8187	0.5909	0.138
H(96C)	0.1119	0.9196	0.5759	0.138
H(97)	0.3504	0.5234	0.1850	0.083
H(98A)	0.5494	0.6469	0.2171	0.194
H(98B)	0.5149	0.6374	0.2870	0.194
H(98C)	0.4416	0.6495	0.2195	0.194
H(99A)	0.5496	0.4196	0.2233	0.118
H(99B)	0.5911	0.4869	0.2872	0.118
H(99C)	0.6138	0.5051	0.2146	0.118
H(100)	0.1210	–0.0360	0.9910	0.051
H(10A)	0.0472	–0.1534	0.9254	0.091
H(10B)	0.0120	–0.1357	0.8478	0.091
H(10C)	–0.0595	–0.1384	0.8985	0.091
H(10D)	–0.0005	0.0886	0.8790	0.143
H(10E)	–0.0920	0.0252	0.8786	0.143
H(10F)	–0.0317	0.0102	0.8215	0.143
H(103)	–0.1030	0.8822	0.3252	0.084
H(10G)	0.0071	0.8484	0.2633	0.130
H(10H)	0.0891	0.8057	0.3104	0.130
H(10I)	0.1053	0.9035	0.2897	0.130
H(10J)	0.0761	0.9457	0.4553	0.142
H(10K)	0.1504	0.9561	0.4071	0.142
H(10L)	0.1294	0.8639	0.4362	0.142

H(106)	0.5872	0.5944	1.0012	0.073
H(10M)	0.3999	0.6154	1.0798	0.134
H(10N)	0.3284	0.5906	1.0099	0.134
H(10O)	0.3672	0.6902	1.0314	0.134
H(10P)	0.4963	0.6207	0.9083	0.130
H(10Q)	0.4149	0.6812	0.9161	0.130
H(10R)	0.3928	0.5776	0.9043	0.130
H(1O)	0.191(3)	0.334(3)	1.103(2)	0.078(15)
H(2O)	0.275(4)	0.377(3)	1.109(3)	0.088(19)
H(3O)	0.200(3)	0.116(3)	1.061(2)	0.060(14)
H(4O)	0.285(3)	0.156(3)	1.076(2)	0.049(13)

Table 6. Torsion angles [°] for *rac*-**6**[b].

C(4)–N(1)–C(1)–O(1)	−176.4(3)	C(4)–N(1)–C(1)–C(2)	2.0(4)
C(3)–N(2)–C(2)–C(1)	−7.8(4)	C(3)–N(2)–C(2)–C(13)	113.9(3)
C(3)–N(2)–C(2)–C(20)	−129.6(3)	O(1)–C(1)–C(2)–N(2)	−173.6(2)
O(1)–C(1)–C(2)–C(13)	64.1(3)	O(1)–C(1)–C(2)–C(20)	−52.1(3)
N(1)–C(1)–C(2)–N(2)	7.9(4)	N(1)–C(1)–C(2)–C(13)	−114.4(3)
N(1)–C(1)–C(2)–C(20)	129.5(3)	C(2)–N(2)–C(3)–O(2)	178.8(3)
C(2)–N(2)–C(3)–C(4)	−2.2(4)	C(1)–N(1)–C(4)–C(3)	−11.7(4)
C(1)–N(1)–C(4)–C(5)	−133.0(3)	C(1)–N(1)–C(4)–C(12)	110.0(3)
O(2)–C(3)–C(4)–N(1)	−169.5(2)	O(2)–C(3)–C(4)–C(5)	−46.5(3)
O(2)–C(3)–C(4)–C(12)	67.9(3)	N(2)–C(3)–C(4)–N(1)	11.4(4)
N(2)–C(3)–C(4)–C(5)	134.5(3)	N(2)–C(3)–C(4)–C(12)	−111.1(3)
N(1)–C(4)–C(5)–C(6)	−135.6(2)	C(3)–C(4)–C(5)–C(6)	101.3(2)
C(12)–C(4)–C(5)–C(6)	−15.5(3)	C(4)–C(5)–C(6)–C(7)	−170.5(3)
C(4)–C(5)–C(6)–C(11)	11.4(3)	C(21)–O(5)–C(7)–C(6)	−177.9(3)
C(21)–O(5)–C(7)–C(8)	2.0(4)	C(5)–C(6)–C(7)–O(5)	1.5(4)
C(5)–C(6)–C(7)–C(8)	−178.3(3)	C(11)–C(6)–C(7)–O(5)	179.6(2)
C(11)–C(6)–C(7)–C(8)	−0.3(4)	O(5)–C(7)–C(8)–C(9)	−178.7(3)
C(6)–C(7)–C(8)–C(9)	1.1(4)	C(7)–C(8)–C(9)–C(10)	−0.1(4)
C(8)–C(9)–C(10)–N(3)	178.2(3)	C(8)–C(9)–C(10)–C(11)	−1.7(4)
O(3)–N(3)–C(10)–C(9)	0.9(4)	O(3)–N(3)–C(10)–C(11)	−179.2(3)
O(4)–N(3)–C(10)–C(9)	−179.7(3)	O(4)–N(3)–C(10)–C(11)	0.2(4)
C(5)–C(6)–C(11)–C(10)	176.8(2)	C(5)–C(6)–C(11)–C(12)	−2.1(3)
C(7)–C(6)–C(11)–C(10)	−1.5(4)	C(7)–C(6)–C(11)–C(12)	179.6(3)
N(3)–C(10)–C(11)–C(6)	−177.4(3)	N(3)–C(10)–C(11)–C(12)	1.2(5)
C(9)–C(10)–C(11)–C(6)	2.5(4)	C(9)–C(10)–C(11)–C(12)	−178.9(3)
C(6)–C(11)–C(12)–C(4)	−8.0(3)	C(10)–C(11)–C(12)–C(4)	173.3(3)
N(1)–C(4)–C(12)–C(11)	135.0(2)	C(3)–C(4)–C(12)–C(11)	−101.8(3)
C(5)–C(4)–C(12)–C(11)	14.5(3)	N(2)–C(2)–C(13)–C(14)	119.9(2)
C(1)–C(2)–C(13)–C(14)	−117.1(2)	C(20)–C(2)–C(13)–C(14)	1.3(3)
C(2)–C(13)–C(14)–C(15)	177.6(3)	C(2)–C(13)–C(14)–C(19)	0.1(3)
C(13)–C(14)–C(15)–N(4)	3.0(4)	C(13)–C(14)–C(15)–C(16)	−175.8(3)
C(19)–C(14)–C(15)–N(4)	−179.6(2)	C(19)–C(14)–C(15)–C(16)	1.6(4)
O(6)–N(4)–C(15)–C(14)	3.1(4)	O(6)–N(4)–C(15)–C(16)	−178.0(3)
O(7)–N(4)–C(15)–C(14)	−177.0(3)	O(7)–N(4)–C(15)–C(16)	1.9(4)

N(4)–C(15)–C(16)–C(17)	−179.1(3)	C(14)–C(15)–C(16)–C(17)	−0.3(4)
C(15)–C(16)–C(17)–C(18)	−0.8(4)	C(22)–O(8)–C(18)–C(17)	−3.9(4)
C(22)–O(8)–C(18)–C(19)	175.1(2)	C(16)–C(17)–C(18)–O(8)	179.4(3)
C(16)–C(17)–C(18)–C(19)	0.4(4)	C(13)–C(14)–C(19)–C(18)	176.0(2)
C(13)–C(14)–C(19)–C(20)	−1.6(3)	C(15)–C(14)–C(19)–C(18)	−1.9(4)
C(15)–C(14)–C(19)–C(20)	−179.5(2)	O(8)–C(18)–C(19)–C(14)	−178.2(2)
O(8)–C(18)–C(19)–C(20)	−1.0(4)	C(17)–C(18)–C(19)–C(14)	0.9(4)
C(17)–C(18)–C(19)–C(20)	178.1(3)	C(14)–C(19)–C(20)–C(2)	2.3(3)
C(18)–C(19)–C(20)–C(2)	−175.1(3)	N(2)–C(2)–C(20)–C(19)	−121.2(2)
C(1)–C(2)–C(20)–C(19)	116.0(2)	C(13)–C(2)–C(20)–C(19)	−2.1(3)
C(34)–N(31)–C(31)–O(31)	176.4(3)	C(34)–N(31)–C(31)–C(32)	−0.8(4)
C(33)–N(32)–C(32)–C(31)	20.5(4)	C(33)–N(32)–C(32)–C(43)	143.6(3)
C(33)–N(32)–C(32)–C(50)	−99.9(3)	O(31)–C(31)–C(32)–N(32)	165.5(2)
O(31)–C(31)–C(32)–C(43)	42.8(3)	O(31)–C(31)–C(32)–C(50)	−73.0(3)
N(31)–C(31)–C(32)–N(32)	−17.2(3)	N(31)–C(31)–C(32)–C(43)	−139.9(3)
N(31)–C(31)–C(32)–C(50)	104.4(3)	C(32)–N(32)–C(33)–O(32)	174.2(3)
C(32)–N(32)–C(33)–C(34)	−4.7(4)	C(31)–N(31)–C(34)–C(33)	16.9(4)
C(31)–N(31)–C(34)–C(35)	−104.1(3)	C(31)–N(31)–C(34)–C(42)	138.9(3)
O(32)–C(33)–C(34)–N(31)	167.2(2)	O(32)–C(33)–C(34)–C(35)	−70.1(3)
O(32)–C(33)–C(34)–C(42)	44.8(3)	N(32)–C(33)–C(34)–N(31)	−13.8(3)
N(32)–C(33)–C(34)–C(35)	108.8(3)	N(32)–C(33)–C(34)–C(42)	−136.2(2)
N(31)–C(34)–C(35)–C(36)	−130.1(2)	C(33)–C(34)–C(35)–C(36)	106.9(2)
C(42)–C(34)–C(35)–C(36)	−10.4(3)	C(34)–C(35)–C(36)–C(37)	−174.5(3)
C(34)–C(35)–C(36)–C(41)	6.6(3)	C(51)–O(37)–C(37)–C(36)	178.8(3)
C(51)–O(37)–C(37)–C(38)	−0.8(4)	C(35)–C(36)–C(37)–O(37)	0.1(4)
C(35)–C(36)–C(37)–C(38)	179.7(3)	C(41)–C(36)–C(37)–O(37)	178.9(2)
C(41)–C(36)–C(37)–C(38)	−1.5(4)	O(37)–C(37)–C(38)–C(39)	−179.3(3)
C(36)–C(37)–C(38)–C(39)	1.2(4)	C(37)–C(38)–C(39)–C(40)	0.0(4)
C(38)–C(39)–C(40)–N(33)	180.0(2)	C(38)–C(39)–C(40)–C(41)	−0.9(4)
O(33)–N(33)–C(40)–C(39)	0.9(4)	O(33)–N(33)–C(40)–C(41)	−178.3(2)
O(34)–N(33)–C(40)–C(39)	−178.2(3)	O(34)–N(33)–C(40)–C(41)	2.6(4)
C(35)–C(36)–C(41)–C(40)	179.6(2)	C(35)–C(36)–C(41)–C(42)	0.4(3)
C(37)–C(36)–C(41)–C(40)	0.6(4)	C(37)–C(36)–C(41)–C(42)	−178.6(2)
N(33)–C(40)–C(41)–C(36)	179.7(2)	N(33)–C(40)–C(41)–C(42)	−1.2(4)
C(39)–C(40)–C(41)–C(36)	0.6(4)	C(39)–C(40)–C(41)–C(42)	179.6(3)
C(36)–C(41)–C(42)–C(34)	−7.1(3)	C(40)–C(41)–C(42)–C(34)	173.8(3)
N(31)–C(34)–C(42)–C(41)	131.0(2)	C(33)–C(34)–C(42)–C(41)	−105.8(2)
C(35)–C(34)–C(42)–C(41)	10.7(3)	N(32)–C(32)–C(43)–C(44)	125.2(2)
C(31)–C(32)–C(43)–C(44)	−111.3(2)	C(50)–C(32)–C(43)–C(44)	6.0(3)
C(32)–C(43)–C(44)–C(45)	175.8(3)	C(32)–C(43)–C(44)–C(49)	−3.9(3)
C(43)–C(44)–C(45)–N(34)	0.3(4)	C(43)–C(44)–C(45)–C(46)	179.5(3)
C(49)–C(44)–C(45)–N(34)	−179.9(2)	C(49)–C(44)–C(45)–C(46)	−0.8(4)
O(35)–N(34)–C(45)–C(44)	3.8(4)	O(35)–N(34)–C(45)–C(46)	−175.3(3)
O(36)–N(34)–C(45)–C(44)	−176.6(3)	O(36)–N(34)–C(45)–C(46)	4.2(4)
N(34)–C(45)–C(46)–C(47)	179.4(2)	C(44)–C(45)–C(46)–C(47)	0.2(4)
C(45)–C(46)–C(47)–C(48)	0.0(4)	C(52)–O(38)–C(48)–C(47)	2.0(4)
C(52)–O(38)–C(48)–C(49)	−178.6(3)	C(46)–C(47)–C(48)–O(38)	179.7(3)
C(46)–C(47)–C(48)–C(49)	0.3(4)	C(43)–C(44)–C(49)–C(48)	−179.1(2)
C(43)–C(44)–C(49)–C(50)	0.0(3)	C(45)–C(44)–C(49)–C(48)	1.1(4)

