Table 1. Crystal data and structure refinement.

Identification code	**2014ncs0729 / MAB/CLJ/3.14R**	
Empirical formula	$C_5H_{17}B_5NO_{11.50}$	
Formula weight	329.24	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Triclinic	
Space group	*P*1	
Unit cell dimensions	a = 9.1164(5) Å	α = 75.798(5)°
	b = 9.1691(5) Å	β = 69.608(4)°
	c = 9.5532(7) Å	γ = 82.611(5)°
Volume	724.81(8) Å^3	
Z	2	
Density (calculated)	1.509 Mg / m^3	
Absorption coefficient	0.136 mm^{-1}	
F(000)	342	
Crystal	Prism; Colourless	
Crystal size	0.140 × 0.110 × 0.070 mm^3	
θ range for data collection	2.731 – 27.493°	
Index ranges	$-11 \le h \le 11$, $-11 \le k \le 11$, $-12 \le l \le 12$	
Reflections collected	11353	
Independent reflections	5960 [R_{int} = 0.0239]	
Completeness to θ = 25.242°	99.5 %	
Absorption correction	Semi–empirical from equivalents	
Max. and min. transmission	1.000 and 0.814	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5960 / 3 / 419	
Goodness-of-fit on F^2	1.027	
Final *R* indices [$F^2 > 2\sigma(F^2)$]	*R1* = 0.0349, *wR2* = 0.0950	
R indices (all data)	*R1* = 0.0360, *wR2* = 0.0960	
Absolute structure parameter	–0.3(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.438 and –0.238 e Å^{-3}	

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with VHF *Varimax* optics (70µm focus). **Cell determination and data collection**: *CrystalClear-SM Expert 3.1 b27* (Rigaku, 2013). **Data reduction, cell refinement and absorption correction**: *CrystalClear-SM Expert 3.1 b 27* (Rigaku, 2013). **Structure solution**: : *SHELXD-2013* (Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122). **Structure refinement**: *SHELXL-2013* (Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122). **Graphics:** *ORTEP3 for Windows* (L. J. Farrugia, J. Appl. Crystallogr. 1997, 30, 565

Special details:

It is not possible to accurately determine absolute structure of the crystal and thus the chirality of the prolinolium cations, but both are the same enantiomer.

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

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
B1	5962(3)	5672(3)	5448(3)	16(1)	1
B2	3765(3)	5995(3)	4397(3)	18(1)	1
B3	3819(3)	3870(3)	6387(3)	20(1)	1
B4	8815(3)	6074(3)	4559(3)	18(1)	1
B5	7097(3)	7413(3)	6387(3)	20(1)	1
O1	5170(2)	6420(2)	4326(2)	17(1)	1
O2	3059(2)	4750(2)	5429(2)	21(1)	1
O3	5214(2)	4280(2)	6377(2)	19(1)	1
O4	7601(2)	5325(2)	4601(2)	18(1)	1
O5	8584(2)	7155(2)	5397(2)	22(1)	1
O6	5862(2)	6688(2)	6457(2)	18(1)	1
O7	2970(2)	6815(2)	3463(2)	21(1)	1
O8	3115(2)	2607(2)	7311(2)	27(1)	1
O9	10280(2)	5697(2)	3681(2)	23(1)	1
O10	6962(2)	8413(2)	7269(2)	28(1)	1
B11	3901(3)	9722(3)	201(3)	17(1)	1
B12	6041(3)	9480(3)	1332(3)	19(1)	1
B13	5986(3)	11575(3)	–706(3)	18(1)	1
B14	1033(3)	9413(3)	1030(3)	17(1)	1
B15	2752(3)	7925(3)	–660(3)	19(1)	1
O11	4692(2)	9008(2)	1331(2)	18(1)	1
O12	6696(2)	10777(2)	344(2)	21(1)	1
O13	4679(2)	11088(2)	–780(2)	18(1)	1
O14	2279(2)	10086(2)	1033(2)	18(1)	1
O15	1257(2)	8288(2)	227(2)	21(1)	1
O16	4004(2)	8660(2)	–761(2)	18(1)	1
O17	6804(2)	8711(2)	2301(2)	24(1)	1
O18	6681(2)	12847(2)	–1619(2)	23(1)	1
O19	–412(2)	9883(2)	1844(2)	21(1)	1
O20	2923(2)	6795(2)	–1412(2)	24(1)	1
C21	9671(3)	3238(3)	–412(3)	26(1)	1
C22	9604(3)	4810(3)	–1386(3)	34(1)	1
C23	8837(4)	5784(3)	–226(4)	36(1)	1
C24	7575(3)	4823(3)	1020(3)	26(1)	1
C25	6026(3)	5084(3)	745(3)	27(1)	1
N21	8190(2)	3203(2)	952(2)	22(1)	1
O21	5026(2)	3963(3)	1799(3)	45(1)	1
C31	2739(4)	1418(3)	4291(4)	37(1)	1
C32	2556(4)	–62(3)	5458(3)	36(1)	1
C33	768(4)	–239(4)	6116(3)	36(1)	1
C34	155(3)	570(3)	4797(3)	30(1)	1
C35	–1156(4)	1729(3)	5244(3)	34(1)	1
N31	1531(3)	1359(2)	3582(3)	29(1)	1
O31	–1469(2)	2595(2)	3900(2)	29(1)	1
O41	2112(2)	4351(2)	1336(2)	29(1)	1