C(45)–C(44)–C(49)–C(50)	−179.8(2)	O(38)–C(48)–C(49)–C(44)	179.7(2)
O(38)–C(48)–C(49)–C(50)	0.6(4)	C(47)–C(48)–C(49)–C(44)	−0.9(4)
C(47)–C(48)–C(49)–C(50)	−179.9(3)	C(44)–C(49)–C(50)–C(32)	3.8(3)
C(48)–C(49)–C(50)–C(32)	−177.1(3)	N(32)–C(32)–C(50)–C(49)	−124.9(2)
C(31)–C(32)–C(50)–C(49)	112.9(2)	C(43)–C(32)–C(50)–C(49)	−5.9(3)
C(64)–N(61)–C(61)–O(61)	177.3(2)	C(64)–N(61)–C(61)–C(62)	−2.6(4)
C(63)–N(62)–C(62)–C(61)	−0.8(4)	C(63)–N(62)–C(62)–C(73)	−122.2(3)
C(63)–N(62)–C(62)–C(80)	120.2(3)	O(61)–C(61)–C(62)–N(62)	175.5(2)
O(61)–C(61)–C(62)–C(73)	−61.0(3)	O(61)–C(61)–C(62)–C(80)	52.7(3)
N(61)–C(61)–C(62)–N(62)	−4.6(3)	N(61)–C(61)–C(62)–C(73)	118.9(3)
N(61)–C(61)–C(62)–C(80)	−127.5(3)	C(62)–N(62)–C(63)–O(62)	−171.2(3)
C(62)–N(62)–C(63)–C(64)	12.4(4)	C(61)–N(61)–C(64)–C(63)	13.3(4)
C(61)–N(61)–C(64)–C(65)	136.7(3)	C(61)–N(61)–C(64)–C(72)	−107.3(3)
O(62)–C(63)–C(64)–N(61)	166.1(2)	O(62)–C(63)–C(64)–C(65)	43.3(3)
O(62)–C(63)–C(64)–C(72)	−72.4(3)	N(62)–C(63)–C(64)–N(61)	−17.3(3)
N(62)–C(63)–C(64)–C(65)	−140.1(3)	N(62)–C(63)–C(64)–C(72)	104.2(3)
N(61)–C(64)–C(65)–C(66)	117.2(2)	C(63)–C(64)–C(65)–C(66)	−118.8(2)
C(72)–C(64)–C(65)–C(66)	−1.4(3)	C(64)–C(65)–C(66)–C(67)	177.0(2)
C(64)–C(65)–C(66)–C(71)	−0.2(3)	C(81)–O(67)–C(67)–C(66)	177.7(2)
C(81)–O(67)–C(67)–C(68)	−3.9(4)	C(65)–C(66)–C(67)–O(67)	2.9(4)
C(65)–C(66)–C(67)–C(68)	−175.6(3)	C(71)–C(66)–C(67)–O(67)	179.9(2)
C(71)–C(66)–C(67)–C(68)	1.4(4)	O(67)–C(67)–C(68)–C(69)	179.1(3)
C(66)–C(67)–C(68)–C(69)	−2.5(4)	C(67)–C(68)–C(69)–C(70)	0.7(4)
C(68)–C(69)–C(70)–N(63)	−178.5(3)	C(68)–C(69)–C(70)–C(71)	2.2(4)
O(63)–N(63)–C(70)–C(69)	0.2(4)	O(63)–N(63)–C(70)–C(71)	179.5(3)
O(64)–N(63)–C(70)–C(69)	179.5(3)	O(64)–N(63)–C(70)–C(71)	−1.2(4)
C(65)–C(66)–C(71)–C(70)	178.8(2)	C(65)–C(66)–C(71)–C(72)	1.8(3)
C(67)–C(66)–C(71)–C(70)	1.5(4)	C(67)–C(66)–C(71)–C(72)	−175.6(2)
N(63)–C(70)–C(71)–C(66)	177.4(2)	N(63)–C(70)–C(71)–C(72)	−6.2(4)
C(69)–C(70)–C(71)–C(66)	−3.3(4)	C(69)–C(70)–C(71)–C(72)	173.1(3)
C(66)–C(71)–C(72)–C(64)	−2.6(3)	C(70)–C(71)–C(72)–C(64)	−179.1(3)
N(61)–C(64)–C(72)–C(71)	−116.1(2)	C(63)–C(64)–C(72)–C(71)	121.2(2)
C(65)–C(64)–C(72)–C(71)	2.3(3)	N(62)–C(62)–C(73)–C(74)	−137.8(2)
C(61)–C(62)–C(73)–C(74)	98.5(2)	C(80)–C(62)–C(73)–C(74)	−16.9(3)
C(62)–C(73)–C(74)–C(75)	−172.7(3)	C(62)–C(73)–C(74)–C(79)	10.4(3)
C(73)–C(74)–C(75)–N(64)	4.8(4)	C(73)–C(74)–C(75)–C(76)	−176.0(3)
C(79)–C(74)–C(75)–N(64)	−178.5(2)	C(79)–C(74)–C(75)–C(76)	0.7(4)
O(65)–N(64)–C(75)–C(74)	−1.6(4)	O(65)–N(64)–C(75)–C(76)	179.2(3)
O(66)–N(64)–C(75)–C(74)	178.0(2)	O(66)–N(64)–C(75)–C(76)	−1.3(4)
N(64)–C(75)–C(76)–C(77)	178.2(2)	C(74)–C(75)–C(76)–C(77)	−1.1(4)
C(75)–C(76)–C(77)–C(78)	−0.1(4)	C(82)–O(68)–C(78)–C(77)	5.1(4)
C(82)–O(68)–C(78)–C(79)	−175.0(2)	C(76)–C(77)–C(78)–O(68)	−178.6(3)
C(76)–C(77)–C(78)–C(79)	1.5(4)	C(73)–C(74)–C(79)–C(78)	178.1(2)
C(73)–C(74)–C(79)–C(80)	0.7(3)	C(75)–C(74)–C(79)–C(78)	0.7(4)
C(75)–C(74)–C(79)–C(80)	−176.7(2)	O(68)–C(78)–C(79)–C(74)	178.3(2)
O(68)–C(78)–C(79)–C(80)	−4.7(4)	C(77)–C(78)–C(79)–C(74)	−1.8(4)
C(77)–C(78)–C(79)–C(80)	175.2(3)	C(74)–C(79)–C(80)–C(62)	−11.5(3)
C(78)–C(79)–C(80)–C(62)	171.2(3)	N(62)–C(62)–C(80)–C(79)	138.4(2)

C(61)–C(62)–C(80)–C(79)	–98.2(2)	C(73)–C(62)–C(80)–C(79)	17.2(3)
C(92)–N(91)–C(91)–O(91)	–178.7(5)	C(93)–N(91)–C(91)–O(91)	3.0(8)
C(95)–N(92)–C(94)–O(92)	0.6(6)	C(96)–N(92)–C(94)–O(92)	–179.8(3)
C(98)–N(93)–C(97)–O(93)	178.2(5)	C(99)–N(93)–C(97)–O(93)	2.1(7)
C(101)–N(94)–C(100)–O(94)	179.7(3)	C(102)–N(94)–C(100)–O(94)	–3.2(6)
C(104)–N(95)–C(103)–O(95)	174.6(4)	C(105)–N(95)–C(103)–O(95)	–1.9(7)
C(107)–N(96)–C(106)–O(96)	–1.4(6)	C(108)–N(96)–C(106)–O(96)	179.0(4)

Table 7. Hydrogen bonds for *rac*-**6**^{b} [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
N(1)–H(1N)...O(31)	0.90(3)	2.03(3)	2.923(3)	172(3)
N(2)–H(2N)...O(97)	0.87(3)	1.96(3)	2.816(4)	165(3)
N(32)–H(31N)...O(62)	0.81(3)	2.11(3)	2.917(3)	173(3)
N(31)–H(32N)...O(1)	0.78(3)	2.17(3)	2.955(3)	179(3)
N(61)–H(61N)...O(98A)	0.92(3)	1.88(3)	2.799(3)	172(3)
N(62)–H(62N)...O(32)	0.79(3)	2.17(3)	2.953(3)	168(3)
O(97)–H(1O)...O(61B)	0.90(5)	1.90(5)	2.779(3)	165(4)
O(97)–H(2O)...O(93B)	0.82(5)	1.97(5)	2.784(4)	178(5)
O(98)–H(3O)...O(94)	0.85(4)	1.91(4)	2.750(4)	168(4)
O(98)–H(4O)...O(2)	0.80(4)	2.00(4)	2.772(3)	160(4)
C(102)–H(10F)...O(92C)	0.98	2.53	3.471(6)	160
C(104)–H(10H)...O(66)	0.98	2.54	3.363(5)	142
C(108)–H(10Q)...O(3D)	0.98	2.47	3.421(6)	164
C(22)–H(22B)...O(3D)	0.98	2.54	3.515(4)	170
C(35)–H(35B)...O(91)	0.99	2.37	3.322(4)	160
C(39)–H(39)...O(32E)	0.95	2.50	3.345(4)	148
C(46)–H(46)...O(62F)	0.95	2.49	3.361(4)	152
C(50)–H(50A)...O(91)	0.99	2.48	3.337(4)	144
C(52)–H(52B)...O(34G)	0.98	2.58	3.172(4)	119
C(92)–H(92B)...O(65)	0.98	2.56	3.408(7)	145
C(95)–H(95C)...O(63H)	0.98	2.58	3.252(5)	126
C(96)–H(96C)...O(95I)	0.98	2.55	3.256(5)	129

Symmetry operations for equivalent atoms

A x,y,z–1 B x,y,z+1 C x,y–1,z D x,y+1,z
E –x,–y+1,–z+1 F –x+1,–y,–z+1 G x+1,y,z
H –x+1,–y+1,–z+1 I –x,–y+2,–z+1

Crystallographic data for *rac*-6c

Table 1. Crystal data and structure refinement for *rac*-**6**[c].

Identification code	*rac*-**6**[c]	
Chemical formula (moiety)	$(C_{22}H_{20}N_4O_8)2.5(SOC_2H_6)$	
Chemical formula (total)	$C_{27}H_{35}N_4O_{10.50}S_{2.50}$	
Formula weight	663.74	
Temperature	170(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 9.603(2) Å	α = 82.504(4)°
	b = 11.614(3) Å	β = 79.188(4)°
	c = 14.295(3) Å	γ = 82.969(4)°
Cell volume	1544.8(6) $Å^3$	
Z	2	
Calculated density	1.427 g/cm^3	
Absorption coefficient μ	0.270 mm^{-1}	
F(000)	698	
Crystal colour and size	colourless, 0.27 × 0.17 × 0.07 mm^3	
Reflections for cell refinement	3443 (θ range 2.2 to 26.3°)	
Data collection method	Bruker SMART 1000 CCD diffractometer thin-slice ω scans	
θ range for data collection	1.5 to 26.0°	
Index ranges	h −11 to 11, k −14 to 14, l −17 to 17	
Completeness to θ = 26.0°	98.5 %	
Reflections collected	15838	
Independent reflections	5988 (R_{int} = 0.0443)	
Reflections with $F^2>2\sigma$	3996	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.7612 and 1.0	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0537, 0.7870	
Data / restraints / parameters	5988 / 0 / 438	
Final R indices [$F^2>2\sigma$]	R1 = 0.0596, wR2 = 0.1172	
R indices (all data)	R1 = 0.1033, wR2 = 0.1325	
Goodness-of-fit on F^2	1.032	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.31 and −0.39 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for *rac*-**6**[c]. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1)	0.2683(2)	–0.47755(16)	0.13082(14)	0.0443(6)
C(1)	0.2200(3)	–0.5200(2)	0.21180(19)	0.0286(6)
N(1)	0.1148(3)	–0.50149(19)	0.38114(16)	0.0332(6)
C(2)	0.1554(3)	–0.4380(2)	0.28694(19)	0.0270(6)
C(3)	0.2654(3)	–0.3516(2)	0.28996(19)	0.0259(6)
C(4)	0.2174(3)	–0.2445(2)	0.22879(17)	0.0212(6)
C(5)	0.2914(3)	–0.1462(2)	0.19936(18)	0.0237(6)
O(6)	0.41955(19)	–0.15260(15)	0.22665(14)	0.0320(5)
C(7)	0.4990(3)	–0.0519(3)	0.2010(2)	0.0421(8)
C(8)	0.2293(3)	–0.0509(2)	0.14659(19)	0.0298(7)
C(9)	0.0959(3)	–0.0545(2)	0.12596(19)	0.0326(7)
C(10)	0.0223(3)	–0.1517(2)	0.15749(19)	0.0277(6)
N(11)	–0.1208(3)	–0.1504(2)	0.13543(17)	0.0393(6)
O(12)	–0.1882(2)	–0.2335(2)	0.16733(19)	0.0560(6)
O(13)	–0.1679(2)	–0.0642(3)	0.08834(18)	0.0735(9)
C(14)	0.0838(3)	–0.2485(2)	0.20901(17)	0.0228(6)
C(15)	0.0256(3)	–0.3611(2)	0.2546(2)	0.0293(6)
C(16)	0.1090(3)	–0.6149(2)	0.40447(19)	0.0263(6)
N(16)	0.2240(3)	–0.63429(19)	0.23716(16)	0.0302(6)
O(16)	0.0641(2)	–0.65692(16)	0.48652(14)	0.0381(5)
C(17)	0.1601(3)	–0.6962(2)	0.32661(19)	0.0269(6)
C(18)	0.2692(3)	–0.7952(2)	0.3619(2)	0.0287(6)
C(19)	0.1940(3)	–0.9035(2)	0.37681(18)	0.0236(6)
C(20)	0.2466(3)	–1.0139(2)	0.41419(18)	0.0275(6)
O(21)	0.3791(2)	–1.02102(15)	0.43496(14)	0.0351(5)
C(22)	0.4438(4)	–1.1347(2)	0.4650(2)	0.0483(9)
C(23)	0.1612(3)	–1.1052(2)	0.42854(19)	0.0312(7)
C(24)	0.0310(3)	–1.0875(2)	0.40051(19)	0.0317(7)
C(25)	–0.0183(3)	–0.9790(2)	0.35941(19)	0.0289(6)
N(26)	–0.1553(3)	–0.9657(2)	0.32938(19)	0.0415(7)
O(27)	–0.2216(2)	–1.0514(2)	0.33850(18)	0.0596(7)
O(28)	–0.2013(2)	–0.8689(2)	0.2949(2)	0.0602(7)
C(29)	0.0630(3)	–0.8840(2)	0.34914(18)	0.0245(6)
C(30)	0.0310(3)	–0.7581(2)	0.3125(2)	0.0339(7)
S(100)	0.46879(11)	0.21938(8)	0.01959(7)	0.0612(3)
O(100)	0.3463(3)	0.21060(18)	0.10154(17)	0.0720(9)
C(100)	0.4283(4)	0.3488(3)	–0.0526(2)	0.0630(11)
C(101)	0.6061(6)	0.2680(5)	0.0652(3)	0.114(2)
S(200)	0.28347(8)	0.54341(7)	0.62122(6)	0.0413(2)
O(200)	0.3015(3)	0.59988(19)	0.52112(16)	0.0560(6)
C(200)	0.3550(3)	0.3951(3)	0.6162(2)	0.0486(9)
C(201)	0.4194(4)	0.5908(3)	0.6721(3)	0.0577(10)
S(300)	–0.0790(4)	–0.5590(3)	0.1057(3)	0.0478(8)

O(300)	–0.2355(10)	–0.5399(7)	0.1341(6)	0.060(2)
C(300)	–0.0411(14)	–0.6916(11)	0.0479(10)	0.048(3)
C(301)	–0.026(2)	–0.4674(14)	0.0045(15)	0.063(6)
S(310)	–0.1291(7)	–0.5476(5)	0.0626(5)	0.0611(17)
O(310)	–0.133(2)	–0.5375(12)	0.1673(12)	0.071(4)
C(310)	–0.035(3)	–0.428(2)	–0.0051(18)	0.051(7)
C(311)	0.001(3)	–0.654(3)	0.030(2)	0.102(10)

Table 3. Bond lengths [Å] and angles [°] for *rac*-**6**[c].