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

B1–O3	1.459(3)	C21–N21	1.512(3)
B1–O4	1.466(3)	C21–C22	1.519(4)
B1–O6	1.470(3)	C21–H21C	0.9900
B1–O1	1.480(3)	C21–H21D	0.9900
B2–O1	1.361(3)	C22–C23	1.516(4)
B2–O7	1.366(3)	C22–H22A	0.9900
B2–O2	1.373(3)	C22–H22B	0.9900
B3–O8	1.352(3)	C23–C24	1.519(4)
B3–O3	1.368(3)	C23–H23A	0.9900
B3–O2	1.380(3)	C23–H23B	0.9900
B4–O9	1.360(3)	C24–C25	1.504(3)
B4–O4	1.360(3)	C24–N21	1.527(3)
B4–O5	1.374(3)	C24–H24	1.0000
B5–O6	1.354(3)	C25–O21	1.412(3)
B5–O10	1.358(3)	C25–H25A	0.9900
B5–O5	1.386(3)	C25–H25B	0.9900
O7–H7	0.8400	N21–H21A	0.9900
O8–H8	0.8400	N21–H21B	0.9900
O9–H9	0.8400	O21–H21	0.8400
O10–H10	0.8400	C31–N31	1.492(3)
B11–O14	1.453(3)	C31–C32	1.516(4)
B11–O13	1.462(3)	C31–H31A	0.9900
B11–O16	1.469(3)	C31–H31B	0.9900
B11–O11	1.480(3)	C32–C33	1.544(5)
B12–O11	1.355(3)	C32–H32A	0.9900
B12–O17	1.357(3)	C32–H32B	0.9900
B12–O12	1.379(3)	C33–C34	1.542(4)
B13–O18	1.352(3)	C33–H33A	0.9900
B13–O13	1.355(3)	C33–H33B	0.9900
B13–O12	1.389(3)	C34–N31	1.500(4)
B14–O19	1.353(3)	C34–C35	1.510(4)
B14–O14	1.362(3)	C34–H34	1.0000
B14–O15	1.386(3)	C35–O31	1.434(3)
B15–O16	1.362(3)	C35–H35A	0.9900
B15–O20	1.364(3)	C35–H35B	0.9900
B15–O15	1.380(3)	N31–H31C	0.9900
O17–H17	0.8400	N31–H31D	0.9900
O18–H18	0.8400	O31–H31	0.8400
O19–H19	0.8400	O41–H41A	0.8703
O20–H20	0.8400	O41–H41B	0.8700
O3–B1–O4	109.36(18)	B2–O1–B1	122.56(19)
O3–B1–O6	108.86(18)	B2–O2–B3	119.2(2)
O4–B1–O6	110.72(18)	B3–O3–B1	124.02(18)
O3–B1–O1	110.57(18)	B4–O4–B1	123.07(18)
O4–B1–O1	108.14(18)	B4–O5–B5	119.1(2)
O6–B1–O1	109.18(18)	B5–O6–B1	123.59(19)
O1–B2–O7	121.3(2)	B2–O7–H7	109.5
O1–B2–O2	121.9(2)	B3–O8–H8	109.5
O7–B2–O2	116.8(2)	B4–O9–H9	109.5
O8–B3–O3	122.8(2)	B5–O10–H10	109.5
O8–B3–O2	116.6(2)	O14–B11–O13	110.27(19)
O3–B3–O2	120.6(2)	O14–B11–O16	111.13(19)
O9–B4–O4	117.8(2)	O13–B11–O16	108.53(18)
O9–B4–O5	120.7(2)	O14–B11–O11	108.08(18)
O4–B4–O5	121.5(2)	O13–B11–O11	110.29(18)
O6–B5–O10	122.7(2)	O16–B11–O11	108.53(18)
O6–B5–O5	120.8(2)	O11–B12–O17	122.0(2)
O10–B5–O5	116.5(2)	O11–B12–O12	121.1(2)