O(1)–C(1)	1.226(3)	C(1)–C(2)	1.522(3)
C(1)–N(16)	1.327(3)	N(1)–H(1A)	0.85(3)
N(1)–C(2)	1.457(3)	N(1)–C(16)	1.322(3)
C(2)–C(3)	1.553(4)	C(2)–C(15)	1.550(4)
C(3)–H(3A)	0.9900	C(3)–H(3B)	0.9900
C(3)–C(4)	1.501(3)	C(4)–C(5)	1.395(3)
C(4)–C(14)	1.372(4)	C(5)–O(6)	1.350(3)
C(5)–C(8)	1.392(4)	O(6)–C(7)	1.445(3)
C(7)–H(7A)	0.9800	C(7)–H(7B)	0.9800
C(7)–H(7C)	0.9800	C(8)–H(8A)	0.9500
C(8)–C(9)	1.375(4)	C(9)–H(9A)	0.9500
C(9)–C(10)	1.386(4)	C(10)–N(11)	1.464(4)
C(10)–C(14)	1.392(4)	N(11)–O(12)	1.219(3)
N(11)–O(13)	1.219(3)	C(14)–C(15)	1.506(3)
C(15)–H(15A)	0.9900	C(15)–H(15B)	0.9900
C(16)–O(16)	1.230(3)	C(16)–C(17)	1.525(4)
N(16)–H(16A)	0.86(3)	N(16)–C(17)	1.450(3)
C(17)–C(18)	1.557(4)	C(17)–C(30)	1.563(4)
C(18)–H(18A)	0.9900	C(18)–H(18B)	0.9900
C(18)–C(19)	1.497(3)	C(19)–C(20)	1.396(4)
C(19)–C(29)	1.373(4)	C(20)–O(21)	1.350(3)
C(20)–C(23)	1.391(4)	O(21)–C(22)	1.437(3)
C(22)–H(22A)	0.9800	C(22)–H(22B)	0.9800
C(22)–H(22C)	0.9800	C(23)–H(23A)	0.9500
C(23)–C(24)	1.368(4)	C(24)–H(24A)	0.9500
C(24)–C(25)	1.387(4)	C(25)–N(26)	1.444(4)
C(25)–C(29)	1.405(4)	N(26)–O(27)	1.225(3)
N(26)–O(28)	1.232(3)	C(29)–C(30)	1.502(4)
C(30)–H(30G)	0.9900	C(30)–H(30H)	0.9900
S(100)–O(100)	1.499(2)	S(100)–C(100)	1.755(4)
S(100)–C(101)	1.756(5)	C(100)–H(10D)	0.9800
C(100)–H(10E)	0.9800	C(100)–H(10F)	0.9800
C(101)–H(10G)	0.9800	C(101)–H(10H)	0.9800
C(101)–H(10I)	0.9800	S(200)–O(200)	1.482(2)
S(200)–C(200)	1.780(3)	S(200)–C(201)	1.781(4)
C(200)–H(20D)	0.9800	C(200)–H(20E)	0.9800
C(200)–H(20F)	0.9800	C(201)–H(20A)	0.9800
C(201)–H(20B)	0.9800	C(201)–H(20C)	0.9800
S(300)–O(300)	1.479(10)	S(300)–C(300)	1.808(13)
S(300)–C(301)	1.71(2)	C(300)–H(30A)	0.9800

C(300)–H(30B)	0.9800	C(300)–H(30C)	0.9800
C(301)–H(30D)	0.9800	C(301)–H(30E)	0.9800
C(301)–H(30F)	0.9800	S(310)–O(310)	1.510(16)
S(310)–C(310)	1.82(2)	S(310)–C(311)	1.70(3)
C(310)–H(31A)	0.9800	C(310)–H(31B)	0.9800
C(310)–H(31C)	0.9800	C(311)–H(31D)	0.9800
C(311)–H(31E)	0.9800	C(311)–H(31F)	0.9800

O(1)–C(1)–C(2)	118.5(2)	O(1)–C(1)–N(16)	122.8(2)
C(2)–C(1)–N(16)	118.6(2)	H(1A)–N(1)–C(2)	114(2)
H(1A)–N(1)–C(16)	116(2)	C(2)–N(1)–C(16)	128.8(2)
C(1)–C(2)–N(1)	111.9(2)	C(1)–C(2)–C(3)	108.4(2)
C(1)–C(2)–C(15)	109.4(2)	N(1)–C(2)–C(3)	110.7(2)
N(1)–C(2)–C(15)	110.9(2)	C(3)–C(2)–C(15)	105.3(2)
C(2)–C(3)–H(3A)	111.1	C(2)–C(3)–H(3B)	111.1
C(2)–C(3)–C(4)	103.5(2)	H(3A)–C(3)–H(3B)	109.0
H(3A)–C(3)–C(4)	111.1	H(3B)–C(3)–C(4)	111.1
C(3)–C(4)–C(5)	125.9(2)	C(3)–C(4)–C(14)	112.3(2)
C(5)–C(4)–C(14)	121.7(2)	C(4)–C(5)–O(6)	115.4(2)
C(4)–C(5)–C(8)	119.1(2)	O(6)–C(5)–C(8)	125.5(2)
C(5)–O(6)–C(7)	117.9(2)	O(6)–C(7)–H(7A)	109.5
O(6)–C(7)–H(7B)	109.5	O(6)–C(7)–H(7C)	109.5
H(7A)–C(7)–H(7B)	109.5	H(7A)–C(7)–H(7C)	109.5
H(7B)–C(7)–H(7C)	109.5	C(5)–C(8)–H(8A)	120.2
C(5)–C(8)–C(9)	119.6(3)	H(8A)–C(8)–C(9)	120.2
C(8)–C(9)–H(9A)	119.6	C(8)–C(9)–C(10)	120.7(3)
H(9A)–C(9)–C(10)	119.6	C(9)–C(10)–N(11)	118.6(2)
C(9)–C(10)–C(14)	120.4(3)	N(11)–C(10)–C(14)	121.0(2)
C(10)–N(11)–O(12)	118.5(2)	C(10)–N(11)–O(13)	118.0(3)
O(12)–N(11)–O(13)	123.4(3)	C(4)–C(14)–C(10)	118.5(2)
C(4)–C(14)–C(15)	110.4(2)	C(10)–C(14)–C(15)	131.0(2)
C(2)–C(15)–C(14)	104.5(2)	C(2)–C(15)–H(15A)	110.9
C(2)–C(15)–H(15B)	110.9	C(14)–C(15)–H(15A)	110.9
C(14)–C(15)–H(15B)	110.9	H(15A)–C(15)–H(15B)	108.9
N(1)–C(16)–O(16)	122.3(2)	N(1)–C(16)–C(17)	118.6(2)
O(16)–C(16)–C(17)	119.1(2)	C(1)–N(16)–H(16A)	116.4(19)
C(1)–N(16)–C(17)	128.7(2)	H(16A)–N(16)–C(17)	114.4(19)
C(16)–C(17)–N(16)	111.9(2)	C(16)–C(17)–C(18)	109.1(2)
C(16)–C(17)–C(30)	108.7(2)	N(16)–C(17)–C(18)	110.1(2)
N(16)–C(17)–C(30)	110.9(2)	C(18)–C(17)–C(30)	105.8(2)
C(17)–C(18)–H(18A)	110.8	C(17)–C(18)–H(18B)	110.8
C(17)–C(18)–C(19)	104.8(2)	H(18A)–C(18)–H(18B)	108.9
H(18A)–C(18)–C(19)	110.8	H(18B)–C(18)–C(19)	110.8
C(18)–C(19)–C(20)	125.8(2)	C(18)–C(19)–C(29)	112.5(2)
C(20)–C(19)–C(29)	121.7(2)	C(19)–C(20)–O(21)	115.2(2)
C(19)–C(20)–C(23)	119.2(3)	O(21)–C(20)–C(23)	125.6(2)
C(20)–O(21)–C(22)	117.5(2)	O(21)–C(22)–H(22A)	109.5
O(21)–C(22)–H(22B)	109.5	O(21)–C(22)–H(22C)	109.5
H(22A)–C(22)–H(22B)	109.5	H(22A)–C(22)–H(22C)	109.5
H(22B)–C(22)–H(22C)	109.5	C(20)–C(23)–H(23A)	120.2
C(20)–C(23)–C(24)	119.7(3)	H(23A)–C(23)–C(24)	120.2

C(23)–C(24)–H(24A)	119.6	C(23)–C(24)–C(25)	120.9(3)
H(24A)–C(24)–C(25)	119.6	C(24)–C(25)–N(26)	118.6(2)
C(24)–C(25)–C(29)	120.3(3)	N(26)–C(25)–C(29)	121.2(3)
C(25)–N(26)–O(27)	118.9(3)	C(25)–N(26)–O(28)	118.9(2)
O(27)–N(26)–O(28)	122.2(3)	C(19)–C(29)–C(25)	118.1(2)
C(19)–C(29)–C(30)	111.2(2)	C(25)–C(29)–C(30)	130.7(3)
C(17)–C(30)–C(29)	105.3(2)	C(17)–C(30)–H(30G)	110.7
C(17)–C(30)–H(30H)	110.7	C(29)–C(30)–H(30G)	110.7
C(29)–C(30)–H(30H)	110.7	H(30G)–C(30)–H(30H)	108.8
O(100)–S(100)–C(100)	106.14(17)	O(100)–S(100)–C(101)	105.9(2)
C(100)–S(100)–C(101)	96.9(2)	S(100)–C(100)–H(10D)	109.5
S(100)–C(100)–H(10E)	109.5	S(100)–C(100)–H(10F)	109.5
H(10D)–C(100)–H(10E)	109.5	H(10D)–C(100)–H(10F)	109.5
H(10E)–C(100)–H(10F)	109.5	S(100)–C(101)–H(10G)	109.5
S(100)–C(101)–H(10H)	109.5	S(100)–C(101)–H(10I)	109.5
H(10G)–C(101)–H(10H)	109.5	H(10G)–C(101)–H(10I)	109.5
H(10H)–C(101)–H(10I)	109.5	O(200)–S(200)–C(200)	106.77(15)
O(200)–S(200)–C(201)	105.47(16)	C(200)–S(200)–C(201)	97.71(17)
S(200)–C(200)–H(20D)	109.5	S(200)–C(200)–H(20E)	109.5
S(200)–C(200)–H(20F)	109.5	H(20D)–C(200)–H(20E)	109.5
H(20D)–C(200)–H(20F)	109.5	H(20E)–C(200)–H(20F)	109.5
S(200)–C(201)–H(20A)	109.5	S(200)–C(201)–H(20B)	109.5
S(200)–C(201)–H(20C)	109.5	H(20A)–C(201)–H(20B)	109.5
H(20A)–C(201)–H(20C)	109.5	H(20B)–C(201)–H(20C)	109.5
O(300)–S(300)–C(300)	106.9(6)	O(300)–S(300)–C(301)	109.2(7)
C(300)–S(300)–C(301)	95.7(8)	S(300)–C(301)–H(30D)	109.5
S(300)–C(301)–H(30E)	109.5	S(300)–C(301)–H(30F)	109.5
H(30D)–C(301)–H(30E)	109.5	H(30D)–C(301)–H(30F)	109.5
H(30E)–C(301)–H(30F)	109.5	O(310)–S(310)–C(310)	106.7(10)
O(310)–S(310)–C(311)	107.4(14)	C(310)–S(310)–C(311)	95.4(16)
S(310)–C(310)–H(31A)	109.5	S(310)–C(310)–H(31B)	109.5
S(310)–C(310)–H(31C)	109.5	H(31A)–C(310)–H(31B)	109.5
H(31A)–C(310)–H(31C)	109.5	H(31B)–C(310)–H(31C)	109.5
S(310)–C(311)–H(31D)	109.5	S(310)–C(311)–H(31E)	109.5
S(310)–C(311)–H(31F)	109.5	H(31D)–C(311)–H(31E)	109.5
H(31D)–C(311)–H(31F)	109.5	H(31E)–C(311)–H(31F)	109.5

Table 4. Anisotropic displacement parameters ($Å^2$) for *rac*-**6**[c]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	0.0749(16)	0.0261(11)	0.0263(11)	–0.0044(9)	0.0113(10)	–0.0126(10)
C(1)	0.0388(17)	0.0203(14)	0.0260(16)	–0.0043(12)	–0.0005(13)	–0.0062(12)
N(1)	0.0541(16)	0.0171(12)	0.0241(13)	–0.0052(10)	0.0088(11)	–0.0079(11)
C(2)	0.0373(16)	0.0156(13)	0.0263(15)	–0.0029(11)	0.0014(12)	–0.0061(12)

C(3)	0.0310(15)	0.0196(14)	0.0266(15)	–0.0021(11)	–0.0037(12)	–0.0033(11)
C(4)	0.0270(15)	0.0171(13)	0.0190(13)	–0.0036(10)	–0.0015(11)	–0.0020(11)
C(5)	0.0249(15)	0.0214(14)	0.0240(14)	–0.0066(11)	0.0025(11)	–0.0054(11)
O(6)	0.0292(11)	0.0256(10)	0.0421(12)	–0.0043(9)	–0.0029(9)	–0.0109(8)
C(7)	0.0335(17)	0.0386(18)	0.055(2)	–0.0117(15)	0.0044(15)	–0.0195(14)
C(8)	0.0361(17)	0.0194(14)	0.0295(16)	0.0014(12)	0.0037(13)	–0.0049(12)
C(9)	0.0398(18)	0.0264(15)	0.0259(15)	0.0035(12)	–0.0014(13)	0.0053(13)
C(10)	0.0249(15)	0.0322(16)	0.0245(15)	–0.0031(12)	–0.0025(12)	0.0007(12)
N(11)	0.0312(15)	0.0544(18)	0.0289(14)	–0.0014(13)	–0.0035(12)	0.0035(13)
O(12)	0.0410(14)	0.0507(15)	0.0824(18)	–0.0121(13)	–0.0203(13)	–0.0092(12)
O(13)	0.0379(14)	0.108(2)	0.0578(16)	0.0434(16)	–0.0111(12)	0.0049(14)
C(14)	0.0299(15)	0.0195(13)	0.0191(13)	–0.0070(11)	0.0006(11)	–0.0051(11)
C(15)	0.0311(16)	0.0258(15)	0.0323(16)	–0.0047(12)	–0.0025(12)	–0.0104(12)
C(16)	0.0300(16)	0.0211(14)	0.0272(15)	0.0005(12)	–0.0029(12)	–0.0062(12)
N(16)	0.0431(15)	0.0172(12)	0.0276(13)	–0.0081(10)	0.0027(11)	0.0000(10)
O(16)	0.0548(14)	0.0213(10)	0.0315(12)	0.0027(9)	0.0061(10)	–0.0048(9)
C(17)	0.0336(16)	0.0177(14)	0.0276(15)	–0.0008(11)	–0.0002(12)	–0.0050(12)
C(18)	0.0327(16)	0.0164(13)	0.0367(16)	–0.0016(12)	–0.0060(13)	–0.0028(12)
C(19)	0.0293(15)	0.0177(13)	0.0229(14)	–0.0051(11)	0.0011(12)	–0.0040(11)
C(20)	0.0403(18)	0.0181(14)	0.0229(14)	–0.0047(11)	–0.0008(13)	–0.0027(12)
O(21)	0.0449(13)	0.0193(10)	0.0433(12)	–0.0030(9)	–0.0170(10)	0.0022(9)
C(22)	0.064(2)	0.0246(17)	0.058(2)	–0.0025(15)	–0.0257(18)	0.0098(15)
C(23)	0.0503(19)	0.0165(14)	0.0246(15)	–0.0033(11)	0.0002(13)	–0.0045(13)
C(24)	0.0453(19)	0.0207(15)	0.0278(15)	–0.0086(12)	0.0092(13)	–0.0153(13)
C(25)	0.0282(16)	0.0301(16)	0.0288(15)	–0.0126(12)	0.0041(12)	–0.0093(12)
N(26)	0.0355(16)	0.0432(17)	0.0476(16)	–0.0184(13)	0.0022(13)	–0.0109(13)
O(27)	0.0463(14)	0.0583(15)	0.0806(18)	–0.0174(13)	–0.0038(13)	–0.0317(12)
O(28)	0.0423(14)	0.0474(15)	0.097(2)	–0.0096(14)	–0.0271(14)	–0.0049(12)
C(29)	0.0315(16)	0.0184(13)	0.0225(14)	–0.0068(11)	0.0023(12)	

–0.0037(11)						
C(30)	0.0319(16)	0.0256(15)	0.0463(18)	–0.0048(13)	–0.0102(14)	
–0.0044(12)						
S(100)	0.0850(7)	0.0432(5)	0.0498(6)	–0.0194(4)	0.0251(5)	–0.0261(5)
O(100)	0.112(2)	0.0271(12)	0.0595(16)	–0.0155(11)	0.0467(15)	
–0.0244(13)						
C(100)	0.083(3)	0.062(2)	0.043(2)	–0.0118(18)	0.0140(19)	–0.035(2)
C(101)	0.154(5)	0.132(5)	0.069(3)	0.016(3)	–0.031(3)	–0.078(4)
S(200)	0.0338(4)	0.0357(4)	0.0495(5)	–0.0011(4)	–0.0031(4)	0.0049(3)
O(200)	0.0700(17)	0.0463(14)	0.0551(15)	0.0112(12)	–0.0293(13)	
–0.0086(12)						
C(200)	0.045(2)	0.0295(17)	0.062(2)	0.0013(16)	0.0062(17)	
–0.0001(15)						
C(201)	0.069(3)	0.052(2)	0.057(2)	–0.0087(18)	–0.028(2)	0.0028(19)
S(300)	0.058(2)	0.052(2)	0.041(2)	–0.0161(17)	–0.0182(19)	
–0.0069(17)						
O(300)	0.065(6)	0.061(6)	0.045(5)	–0.014(4)	0.009(5)	0.008(5)
S(310)	0.070(4)	0.054(3)	0.075(4)	–0.023(3)	–0.042(4)	–0.005(3)
O(310)	0.085(12)	0.069(10)	0.061(10)	–0.033(8)	0.006(9)	–0.025(8)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for *rac*-**6**[c].

	x	y	z	U
H(1A)	0.075(3)	–0.458(3)	0.424(2)	0.040
H(3A)	0.2630	–0.3346	0.3563	0.031
H(3B)	0.3631	–0.3834	0.2632	0.031
H(7A)	0.5894	–0.0682	0.2250	0.063
H(7B)	0.4433	0.0153	0.2295	0.063
H(7C)	0.5183	–0.0345	0.1311	0.063
H(8A)	0.2789	0.0162	0.1250	0.036
H(9A)	0.0536	0.0103	0.0897	0.039
H(15A)	–0.0130	–0.3984	0.2078	0.035
H(15B)	–0.0508	–0.3474	0.3101	0.035
H(16A)	0.260(3)	–0.678(2)	0.193(2)	0.036
H(18A)	0.3570	–0.8029	0.3133	0.034
H(18B)	0.2948	–0.7792	0.4226	0.034
H(22A)	0.5390	–1.1279	0.4778	0.072
H(22B)	0.4516	–1.1854	0.4142	0.072
H(22C)	0.3850	–1.1682	0.5234	0.072
H(23A)	0.1932	–1.1796	0.4577	0.037
H(24A)	–0.0265	–1.1504	0.4093	0.038
H(30G)	–0.0589	–0.7241	0.3494	0.041
H(30H)	0.0224	–0.7502	0.2440	0.041
H(10D)	0.3507	0.3388	–0.0857	0.095
H(10E)	0.5128	0.3671	–0.1000	0.095
H(10F)	0.3989	0.4128	–0.0125	0.095

H(10G)	0.6446	0.2052	0.1088	0.171
H(10H)	0.5683	0.3356	0.1000	0.171
H(10I)	0.6819	0.2904	0.0121	0.171
H(20D)	0.2917	0.3534	0.5893	0.073
H(20E)	0.3631	0.3585	0.6810	0.073
H(20F)	0.4494	0.3917	0.5757	0.073
H(20A)	0.3974	0.6739	0.6804	0.087
H(20B)	0.5113	0.5788	0.6294	0.087
H(20C)	0.4243	0.5458	0.7345	0.087
H(30A)	–0.0861	–0.7550	0.0904	0.073
H(30B)	0.0621	–0.7121	0.0342	0.073
H(30C)	–0.0789	–0.6795	–0.0121	0.073
H(30D)	–0.0395	–0.3867	0.0201	0.095
H(30E)	–0.0835	–0.4748	–0.0440	0.095
H(30F)	0.0746	–0.4885	–0.0206	0.095
H(31A)	–0.0942	–0.3540	0.0036	0.076
H(31B)	–0.0144	–0.4394	–0.0732	0.076
H(31C)	0.0547	–0.4262	0.0179	0.076
H(31D)	–0.0298	–0.7306	0.0574	0.153
H(31E)	0.0879	–0.6426	0.0526	0.153
H(31F)	0.0212	–0.6513	–0.0405	0.153

Table 6. Torsion angles [°] for *rac*-**6**[c]

C(16)–N(1)–C(2)–C(1)	–10.2(4)	C(16)–N(1)–C(2)–C(3)	–131.3(3)
C(16)–N(1)–C(2)–C(15)	112.2(3)	O(1)–C(1)–C(2)–N(1)	–174.8(3)
O(1)–C(1)–C(2)–C(3)	–52.4(3)	O(1)–C(1)–C(2)–C(15)	61.9(3)
N(16)–C(1)–C(2)–N(1)	4.0(4)	N(16)–C(1)–C(2)–C(3)	126.4(3)
N(16)–C(1)–C(2)–C(15)	–119.3(3)	C(1)–C(2)–C(3)–C(4)	97.9(2)
N(1)–C(2)–C(3)–C(4)	–139.0(2)	C(15)–C(2)–C(3)–C(4)	–19.1(3)
C(2)–C(3)–C(4)–C(5)	–171.8(2)	C(2)–C(3)–C(4)–C(14)	12.7(3)
C(3)–C(4)–C(5)–O(6)	2.6(4)	C(3)–C(4)–C(5)–C(8)	–176.7(2)
C(14)–C(4)–C(5)–O(6)	177.7(2)	C(14)–C(4)–C(5)–C(8)	–1.6(4)
C(4)–C(5)–O(6)–C(7)	–178.0(2)	C(8)–C(5)–O(6)–C(7)	1.3(4)
C(4)–C(5)–C(8)–C(9)	1.1(4)	O(6)–C(5)–C(8)–C(9)	–178.1(2)
C(5)–C(8)–C(9)–C(10)	0.3(4)	C(8)–C(9)–C(10)–N(11)	178.7(2)
C(8)–C(9)–C(10)–C(14)	–1.3(4)	C(9)–C(10)–N(11)–O(12)	–176.4(3)
C(9)–C(10)–N(11)–O(13)	1.5(4)	C(14)–C(10)–N(11)–O(12)	3.7(4)
C(14)–C(10)–N(11)–O(13)	–178.5(3)	C(3)–C(4)–C(14)–C(10)	176.3(2)
C(3)–C(4)–C(14)–C(15)	–0.5(3)	C(5)–C(4)–C(14)–C(10)	0.6(4)
C(5)–C(4)–C(14)–C(15)	–176.3(2)	C(9)–C(10)–C(14)–C(4)	0.9(4)
C(9)–C(10)–C(14)–C(15)	176.9(3)	N(11)–C(10)–C(14)–C(4)	–179.1(2)
N(11)–C(10)–C(14)–C(15)	–3.1(4)	C(4)–C(14)–C(15)–C(2)	–12.0(3)
C(10)–C(14)–C(15)–C(2)	171.7(3)	C(1)–C(2)–C(15)–C(14)	–97.3(2)
N(1)–C(2)–C(15)–C(14)	138.9(2)	C(3)–C(2)–C(15)–C(14)	19.1(3)
C(2)–N(1)–C(16)–O(16)	–175.3(3)	C(2)–N(1)–C(16)–C(17)	4.8(4)
O(1)–C(1)–N(16)–C(17)	–173.7(3)	C(2)–C(1)–N(16)–C(17)	7.5(4)
C(1)–N(16)–C(17)–C(16)	–12.9(4)	C(1)–N(16)–C(17)–C(18)	–134.5(3)
C(1)–N(16)–C(17)–C(30)	108.7(3)	N(1)–C(16)–C(17)–N(16)	6.3(4)

N(1)–C(16)–C(17)–C(18)	128.5(3)	N(1)–C(16)–C(17)–C(30)	−116.5(3)
O(16)–C(16)–C(17)–N(16)	−173.6(2)	O(16)–C(16)–C(17)–C(18)	−51.4(3)
O(16)–C(16)–C(17)–C(30)	63.6(3)	C(16)–C(17)–C(18)–C(19)	110.7(2)
N(16)–C(17)–C(18)–C(19)	−126.0(2)	C(30)–C(17)–C(18)–C(19)	−6.1(3)
C(17)–C(18)–C(19)–C(20)	−175.7(2)	C(17)–C(18)–C(19)–C(29)	4.4(3)
C(18)–C(19)–C(20)–O(21)	−2.3(4)	C(18)–C(19)–C(20)–C(23)	176.6(2)
C(29)–C(19)–C(20)–O(21)	177.6(2)	C(29)–C(19)–C(20)–C(23)	−3.5(4)
C(19)–C(20)–O(21)–C(22)	−174.2(2)	C(23)–C(20)–O(21)–C(22)	6.9(4)
C(19)–C(20)–C(23)–C(24)	4.0(4)	O(21)–C(20)–C(23)–C(24)	−177.2(2)
C(20)–C(23)–C(24)–C(25)	−1.1(4)	C(23)–C(24)–C(25)–N(26)	178.8(2)
C(23)–C(24)–C(25)–C(29)	−2.4(4)	C(24)–C(25)–N(26)–O(27)	−2.2(4)
C(24)–C(25)–N(26)–O(28)	178.3(3)	C(29)–C(25)–N(26)–O(27)	179.0(2)
C(29)–C(25)–N(26)–O(28)	−0.5(4)	C(18)–C(19)–C(29)–C(25)	179.9(2)
C(18)–C(19)–C(29)–C(30)	−0.7(3)	C(20)–C(19)–C(29)–C(25)	0.0(4)
C(20)–C(19)–C(29)–C(30)	179.4(2)	C(24)–C(25)–C(29)–C(19)	2.9(4)
C(24)–C(25)–C(29)–C(30)	−176.3(3)	N(26)–C(25)–C(29)–C(19)	−178.3(2)
N(26)–C(25)–C(29)–C(30)	2.5(4)	C(19)–C(29)–C(30)–C(17)	−3.3(3)
C(25)–C(29)–C(30)–C(17)	176.0(3)	C(16)–C(17)–C(30)–C(29)	−111.4(2)
N(16)–C(17)–C(30)–C(29)	125.2(2)	C(18)–C(17)–C(30)–C(29)	5.7(3)

Table 7. Hydrogen bonds for *rac*-**6**[c] [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
N(1)–H(1A)...O(16A)	0.85(3)	2.13(3)	2.972(3)	166(3)
N(16)–H(16A)...O(100B)	0.86(3)	1.96(3)	2.815(3)	175(3)

Symmetry operations for equivalent atoms
A −x,−y−1,−z+1 B x,y−1,z

Crystallographic data for *meso*-6.