O17–B12–O12	116.9(2)	C24–C25–H25B	110.2
O18–B13–O13	123.4(2)	H25A–C25–H25B	108.5
O18–B13–O12	115.7(2)	C21–N21–C24	108.37(19)
O13–B13–O12	121.0(2)	C21–N21–H21A	110.0
O19–B14–O14	117.3(2)	C24–N21–H21A	110.0
O19–B14–O15	122.0(2)	C21–N21–H21B	110.0
O14–B14–O15	120.6(2)	C24–N21–H21B	110.0
O16–B15–O20	121.6(2)	H21A–N21–H21B	108.4
O16–B15–O15	121.0(2)	C25–O21–H21	109.5
O20–B15–O15	117.4(2)	N31–C31–C32	102.3(2)
B12–O11–B11	123.89(18)	N31–C31–H31A	111.3
B12–O12–B13	119.1(2)	C32–C31–H31A	111.3
B13–O13–B11	124.37(18)	N31–C31–H31B	111.3
B14–O14–B11	124.00(18)	C32–C31–H31B	111.3
B15–O15–B14	119.3(2)	H31A–C31–H31B	109.2
B15–O16–B11	123.12(19)	C31–C32–C33	103.8(2)
B12–O17–H17	109.5	C31–C32–H32A	111.0
B13–O18–H18	109.5	C33–C32–H32A	111.0
B14–O19–H19	109.5	C31–C32–H32B	111.0
B15–O20–H20	109.5	C33–C32–H32B	111.0
N21–C21–C22	103.81(19)	H32A–C32–H32B	109.0
N21–C21–H21C	111.0	C34–C33–C32	104.9(2)
C22–C21–H21C	111.0	C34–C33–H33A	110.8
N21–C21–H21D	111.0	C32–C33–H33A	110.8
C22–C21–H21D	111.0	C34–C33–H33B	110.8
H21C–C21–H21D	109.0	C32–C33–H33B	110.8
C23–C22–C21	103.9(2)	H33A–C33–H33B	108.8
C23–C22–H22A	111.0	N31–C34–C35	108.6(2)
C21–C22–H22A	111.0	N31–C34–C33	105.2(2)
C23–C22–H22B	111.0	C35–C34–C33	113.2(2)
C21–C22–H22B	111.0	N31–C34–H34	109.9
H22A–C22–H22B	109.0	C35–C34–H34	109.9
C22–C23–C24	104.3(2)	C33–C34–H34	109.9
C22–C23–H23A	110.9	O31–C35–C34	109.3(2)
C24–C23–H23A	110.9	O31–C35–H35A	109.8
C22–C23–H23B	110.9	C34–C35–H35A	109.8
C24–C23–H23B	110.9	O31–C35–H35B	109.8
H23A–C23–H23B	108.9	C34–C35–H35B	109.8
C25–C24–C23	112.5(2)	H35A–C35–H35B	108.3
C25–C24–N21	109.6(2)	C31–N31–C34	108.3(2)
C23–C24–N21	104.5(2)	C31–N31–H31C	110.0
C25–C24–H24	110.0	C34–N31–H31C	110.0
C23–C24–H24	110.0	C31–N31–H31D	110.0
N21–C24–H24	110.0	C34–N31–H31D	110.0
O21–C25–C24	107.8(2)	H31C–N31–H31D	108.4
O21–C25–H25A	110.2	C35–O31–H31	109.5
C24–C25–H25A	110.2	H41A–O41–H41B	109.5
O21–C25–H25B	110.2		