Table 1. Crystal data and structure refinement for *meso*-**6**.

Identification code	*meso*-**6**	
Chemical formula (moiety)	$C_{22}H_{20}N_4O_8$	
Chemical formula (total)	$C_{22}H_{20}N_4O_8$	
Formula weight	468.42	
Temperature	120(2) K	
Radiation, wavelength	synchrotron, 0.77490 Å	
Crystal system, space group	monoclinic, C2/m	
Unit cell parameters	a = 17.149(7) Å	α = 90°
	b = 6.368(3) Å	β = 106.207(6)°
	c = 9.310(4) Å	γ = 90°
Cell volume	976.3(7) $Å^3$	
Z	2	
Calculated density	1.593 g/cm^3	
Absorption coefficient μ	0.124 mm^{-1}	
F(000)	488	
Crystal colour and size	colourless, 0.10 × 0.01 × 0.01 mm^3	
Reflections for cell refinement	728 (θ range 2.5 to 27.2°)	
Data collection method	Bruker SMART 1000 CCD diffractometer thin-slice ω scans	
θ range for data collection	2.5 to 31.3°	
Index ranges	h −20 to 22, k −8 to 7, l −12 to 12	
Completeness to θ = 31.3°	95.3 %	
Reflections collected	3228	
Independent reflections	1283 (R_{int} = 0.0536)	
Reflections with $F^2>2\sigma$	752	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.9877 and 0.9988	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0865, 0.0435	
Data / restraints / parameters	1283 / 0 / 118	
Final R indices [$F^2>2\sigma$]	R1 = 0.0598, wR2 = 0.1498	
R indices (all data)	R1 = 0.1094, wR2 = 0.1715	
Goodness-of-fit on F^2	1.046	
Extinction coefficient	0.033(6)	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.25 and −0.19 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for *meso*-**6**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
C(10)	0.03413(12)	0.1924(3)	0.0526(2)	0.0389(6)
O(1)	0.07378(18)	0.3528(5)	0.1229(3)	0.0420(9)
O(2)	0.0913(2)	0.0000	0.5946(3)	0.0603(13)

O(3)	0.2001(2)	0.0000	0.7683(2)	0.0609(9)
N(2)	0.1614(2)	0.0000	0.6287(3)	0.0494(9)
C(11)	0.4255(2)	0.0000	0.2674(6)	0.0811(15)
O(4)	0.33992(16)	0.0000	0.2155(4)	0.0518(8)
N(1)	0.03413(12)	0.1924(3)	0.0526(2)	0.0389(6)
O(4')	0.1614(2)	0.0000	0.6287(3)	0.0494(9)
C(11')	0.2001(2)	0.0000	0.7683(2)	0.0609(9)
O(3')	0.4255(2)	0.0000	0.2674(6)	0.0811(15)
N(2')	0.33992(16)	0.0000	0.2155(4)	0.0518(8)
O(2')	0.3273(7)	0.0000	0.1007(13)	0.059(4)
C(1)	0.20886(17)	0.0000	0.5253(3)	0.0296(7)
C(2)	0.29192(19)	0.0000	0.5764(3)	0.0382(8)
C(3)	0.33682(18)	0.0000	0.4760(4)	0.0414(9)
C(4)	0.30012(17)	0.0000	0.3250(3)	0.0330(7)
C(5)	0.21569(16)	0.0000	0.2739(3)	0.0293(7)
C(6)	0.17011(16)	0.0000	0.3728(3)	0.0298(7)
C(7)	0.08183(19)	0.0000	0.2930(3)	0.0501(11)
C(8)	0.07693(17)	0.0000	0.1240(3)	0.0368(8)
C(9)	0.16563(19)	0.0000	0.1145(3)	0.0460(9)

Table 3. Bond lengths [Å] and angles [°] for *meso*-**6**.

C(10)–C(10A)	1.300(4)	C(10)–O(1)	1.298(3)
C(10)–C(8)	1.486(3)	O(2)–N(2)	1.154(4)
O(3)–N(2)	1.284(4)	N(2)–C(1)	1.424(4)
C(11)–H(11A)	0.9800	C(11)–H(11B)	0.9800
C(11)–H(11C)	0.9800	C(11)–O(4)	1.411(4)
O(4)–C(4)	1.376(4)	C(1)–C(2)	1.370(4)
C(1)–C(6)	1.389(4)	C(2)–H(2)	0.9500
C(2)–C(3)	1.367(5)	C(3)–H(3)	0.9500
C(3)–C(4)	1.371(4)	C(4)–C(5)	1.392(4)
C(5)–C(6)	1.365(4)	C(5)–C(9)	1.493(4)
C(6)–C(7)	1.489(4)	C(7)–H(7)	0.90(3)
C(7)–C(8)	1.552(4)	C(8)–C(10B)	1.486(3)
C(8)–N(1B)	1.486(3)	C(8)–C(9)	1.548(5)
C(9)–H(9)	1.04(3)		

C(10A)–C(10)–O(1)	127.92(15)	C(10A)–C(10)–C(8)	124.43(11)
O(1)–C(10)–C(8)	107.43(19)	O(2)–N(2)–O(3)	118.8(3)
O(2)–N(2)–C(1)	124.2(3)	O(3)–N(2)–C(1)	116.9(3)
H(11A)–C(11)–H(11B)	109.5	H(11A)–C(11)–H(11C)	109.5
H(11A)–C(11)–O(4)	109.5	H(11B)–C(11)–H(11C)	109.5
H(11B)–C(11)–O(4)	109.5	H(11C)–C(11)–O(4)	109.5
C(11)–O(4)–C(4)	115.5(3)	N(2)–C(1)–C(2)	120.0(3)
N(2)–C(1)–C(6)	119.3(3)	C(2)–C(1)–C(6)	120.6(3)
C(1)–C(2)–H(2)	120.3	C(1)–C(2)–C(3)	119.4(3)
H(2)–C(2)–C(3)	120.3	C(2)–C(3)–H(3)	119.5
C(2)–C(3)–C(4)	121.1(3)	H(3)–C(3)–C(4)	119.5
O(4)–C(4)–C(3)	125.4(3)	O(4)–C(4)–C(5)	115.5(3)
C(3)–C(4)–C(5)	119.1(3)	C(4)–C(5)–C(6)	120.4(2)
C(4)–C(5)–C(9)	126.5(3)	C(6)–C(5)–C(9)	113.1(3)

C(1)–C(6)–C(5)	119.3(3)	C(1)–C(6)–C(7)	129.8(3)
C(5)–C(6)–C(7)	110.9(2)	C(6)–C(7)–H(7)	117.8(17)
C(6)–C(7)–C(8)	105.4(2)	H(7)–C(7)–C(8)	116.2(17)
C(10)–C(8)–C(10B)	111.0(2)	C(10B)–C(8)–N(1B)	0.0(3)
C(10)–C(8)–N(1B)	111.0(2)	C(10)–C(8)–C(7)	109.48(15)
C(10B)–C(8)–C(7)	109.48(15)	C(10)–C(8)–C(9)	110.17(16)
C(10B)–C(8)–C(9)	110.17(16)	N(1B)–C(8)–C(7)	109.48(15)
N(1B)–C(8)–C(9)	110.17(16)	C(7)–C(8)–C(9)	106.4(2)
C(5)–C(9)–C(8)	104.2(3)	C(5)–C(9)–H(9)	109.1(14)
C(8)–C(9)–H(9)	111.8(15)		

Symmetry operations for equivalent atoms
A −x,y,−z B x,−y,z

Table 4. Anisotropic displacement parameters (Å^2) for *meso*-**6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(10)	0.0414(11)	0.0351(13)	0.0363(11)	–0.0021(8)	0.0043(8)	–0.0015(10)
O(1)	0.0412(18)	0.0355(18)	0.0385(19)	–0.0044(13)	–0.0067(14)	
–0.0087(14)						
O(2)	0.046(2)	0.098(3)	0.0416(19)	0.000	0.0205(15)	0.000
O(3)	0.104(2)	0.0605(19)	0.0182(12)	0.000	0.0168(13)	0.000
N(2)	0.072(2)	0.0410(17)	0.0431(16)	0.000	0.0280(16)	0.000
C(11)	0.043(2)	0.078(3)	0.137(4)	0.000	0.050(2)	0.000
O(4)	0.0528(17)	0.0468(16)	0.068(2)	0.000	0.0364(14)	0.000
N(1)	0.0414(11)	0.0351(13)	0.0363(11)	–0.0021(8)	0.0043(8)	–0.0015(10)
O(4')	0.072(2)	0.0410(17)	0.0431(16)	0.000	0.0280(16)	0.000
C(11')	0.104(2)	0.0605(19)	0.0182(12)	0.000	0.0168(13)	0.000
O(3')	0.043(2)	0.078(3)	0.137(4)	0.000	0.050(2)	0.000
N(2')	0.0528(17)	0.0468(16)	0.068(2)	0.000	0.0364(14)	0.000
O(2')	0.078(6)	0.072(8)	0.045(8)	0.000	0.045(5)	0.000
C(1)	0.0372(16)	0.0316(16)	0.0188(12)	0.000	0.0059(11)	0.000
C(2)	0.0394(17)	0.0344(18)	0.0278(15)	0.000	–0.0120(13)	0.000
C(3)	0.0261(15)	0.045(2)	0.0438(18)	0.000	–0.0063(13)	0.000
C(4)	0.0295(16)	0.0302(17)	0.0406(17)	0.000	0.0121(13)	0.000
C(5)	0.0253(15)	0.0376(17)	0.0207(13)	0.000	–0.0005(10)	0.000
C(6)	0.0242(14)	0.0426(18)	0.0195(13)	0.000	0.0008(10)	0.000
C(7)	0.0228(16)	0.105(3)	0.0204(15)	0.000	0.0028(12)	0.000
C(8)	0.0281(15)	0.055(2)	0.0227(14)	0.000	0.0005(12)	0.000
C(9)	0.0327(17)	0.081(3)	0.0220(15)	0.000	0.0043(12)	0.000

Table 5. Hydrogen coordinates and isotropic displacement parameters (Å^2) for *meso*-**6**.

	x	y	z	U
H(11A)	0.4482	0.0000	0.1817	0.122
H(11B)	0.4438	–0.1257	0.3282	0.122

H(11C)	0.4438	0.1257	0.3282	0.122
H(1)	0.0565	0.3145	0.0837	0.047
H(11D)	0.1612	0.0000	0.8280	0.091
H(11E)	0.2343	0.1257	0.7917	0.091
H(11F)	0.2343	–0.1257	0.7917	0.091
H(2)	0.3181	0.0000	0.6808	0.046
H(3)	0.3944	0.0000	0.5115	0.050
H(7)	0.0501(16)	0.093(4)	0.322(3)	0.060
H(9)	0.1786(16)	0.134(5)	0.062(3)	0.055

Table 6. Torsion angles [°] for *meso*-**6**.

O(2)–N(2)–C(1)–C(2)	180.0	O(2)–N(2)–C(1)–C(6)	0.0
O(3)–N(2)–C(1)–C(2)	0.0	O(3)–N(2)–C(1)–C(6)	180.0
N(2)–C(1)–C(2)–C(3)	180.0	C(6)–C(1)–C(2)–C(3)	0.0
C(1)–C(2)–C(3)–C(4)	0.0	C(2)–C(3)–C(4)–O(4)	180.0
C(2)–C(3)–C(4)–C(5)	0.0	C(11)–O(4)–C(4)–C(3)	0.0
C(11)–O(4)–C(4)–C(5)	180.0	O(4)–C(4)–C(5)–C(6)	180.0
O(4)–C(4)–C(5)–C(9)	0.0	C(3)–C(4)–C(5)–C(6)	0.0
C(3)–C(4)–C(5)–C(9)	180.0	C(4)–C(5)–C(6)–C(1)	0.0
C(4)–C(5)–C(6)–C(7)	180.0	C(9)–C(5)–C(6)–C(1)	180.0
C(9)–C(5)–C(6)–C(7)	0.0	N(2)–C(1)–C(6)–C(5)	180.0
N(2)–C(1)–C(6)–C(7)	0.0	C(2)–C(1)–C(6)–C(5)	0.0
C(2)–C(1)–C(6)–C(7)	180.0	C(1)–C(6)–C(7)–C(8)	180.0
C(5)–C(6)–C(7)–C(8)	0.0	C(10A)–C(10)–C(8)–C(10B)	3.6(4)
C(10A)–C(10)–C(8)–N(1B)	3.6(4)	C(10A)–C(10)–C(8)–C(7)	–117.4(3)
C(10A)–C(10)–C(8)–C(9)	125.9(3)	O(1)–C(10)–C(8)–C(10B)	178.5(2)
O(1)–C(10)–C(8)–N(1B)	178.5(2)	O(1)–C(10)–C(8)–C(7)	57.5(3)
O(1)–C(10)–C(8)–C(9)	–59.2(3)	C(6)–C(7)–C(8)–C(10)	–119.03(16)
C(6)–C(7)–C(8)–C(10B)	119.03(16)	C(6)–C(7)–C(8)–N(1B)	119.03(16)
C(6)–C(7)–C(8)–C(9)	0.0	C(4)–C(5)–C(9)–C(8)	180.0
C(6)–C(5)–C(9)–C(8)	0.0	C(10)–C(8)–C(9)–C(5)	118.57(15)
C(10B)–C(8)–C(9)–C(5)	–118.57(15)	N(1B)–C(8)–C(9)–C(5)	–118.57(15)
C(7)–C(8)–C(9)–C(5)	0.0		

Symmetry operations for equivalent atoms
A –x,y,–z B x,–y,z

Crystallographic data for (*R,S*)-9

Table 1. Crystal data and structure refinement for (*R,S*)-**9**.

Identification code	(*R,S*)-**9**	
Chemical formula (moiety)	$C_{20}H_{19}N_3O_5$	
Chemical formula (total)	$C_{20}H_{19}N_3O_5$	
Formula weight	381.38	
Temperature	173(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1$	
Unit cell parameters	a = 11.872(5) Å	α = 90°
	b = 6.262(3) Å	β = 111.215(12)°
	c = 12.819(6) Å	γ = 90°
Cell volume	888.4(7) $Å^3$	
Z	2	
Calculated density	1.426 g/cm^3	
Absorption coefficient μ	0.104 mm^{-1}	
F(000)	400	
Crystal colour and size	colourless, 0.13 × 0.07 × 0.04 mm^3	
Reflections for cell refinement	1814 (θ range 2.9 to 21.5°)	
Data collection method	Bruker SMART 1000 CCD diffractometer thin-slice ω scans	
θ range for data collection	1.7 to 26.0°	
Index ranges	h −14 to 14, k −7 to 7, l −15 to 15	
Completeness to θ = 26.0°	100.0 %	
Reflections collected	9941	
Independent reflections	1919 (R_{int} = 0.0996)	
Reflections with $F^2>2\sigma$	1144	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.9866 and 0.9958	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0880, 0.0620	
Data / restraints / parameters	1919 / 1 / 254	
Final R indices [$F^2>2\sigma$]	R1 = 0.0537, wR2 = 0.1247	
R indices (all data)	R1 = 0.1210, wR2 = 0.1702	
Goodness-of-fit on F^2	1.052	
Absolute structure parameter	3(3)	
Extinction coefficient	0.026(6)	
Largest and mean shift/su	0.000 and 0.000	
Largest diff. peak and hole	0.28 and −0.28 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for (*R,S*)-**9**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.8882(5)	0.0222(10)	0.6132(5)	0.0254(14)
N(1)	0.8591(4)	0.0135(7)	0.5027(4)	0.0251(12)

O(1)	0.8991(4)	–0.1442(6)	0.6693(3)	0.0328(10)
C(2)	0.9114(5)	0.2334(11)	0.6719(4)	0.0255(12)
C(3)	1.0496(5)	0.2522(11)	0.7430(4)	0.0296(13)
C(4)	1.0577(5)	0.2413(11)	0.8614(4)	0.0262(12)
O(5)	1.2676(3)	0.2400(9)	0.9322(3)	0.0438(11)
C(5)	1.1635(5)	0.2405(12)	0.9553(5)	0.0328(13)
C(5A)	1.3799(5)	0.2456(15)	1.0254(6)	0.060(2)
C(6)	1.1568(6)	0.2420(11)	1.0619(5)	0.0388(15)
C(7)	1.0462(6)	0.2409(12)	1.0723(5)	0.0378(15)
N(8)	0.8257(5)	0.2411(10)	0.9952(4)	0.0396(13)
C(8)	0.9402(5)	0.2407(11)	0.9782(4)	0.0320(13)
O(8B)	0.8262(4)	0.2348(10)	1.0921(4)	0.0564(13)
O(8A)	0.7328(4)	0.2458(9)	0.9122(4)	0.0492(12)
C(9)	0.9456(5)	0.2411(10)	0.8714(4)	0.0256(12)
C(10)	0.8468(5)	0.2451(11)	0.7582(4)	0.0283(12)
N(11)	0.8720(4)	0.4108(8)	0.5930(4)	0.0294(12)
C(11)	0.8519(5)	0.4084(10)	0.4831(5)	0.0253(13)
O(11)	0.8335(4)	0.5724(6)	0.4259(3)	0.0312(10)
C(12)	0.8515(5)	0.1933(9)	0.4274(5)	0.0242(13)
C(13)	0.7423(5)	0.1700(9)	0.3194(4)	0.0303(15)
C(14)	0.6222(5)	0.1959(11)	0.3334(4)	0.0322(15)
C(15)	0.5692(6)	0.0296(12)	0.3698(5)	0.0430(17)
C(16)	0.4593(6)	0.0575(15)	0.3855(6)	0.054(2)
C(17)	0.4020(6)	0.2562(16)	0.3597(6)	0.057(2)
C(18)	0.4525(7)	0.4202(14)	0.3236(7)	0.058(2)
C(19)	0.5625(6)	0.3916(12)	0.3091(5)	0.0455(18)

Table 3. Bond lengths [Å] and angles [°] for (*R,S*)-**9**.

C(1)–N(1)	1.333(7)	C(1)–O(1)	1.246(7)
C(1)–C(2)	1.497(8)	N(1)–H(1A)	0.8800
N(1)–C(12)	1.464(7)	C(2)–C(3)	1.566(7)
C(2)–C(10)	1.560(7)	C(2)–N(11)	1.460(8)
C(3)–H(3A)	0.9900	C(3)–H(3B)	0.9900
C(3)–C(4)	1.487(7)	C(4)–C(5)	1.390(7)
C(4)–C(9)	1.382(7)	O(5)–C(5)	1.371(7)
O(5)–C(5A)	1.434(7)	C(5)–C(6)	1.398(8)
C(5A)–H(5A)	0.9800	C(5A)–H(5B)	0.9800
C(5A)–H(5C)	0.9800	C(6)–H(6A)	0.9500
C(6)–C(7)	1.366(8)	C(7)–H(7A)	0.9500
C(7)–C(8)	1.393(8)	N(8)–C(8)	1.453(7)
N(8)–O(8B)	1.240(6)	N(8)–O(8A)	1.225(6)
C(8)–C(9)	1.395(7)	C(9)–C(10)	1.500(7)
C(10)–H(10A)	0.9900	C(10)–H(10B)	0.9900
N(11)–H(11A)	0.8800	N(11)–C(11)	1.341(7)
C(11)–O(11)	1.235(7)	C(11)–C(12)	1.524(8)
C(12)–H(12A)	1.0000	C(12)–C(13)	1.523(7)
C(13)–H(13A)	0.9900	C(13)–H(13B)	0.9900
C(13)–C(14)	1.509(8)	C(14)–C(15)	1.382(9)
C(14)–C(19)	1.393(10)	C(15)–H(15A)	0.9500
C(15)–C(16)	1.401(9)	C(16)–H(16A)	0.9500

C(16)–C(17)	1.399(12)	C(17)–H(17A)	0.9500
C(17)–C(18)	1.352(12)	C(18)–H(18A)	0.9500
C(18)–C(19)	1.396(10)	C(19)–H(19A)	0.9500

N(1)–C(1)–O(1)	120.8(5)	N(1)–C(1)–C(2)	120.0(5)
O(1)–C(1)–C(2)	119.1(5)	C(1)–N(1)–H(1A)	116.6
C(1)–N(1)–C(12)	126.8(5)	H(1A)–N(1)–C(12)	116.6
C(1)–C(2)–C(3)	108.9(5)	C(1)–C(2)–C(10)	110.5(5)
C(1)–C(2)–N(11)	111.7(4)	C(3)–C(2)–C(10)	105.3(4)
C(3)–C(2)–N(11)	110.6(5)	C(10)–C(2)–N(11)	109.8(5)
C(2)–C(3)–H(3A)	110.8	C(2)–C(3)–H(3B)	110.8
C(2)–C(3)–C(4)	104.9(4)	H(3A)–C(3)–H(3B)	108.8
H(3A)–C(3)–C(4)	110.8	H(3B)–C(3)–C(4)	110.8
C(3)–C(4)–C(5)	126.0(5)	C(3)–C(4)–C(9)	112.7(4)
C(5)–C(4)–C(9)	121.2(5)	C(5)–O(5)–C(5A)	117.4(5)
C(4)–C(5)–O(5)	114.5(5)	C(4)–C(5)–C(6)	119.6(5)
O(5)–C(5)–C(6)	125.9(5)	O(5)–C(5A)–H(5A)	109.5
O(5)–C(5A)–H(5B)	109.5	O(5)–C(5A)–H(5C)	109.5
H(5A)–C(5A)–H(5B)	109.5	H(5A)–C(5A)–H(5C)	109.5
H(5B)–C(5A)–H(5C)	109.5	C(5)–C(6)–H(6A)	120.3
C(5)–C(6)–C(7)	119.5(5)	H(6A)–C(6)–C(7)	120.3
C(6)–C(7)–H(7A)	119.5	C(6)–C(7)–C(8)	121.0(5)
H(7A)–C(7)–C(8)	119.5	C(8)–N(8)–O(8B)	118.9(6)
C(8)–N(8)–O(8A)	117.8(4)	O(8B)–N(8)–O(8A)	123.2(5)
C(7)–C(8)–N(8)	118.2(5)	C(7)–C(8)–C(9)	120.1(5)
N(8)–C(8)–C(9)	121.7(5)	C(4)–C(9)–C(8)	118.6(5)
C(4)–C(9)–C(10)	110.7(4)	C(8)–C(9)–C(10)	130.7(5)
C(2)–C(10)–C(9)	105.8(4)	C(2)–C(10)–H(10A)	110.6
C(2)–C(10)–H(10B)	110.6	C(9)–C(10)–H(10A)	110.6
C(9)–C(10)–H(10B)	110.6	H(10A)–C(10)–H(10B)	108.7
C(2)–N(11)–H(11A)	116.2	C(2)–N(11)–C(11)	127.5(5)
H(11A)–N(11)–C(11)	116.2	N(11)–C(11)–O(11)	122.8(5)
N(11)–C(11)–C(12)	118.1(5)	O(11)–C(11)–C(12)	119.1(5)
N(1)–C(12)–C(11)	112.5(4)	N(1)–C(12)–H(12A)	107.3
N(1)–C(12)–C(13)	110.7(5)	C(11)–C(12)–H(12A)	107.3
C(11)–C(12)–C(13)	111.6(5)	H(12A)–C(12)–C(13)	107.3
C(12)–C(13)–H(13A)	108.7	C(12)–C(13)–H(13B)	108.7
C(12)–C(13)–C(14)	114.3(4)	H(13A)–C(13)–H(13B)	107.6
H(13A)–C(13)–C(14)	108.7	H(13B)–C(13)–C(14)	108.7
C(13)–C(14)–C(15)	121.7(6)	C(13)–C(14)–C(19)	119.6(6)
C(15)–C(14)–C(19)	118.7(6)	C(14)–C(15)–H(15A)	119.5
C(14)–C(15)–C(16)	121.1(7)	H(15A)–C(15)–C(16)	119.5
C(15)–C(16)–H(16A)	120.8	C(15)–C(16)–C(17)	118.4(8)
H(16A)–C(16)–C(17)	120.8	C(16)–C(17)–H(17A)	119.4
C(16)–C(17)–C(18)	121.2(7)	H(17A)–C(17)–C(18)	119.4
C(17)–C(18)–H(18A)	120.0	C(17)–C(18)–C(19)	120.0(8)
H(18A)–C(18)–C(19)	120.0	C(14)–C(19)–C(18)	120.5(7)
C(14)–C(19)–H(19A)	119.7	C(18)–C(19)–H(19A)	119.7

Table 4. Anisotropic displacement parameters (Å^2) for(*R,S*)-**9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	0.023(3)	0.033(4)	0.020(3)	–0.002(3)	0.007(2)	–0.002(3)
N(1)	0.030(3)	0.017(3)	0.027(3)	–0.003(2)	0.009(2)	–0.002(2)
O(1)	0.045(3)	0.024(2)	0.030(2)	0.0005(19)	0.0136(19)	–0.002(2)
C(2)	0.032(3)	0.025(3)	0.019(3)	0.006(3)	0.007(2)	–0.003(3)
C(3)	0.029(3)	0.028(3)	0.032(3)	–0.006(3)	0.011(2)	–0.006(3)
C(4)	0.034(3)	0.024(3)	0.019(3)	–0.004(3)	0.007(2)	–0.001(3)
O(5)	0.029(2)	0.045(3)	0.049(3)	–0.006(3)	0.004(2)	–0.001(3)
C(5)	0.033(3)	0.028(3)	0.032(3)	–0.007(3)	0.005(3)	–0.001(3)
C(5A)	0.032(4)	0.061(5)	0.062(5)	–0.010(5)	–0.011(3)	0.004(4)
C(6)	0.053(4)	0.026(3)	0.028(3)	–0.005(3)	0.004(3)	–0.006(4)
C(7)	0.064(4)	0.023(3)	0.026(3)	0.002(3)	0.015(3)	0.007(4)
N(8)	0.062(4)	0.028(3)	0.040(3)	–0.002(3)	0.031(3)	–0.002(3)
C(8)	0.045(3)	0.023(3)	0.032(3)	0.001(3)	0.020(3)	0.006(3)
O(8B)	0.094(4)	0.049(3)	0.046(3)	0.000(3)	0.050(3)	0.001(3)
O(8A)	0.056(3)	0.047(3)	0.058(3)	–0.002(3)	0.037(3)	–0.004(3)
C(9)	0.036(3)	0.019(3)	0.023(3)	–0.005(3)	0.012(2)	–0.002(3)
C(10)	0.030(3)	0.029(3)	0.031(3)	–0.001(3)	0.017(2)	0.000(3)
N(11)	0.043(3)	0.022(3)	0.026(3)	0.000(2)	0.016(2)	0.000(2)
C(11)	0.024(3)	0.026(3)	0.028(3)	–0.003(3)	0.010(3)	–0.003(3)
O(11)	0.044(3)	0.024(2)	0.027(2)	0.0049(18)	0.0142(19)	
–0.0014(19)						
C(12)	0.029(3)	0.019(3)	0.027(3)	0.001(2)	0.013(2)	–0.001(2)
C(13)	0.035(3)	0.034(4)	0.018(3)	–0.002(2)	0.005(3)	0.003(3)
C(14)	0.031(3)	0.039(4)	0.022(3)	–0.005(3)	0.003(3)	0.007(3)
C(15)	0.034(4)	0.050(5)	0.043(4)	0.004(4)	0.011(3)	0.003(3)
C(16)	0.031(4)	0.069(6)	0.056(5)	–0.003(4)	0.008(3)	–0.012(4)
C(17)	0.031(4)	0.080(6)	0.059(5)	–0.026(5)	0.016(3)	0.005(5)
C(18)	0.031(4)	0.054(5)	0.075(5)	–0.018(4)	0.003(4)	0.002(4)
C(19)	0.032(4)	0.046(4)	0.049(4)	–0.004(4)	0.002(3)	0.005(3)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for (*R,S*)-**9**.

	x	y	z	U
H(1A)	0.8428	–0.1137	0.4717	0.030
H(3A)	1.0951	0.1334	0.7258	0.036
H(3B)	1.0824	0.3893	0.7279	0.036
H(5A)	1.4470	0.2446	0.9980	0.089
H(5B)	1.3858	0.1203	1.0729	0.089
H(5C)	1.3838	0.3757	1.0691	0.089
H(6A)	1.2285	0.2438	1.1267	0.047
H(7A)	1.0416	0.2403	1.1447	0.045
H(10A)	0.7990	0.3783	0.7480	0.034
H(10B)	0.7919	0.1217	0.7491	0.034
H(11A)	0.8601	0.5335	0.6209	0.035
H(12A)	0.9252	0.1882	0.4070	0.029
H(13A)	0.7482	0.2779	0.2652	0.036
H(13B)	0.7450	0.0272	0.2873	0.036
H(15A)	0.6078	–0.1058	0.3843	0.052
H(16A)	0.4246	–0.0557	0.4130	0.065
H(17A)	0.3262	0.2763	0.3677	0.068
H(18A)	0.4131	0.5548	0.3081	0.069
H(19A)	0.5969	0.5064	0.2825	0.055

Table 6. Torsion angles [°] for (*R,S*)-**9**.

O(1)–C(1)–N(1)–C(12)	–175.4(5)	C(2)–C(1)–N(1)–C(12)	3.0(8)
N(1)–C(1)–C(2)–C(3)	–109.5(6)	N(1)–C(1)–C(2)–C(10)	135.3(5)
N(1)–C(1)–C(2)–N(11)	12.8(7)	O(1)–C(1)–C(2)–C(3)	68.8(6)
O(1)–C(1)–C(2)–C(10)	–46.4(7)	O(1)–C(1)–C(2)–N(11)	–168.8(5)
C(1)–C(2)–C(3)–C(4)	–110.6(5)	C(10)–C(2)–C(3)–C(4)	7.9(7)
N(11)–C(2)–C(3)–C(4)	126.4(5)	C(2)–C(3)–C(4)–C(5)	176.5(6)
C(2)–C(3)–C(4)–C(9)	–6.2(8)	C(5A)–O(5)–C(5)–C(4)	178.2(7)
C(5A)–O(5)–C(5)–C(6)	–1.3(11)	C(3)–C(4)–C(5)–O(5)	–3.1(10)
C(3)–C(4)–C(5)–C(6)	176.3(7)	C(9)–C(4)–C(5)–O(5)	179.8(7)
C(9)–C(4)–C(5)–C(6)	–0.8(11)	C(4)–C(5)–C(6)–C(7)	1.0(11)
O(5)–C(5)–C(6)–C(7)	–179.6(7)	C(5)–C(6)–C(7)–C(8)	–0.7(12)
C(6)–C(7)–C(8)–N(8)	–179.6(7)	C(6)–C(7)–C(8)–C(9)	0.2(11)
O(8B)–N(8)–C(8)–C(7)	–2.2(10)	O(8B)–N(8)–C(8)–C(9)	178.0(6)
O(8A)–N(8)–C(8)–C(7)	178.4(6)	O(8A)–N(8)–C(8)–C(9)	–1.3(10)
C(3)–C(4)–C(9)–C(8)	–177.3(6)	C(3)–C(4)–C(9)–C(10)	1.8(8)
C(5)–C(4)–C(9)–C(8)	0.2(11)	C(5)–C(4)–C(9)–C(10)	179.2(6)
C(7)–C(8)–C(9)–C(4)	0.1(10)	C(7)–C(8)–C(9)–C(10)	–178.7(7)
N(8)–C(8)–C(9)–C(4)	179.8(6)	N(8)–C(8)–C(9)–C(10)	1.0(11)
C(4)–C(9)–C(10)–C(2)	3.5(7)	C(8)–C(9)–C(10)–C(2)	–177.6(7)
C(1)–C(2)–C(10)–C(9)	110.4(5)	C(3)–C(2)–C(10)–C(9)	–7.0(7)
N(11)–C(2)–C(10)–C(9)	–126.0(5)	C(1)–C(2)–N(11)–C(11)	–19.8(7)
C(3)–C(2)–N(11)–C(11)	101.6(6)	C(10)–C(2)–N(11)–C(11)	–142.7(6)

C(2)–N(11)–C(11)–O(11)	−170.5(5)	C(2)–N(11)–C(11)–C(12)	9.7(8)
C(1)–N(1)–C(12)–C(11)	−13.5(7)	C(1)–N(1)–C(12)–C(13)	−139.1(6)
N(11)–C(11)–C(12)–N(1)	7.2(7)	N(11)–C(11)–C(12)–C(13)	132.3(5)
O(11)–C(11)–C(12)–N(1)	−172.7(5)	O(11)–C(11)–C(12)–C(13)	−47.5(7)
N(1)–C(12)–C(13)–C(14)	68.9(6)	C(11)–C(12)–C(13)–C(14)	−57.2(6)
C(12)–C(13)–C(14)–C(15)	−82.0(7)	C(12)–C(13)–C(14)–C(19)	98.2(6)
C(13)–C(14)–C(15)–C(16)	178.1(5)	C(19)–C(14)–C(15)–C(16)	−2.0(9)
C(14)–C(15)–C(16)–C(17)	2.3(10)	C(15)–C(16)–C(17)–C(18)	−2.0(11)
C(16)–C(17)–C(18)–C(19)	1.4(12)	C(13)–C(14)–C(19)–C(18)	−178.7(6)
C(15)–C(14)–C(19)–C(18)	1.4(9)	C(17)–C(18)–C(19)–C(14)	−1.1(11)

Table 7. Hydrogen bonds for (*R,S*)-**9** [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
N(1)–H(1A)...O(11A)	0.88	2.04	2.911(6)	169
N(11)–H(11A)...O(1B)	0.88	2.11	2.932(7)	154

Symmetry operations for equivalent atoms
A x,y−1,z B x,y+1,z

Crystallographic data for (*S,S*)-9

Table 1. Crystal data and structure refinement for (*S,S*)-**9**.

Identification code	(*S,S*)-**9**	
Chemical formula (moiety)	$C_{20}H_{19}N_3O_5$	
Chemical formula (total)	$C_{20}H_{19}N_3O_5$	
Formula weight	381.38	
Temperature	170(2) K	
Radiation, wavelength	MoKα, 0.71073 Å	
Crystal system, space group	monoclinic, $P2_1$	
Unit cell parameters	a = 10.6551(10) Å	α = 90°
	b = 6.0480(6) Å	β = 91.171(2)°
	c = 13.9914(13) Å	γ = 90°
Cell volume	901.45(15) $Å^3$	
Z	2	
Calculated density	1.405 g/cm^3	
Absorption coefficient μ	0.103 mm^{-1}	
F(000)	400	
Crystal colour and size	colourless, 0.33 × 0.08 × 0.07 mm^3	
Reflections for cell refinement	1433 (θ range 2.4 to 19.8°)	
Data collection method	Bruker SMART 1000 CCD diffractometer thin-slice ω scans	
θ range for data collection	1.5 to 27.0°	
Index ranges	h −13 to 13, k −7 to 7, l −17 to 17	
Completeness to θ = 27.0°	100.0 %	
Reflections collected	10707	
Independent reflections	2173 (R_{int} = 0.0646)	
Reflections with $F^2>2\sigma$	1683	
Absorption correction	semi-empirical from equivalents	
Min. and max. transmission	0.9669 and 0.9928	
Structure solution	direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting parameters a, b	0.0545, 0.0577	
Data / restraints / parameters	2173 / 1 / 259	
Final R indices [$F^2>2\sigma$]	R1 = 0.0579, wR2 = 0.1039	
R indices (all data)	R1 = 0.0823, wR2 = 0.1118	
Goodness-of-fit on F^2	1.085	
Absolute structure parameter	0.5(19)	
Largest and mean shift/su	0.001 and 0.000	
Largest diff. peak and hole	0.25 and −0.22 e $Å^{-3}$	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for (*S,S*)-**9**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
O(1)	0.4602(2)	0.6478(4)	0.31464(16)	0.0311(6)
N(1)	0.4001(3)	0.0811(5)	0.3778(2)	0.0237(7)
O(11)	0.3226(2)	–0.0680(4)	0.51215(17)	0.0293(6)
O(5)	0.1727(2)	–0.0233(5)	0.10032(17)	0.0356(7)
N(11)	0.3857(3)	0.4988(5)	0.4491(2)	0.0240(7)
C(12)	0.3292(3)	0.3231(5)	0.5059(2)	0.0215(8)
C(8)	0.5561(3)	–0.1155(6)	0.1291(2)	0.0255(8)
C(9)	0.4952(3)	0.0510(6)	0.1804(2)	0.0237(8)
C(2)	0.4210(3)	0.2610(6)	0.3106(2)	0.0230(8)
C(11)	0.3495(3)	0.0958(5)	0.4638(2)	0.0207(8)
C(10)	0.5428(3)	0.2095(6)	0.2566(2)	0.0240(8)
C(1)	0.4242(3)	0.4841(6)	0.3600(2)	0.0235(8)
C(5A)	0.0975(4)	–0.1718(8)	0.0449(3)	0.0508(13)
C(13)	0.1906(3)	0.3716(6)	0.5219(2)	0.0259(8)
C(6)	0.3613(4)	–0.2298(6)	0.0572(2)	0.0303(9)
C(5)	0.2985(3)	–0.0615(6)	0.1062(2)	0.0270(8)
N(8)	0.6906(3)	–0.1479(6)	0.1391(2)	0.0362(8)
C(17)	–0.0256(4)	0.4455(8)	0.2607(3)	0.0429(11)
C(4)	0.3671(3)	0.0742(6)	0.1671(2)	0.0229(8)
C(16)	0.0441(4)	0.6202(8)	0.2966(3)	0.0417(11)
O(8B)	0.7533(3)	–0.0041(6)	0.1747(2)	0.0629(10)
C(3)	0.3180(3)	0.2557(6)	0.2309(2)	0.0249(8)
O(8A)	0.7361(3)	–0.3178(6)	0.1076(3)	0.0682(11)
C(7)	0.4880(4)	–0.2548(6)	0.0693(2)	0.0291(9)
C(14)	0.1140(3)	0.3962(6)	0.4302(2)	0.0277(9)
C(15)	0.1125(4)	0.5977(6)	0.3815(3)	0.0328(9)
C(19)	0.0460(3)	0.2219(7)	0.3922(3)	0.0320(9)
C(18)	–0.0230(4)	0.2466(8)	0.3080(3)	0.0392(10)

Table 3. Bond lengths [Å] and angles [°] for (*S,S*)-**9**.

O(1)–C(1)	1.241(4)	N(1)–H(1A)	0.85(4)
N(1)–C(2)	1.458(4)	N(1)–C(11)	1.332(4)
O(11)–C(11)	1.236(4)	O(5)–C(5A)	1.423(5)
O(5)–C(5)	1.361(4)	N(11)–H(11A)	0.92(4)
N(11)–C(12)	1.464(4)	N(11)–C(1)	1.324(4)
C(12)–H(12A)	1.0000	C(12)–C(11)	1.513(4)
C(12)–C(13)	1.526(5)	C(8)–C(9)	1.404(5)
C(8)–N(8)	1.451(5)	C(8)–C(7)	1.382(5)
C(9)–C(10)	1.514(5)	C(9)–C(4)	1.381(5)
C(2)–C(10)	1.547(5)	C(2)–C(1)	1.516(5)
C(2)–C(3)	1.549(5)	C(10)–H(10A)	0.9900
C(10)–H(10B)	0.9900	C(5A)–H(5AA)	0.9800
C(5A)–H(5AB)	0.9800	C(5A)–H(5AC)	0.9800
C(13)–H(13A)	0.9900	C(13)–H(13B)	0.9900

C(13)–C(14)	1.513(5)	C(6)–H(6A)	0.9500
C(6)–C(5)	1.405(5)	C(6)–C(7)	1.365(5)
C(5)–C(4)	1.381(5)	N(8)–O(8B)	1.198(4)
N(8)–O(8A)	1.222(4)	C(17)–H(17A)	0.9500
C(17)–C(16)	1.381(6)	C(17)–C(18)	1.373(6)
C(4)–C(3)	1.515(5)	C(16)–H(16A)	0.9500
C(16)–C(15)	1.388(5)	C(3)–H(3A)	0.9900
C(3)–H(3B)	0.9900	C(7)–H(7A)	0.9500
C(14)–C(15)	1.396(5)	C(14)–C(19)	1.380(5)
C(15)–H(15A)	0.9500	C(19)–H(19A)	0.9500
C(19)–C(18)	1.384(5)	C(18)–H(18A)	0.9500

H(1A)–N(1)–C(2)	111(3)	H(1A)–N(1)–C(11)	121(3)
C(2)–N(1)–C(11)	127.1(3)	C(5A)–O(5)–C(5)	118.0(3)
H(11A)–N(11)–C(12)	110(2)	H(11A)–N(11)–C(1)	122(2)
C(12)–N(11)–C(1)	127.0(3)	N(11)–C(12)–H(12A)	107.1
N(11)–C(12)–C(11)	112.6(3)	N(11)–C(12)–C(13)	110.5(3)
H(12A)–C(12)–C(11)	107.1	H(12A)–C(12)–C(13)	107.1
C(11)–C(12)–C(13)	112.2(3)	C(9)–C(8)–N(8)	120.9(3)
C(9)–C(8)–C(7)	120.3(3)	N(8)–C(8)–C(7)	118.8(3)
C(8)–C(9)–C(10)	131.5(3)	C(8)–C(9)–C(4)	118.0(3)
C(10)–C(9)–C(4)	110.3(3)	N(1)–C(2)–C(10)	107.8(3)
N(1)–C(2)–C(1)	111.9(3)	N(1)–C(2)–C(3)	109.5(3)
C(10)–C(2)–C(1)	113.0(3)	C(10)–C(2)–C(3)	103.5(3)
C(1)–C(2)–C(3)	110.9(3)	N(1)–C(11)–O(11)	122.9(3)
N(1)–C(11)–C(12)	118.4(3)	O(11)–C(11)–C(12)	118.6(3)
C(9)–C(10)–C(2)	101.4(3)	C(9)–C(10)–H(10A)	111.5
C(9)–C(10)–H(10B)	111.5	C(2)–C(10)–H(10A)	111.5
C(2)–C(10)–H(10B)	111.5	H(10A)–C(10)–H(10B)	109.3
O(1)–C(1)–N(11)	122.2(3)	O(1)–C(1)–C(2)	118.8(3)
N(11)–C(1)–C(2)	119.0(3)	O(5)–C(5A)–H(5AA)	109.5
O(5)–C(5A)–H(5AB)	109.5	O(5)–C(5A)–H(5AC)	109.5
H(5AA)–C(5A)–H(5AB)	109.5	H(5AA)–C(5A)–H(5AC)	109.5
H(5AB)–C(5A)–H(5AC)	109.5	C(12)–C(13)–H(13A)	108.8
C(12)–C(13)–H(13B)	108.8	C(12)–C(13)–C(14)	113.7(3)
H(13A)–C(13)–H(13B)	107.7	H(13A)–C(13)–C(14)	108.8
H(13B)–C(13)–C(14)	108.8	H(6A)–C(6)–C(5)	120.0
H(6A)–C(6)–C(7)	120.0	C(5)–C(6)–C(7)	120.0(3)
O(5)–C(5)–C(6)	124.9(3)	O(5)–C(5)–C(4)	116.4(3)
C(6)–C(5)–C(4)	118.7(3)	C(8)–N(8)–O(8B)	118.9(3)
C(8)–N(8)–O(8A)	118.5(3)	O(8B)–N(8)–O(8A)	122.6(4)
H(17A)–C(17)–C(16)	120.3	H(17A)–C(17)–C(18)	120.3
C(16)–C(17)–C(18)	119.3(4)	C(9)–C(4)–C(5)	122.1(3)
C(9)–C(4)–C(3)	110.3(3)	C(5)–C(4)–C(3)	127.6(3)
C(17)–C(16)–H(16A)	119.8	C(17)–C(16)–C(15)	120.4(4)
H(16A)–C(16)–C(15)	119.8	C(2)–C(3)–C(4)	101.0(3)
C(2)–C(3)–H(3A)	111.6	C(2)–C(3)–H(3B)	111.6
C(4)–C(3)–H(3A)	111.6	C(4)–C(3)–H(3B)	111.6
H(3A)–C(3)–H(3B)	109.4	C(8)–C(7)–C(6)	120.9(3)
C(8)–C(7)–H(7A)	119.6	C(6)–C(7)–H(7A)	119.6
C(13)–C(14)–C(15)	120.0(3)	C(13)–C(14)–C(19)	121.4(3)

C(15)–C(14)–C(19)	118.6(3)	C(16)–C(15)–C(14)	120.3(4)
C(16)–C(15)–H(15A)	119.9	C(14)–C(15)–H(15A)	119.9
C(14)–C(19)–H(19A)	119.6	C(14)–C(19)–C(18)	120.7(4)
H(19A)–C(19)–C(18)	119.6	C(17)–C(18)–C(19)	120.7(4)
C(17)–C(18)–H(18A)	119.7	C(19)–C(18)–H(18A)	119.7

Table 4. Anisotropic displacement parameters ($Å^2$) for (*S*,*S*)-**9**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	0.0529(17)	0.0104(13)	0.0302(13)	0.0022(11)	0.0068(12)	0.0001(12)
N(1)	0.0396(18)	0.0067(15)	0.0248(16)	–0.0017(12)	0.0010(13)	0.0011(14)
O(11)	0.0409(15)	0.0110(13)	0.0364(14)	0.0019(11)	0.0094(11)	
–0.0021(11)						
O(5)	0.0332(15)	0.0345(17)	0.0388(14)	–0.0020(14)	–0.0040(11)	
–0.0037(14)						
N(11)	0.0350(17)	0.0082(15)	0.0288(17)	–0.0051(13)	0.0032(13)	0.0000(14)
C(12)	0.030(2)	0.0090(18)	0.0260(18)	–0.0018(14)	–0.0007(15)	
–0.0033(14)						
C(8)	0.032(2)	0.0172(19)	0.0271(18)	0.0028(16)	0.0013(16)	0.0037(17)
C(9)	0.032(2)	0.0156(19)	0.0235(17)	0.0043(15)	0.0037(15)	
–0.0018(16)						
C(2)	0.038(2)	0.0087(17)	0.0224(17)	0.0014(14)	0.0018(15)	
–0.0001(16)						
C(11)	0.0233(19)	0.0113(18)	0.0274(18)	–0.0008(15)	–0.0034(15)	
–0.0001(15)						
C(10)	0.030(2)	0.0151(19)	0.0269(18)	–0.0004(15)	–0.0006(15)	0.0028(16)
C(1)	0.032(2)	0.0120(18)	0.0261(19)	–0.0012(16)	–0.0026(15)	0.0020(16)
C(5A)	0.044(3)	0.054(3)	0.055(3)	–0.007(3)	–0.015(2)	–0.008(2)
C(13)	0.038(2)	0.0149(18)	0.0250(17)	–0.0009(15)	0.0037(15)	0.0029(17)
C(6)	0.047(3)	0.019(2)	0.0252(18)	–0.0057(16)	–0.0002(16)	
–0.0064(19)						
C(5)	0.031(2)	0.026(2)	0.0237(18)	0.0038(17)	0.0015(15)	
–0.0044(17)						
N(8)	0.040(2)	0.035(2)	0.0336(18)	–0.0049(16)	0.0017(15)	0.0074(19)
C(17)	0.038(2)	0.054(3)	0.036(2)	0.000(2)	–0.0111(18)	0.006(2)
C(4)	0.038(2)	0.0124(18)	0.0180(16)	0.0027(14)	0.0028(14)	
–0.0010(16)						
C(16)	0.048(3)	0.033(3)	0.044(2)	0.008(2)	0.001(2)	0.014(2)
O(8B)	0.0370(18)	0.060(2)	0.091(2)	–0.032(2)	–0.0049(16)	0.0024(18)
C(3)	0.033(2)	0.0151(19)	0.0270(18)	–0.0002(16)	0.0025(15)	0.0021(16)
O(8A)	0.060(2)	0.058(3)	0.086(2)	–0.037(2)	–0.0108(18)	0.0354(19)
C(7)	0.046(2)	0.018(2)	0.0236(17)	–0.0008(17)	0.0052(16)	0.0042(19)
C(14)	0.0253(19)	0.024(2)	0.0340(19)	–0.0028(17)	0.0079(16)	0.0041(17)
C(15)	0.038(2)	0.018(2)	0.042(2)	–0.0007(18)	0.0023(17)	0.0037(18)
C(19)	0.029(2)	0.024(2)	0.043(2)	0.0014(19)	0.0095(17)	0.0008(18)
C(18)	0.030(2)	0.041(3)	0.046(2)	–0.005(2)	–0.0035(18)	–0.001(2)

Table 5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for (*S,S*)-**9**.

	x	y	z	U
H(1A)	0.411(3)	–0.044(7)	0.351(3)	0.028
H(11A)	0.373(3)	0.633(7)	0.478(2)	0.029
H(12A)	0.3722	0.3250	0.5701	0.026
H(10A)	0.5788	0.3447	0.2281	0.029
H(10B)	0.6066	0.1391	0.2991	0.029
H(5AA)	0.0094	–0.1252	0.0467	0.076
H(5AB)	0.1056	–0.3214	0.0711	0.076
H(5AC)	0.1255	–0.1709	–0.0214	0.076
H(13A)	0.1546	0.2502	0.5601	0.031
H(13B)	0.1836	0.5095	0.5595	0.031
H(6A)	0.3157	–0.3261	0.0156	0.036
H(17A)	–0.0749	0.4627	0.2038	0.051
H(16A)	0.0453	0.7567	0.2630	0.050
H(3A)	0.2349	0.2174	0.2567	0.030
H(3B)	0.3120	0.3987	0.1967	0.030
H(7A)	0.5299	–0.3694	0.0362	0.035
H(15A)	0.1586	0.7199	0.4066	0.039
H(19A)	0.0465	0.0833	0.4242	0.038
H(18A)	–0.0689	0.1246	0.2826	0.047

Table 6. Torsion angles [°] for (*S,S*)-**9**.

C(1)–N(11)–C(12)–C(11)	16.0(5)	C(1)–N(11)–C(12)–C(13)	−110.3(4)
N(8)–C(8)–C(9)–C(10)	−5.4(6)	N(8)–C(8)–C(9)–C(4)	179.5(3)
C(7)–C(8)–C(9)–C(10)	173.3(3)	C(7)–C(8)–C(9)–C(4)	−1.8(5)
C(11)–N(1)–C(2)–C(10)	146.0(3)	C(11)–N(1)–C(2)–C(1)	21.2(5)
C(11)–N(1)–C(2)–C(3)	−102.1(4)	C(2)–N(1)–C(11)–O(11)	171.9(3)
C(2)–N(1)–C(11)–C(12)	−10.7(5)	N(11)–C(12)–C(11)–N(1)	−8.0(4)
N(11)–C(12)–C(11)–O(11)	169.6(3)	C(13)–C(12)–C(11)–N(1)	117.4(3)
C(13)–C(12)–C(11)–O(11)	−65.1(4)	C(8)–C(9)–C(10)–C(2)	−154.8(3)
C(4)–C(9)–C(10)–C(2)	20.6(3)	N(1)–C(2)–C(10)–C(9)	81.8(3)
C(1)–C(2)–C(10)–C(9)	−154.1(3)	C(3)–C(2)–C(10)–C(9)	−34.1(3)
C(12)–N(11)–C(1)–O(1)	173.0(3)	C(12)–N(11)–C(1)–C(2)	−5.2(5)
N(1)–C(2)–C(1)–O(1)	169.1(3)	N(1)–C(2)–C(1)–N(11)	−12.6(4)
C(10)–C(2)–C(1)–O(1)	47.3(4)	C(10)–C(2)–C(1)–N(11)	−134.4(3)
C(3)–C(2)–C(1)–O(1)	−68.4(4)	C(3)–C(2)–C(1)–N(11)	109.9(3)
N(11)–C(12)–C(13)–C(14)	58.2(4)	C(11)–C(12)–C(13)–C(14)	−68.3(4)
C(5A)–O(5)–C(5)–C(6)	3.8(5)	C(5A)–O(5)–C(5)–C(4)	−174.6(3)
C(7)–C(6)–C(5)–O(5)	−179.2(3)	C(7)–C(6)–C(5)–C(4)	−0.8(5)
C(9)–C(8)–N(8)–O(8B)	−16.1(5)	C(9)–C(8)–N(8)–O(8A)	166.6(4)
C(7)–C(8)–N(8)–O(8B)	165.2(4)	C(7)–C(8)–N(8)–O(8A)	−12.1(5)
C(8)–C(9)–C(4)–C(5)	0.7(5)	C(8)–C(9)–C(4)–C(3)	177.9(3)
C(10)–C(9)–C(4)–C(5)	−175.5(3)	C(10)–C(9)–C(4)–C(3)	1.8(4)
O(5)–C(5)–C(4)–C(9)	179.2(3)	O(5)–C(5)–C(4)–C(3)	2.4(5)

C(6)–C(5)–C(4)–C(9)	0.6(5)	C(6)–C(5)–C(4)–C(3)	−176.1(3)
C(18)–C(17)–C(16)–C(15)	−2.4(6)	C(9)–C(4)–C(3)–C(2)	−23.4(4)
C(5)–C(4)–C(3)–C(2)	153.7(3)	N(1)–C(2)–C(3)–C(4)	−79.7(3)
C(10)–C(2)–C(3)–C(4)	35.0(3)	C(1)–C(2)–C(3)–C(4)	156.4(3)
C(5)–C(6)–C(7)–C(8)	−0.4(5)	C(9)–C(8)–C(7)–C(6)	1.7(5)
N(8)–C(8)–C(7)–C(6)	−179.6(3)	C(12)–C(13)–C(14)–C(15)	−82.5(4)
C(12)–C(13)–C(14)–C(19)	96.6(4)	C(17)–C(16)–C(15)–C(14)	1.6(6)
C(13)–C(14)–C(15)–C(16)	178.9(3)	C(19)–C(14)–C(15)–C(16)	−0.2(5)
C(13)–C(14)–C(19)–C(18)	−179.6(3)	C(15)–C(14)–C(19)–C(18)	−0.5(6)
C(16)–C(17)–C(18)–C(19)	1.7(6)	C(14)–C(19)–C(18)–C(17)	−0.3(6)

Table 7. Hydrogen bonds for (*S,S*)-**9** [Å and °].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)
N(1)–H(1A)...O(1A)	0.85(4)	2.01(4)	2.843(4)	168(3)
N(11)–H(11A)...O(11B)	0.92(4)	1.95(4)	2.850(4)	166(3)

Symmetry operations for equivalent atoms
A x,y−1,z B x,y+1,z