Symmetry transformations used to generate equivalent atoms:

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

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B1	13(1)	18(1)	17(1)	−4(1)	−6(1)	−1(1)
B2	15(1)	20(1)	17(1)	−2(1)	−5(1)	−2(1)
B3	14(1)	22(1)	22(1)	−1(1)	−6(1)	−3(1)
B4	17(1)	21(1)	17(1)	−3(1)	−6(1)	−2(1)
B5	18(1)	24(1)	19(1)	−7(1)	−7(1)	−2(1)
O1	16(1)	19(1)	18(1)	−1(1)	−7(1)	−4(1)
O2	17(1)	21(1)	23(1)	3(1)	−9(1)	−6(1)
O3	17(1)	20(1)	19(1)	0(1)	−8(1)	−4(1)
O4	14(1)	20(1)	20(1)	−6(1)	−6(1)	−2(1)
O5	15(1)	27(1)	26(1)	−11(1)	−4(1)	−5(1)
O6	14(1)	22(1)	19(1)	−6(1)	−4(1)	−1(1)
O7	16(1)	22(1)	23(1)	3(1)	−9(1)	−5(1)
O8	23(1)	26(1)	32(1)	10(1)	−15(1)	−10(1)
O9	14(1)	30(1)	27(1)	−11(1)	−6(1)	−3(1)
O10	18(1)	35(1)	33(1)	−19(1)	−3(1)	−5(1)
B11	15(1)	17(1)	18(1)	−2(1)	−7(1)	−3(1)
B12	16(1)	20(1)	19(1)	−2(1)	−6(1)	−4(1)
B13	20(1)	18(1)	17(1)	−3(1)	−8(1)	−2(1)
B14	14(1)	19(1)	19(1)	−3(1)	−7(1)	−2(1)
B15	19(1)	20(1)	19(1)	−3(1)	−7(1)	−3(1)
O11	16(1)	19(1)	20(1)	1(1)	−9(1)	−5(1)
O12	18(1)	22(1)	23(1)	2(1)	−11(1)	−7(1)
O13	17(1)	18(1)	19(1)	0(1)	−8(1)	−4(1)
O14	16(1)	21(1)	21(1)	−6(1)	−7(1)	−2(1)
O15	16(1)	24(1)	24(1)	−10(1)	−4(1)	−4(1)
O16	15(1)	20(1)	20(1)	−6(1)	−5(1)	−3(1)
O17	19(1)	25(1)	27(1)	7(1)	−13(1)	−9(1)
O18	23(1)	23(1)	25(1)	2(1)	−13(1)	−8(1)
O19	14(1)	24(1)	25(1)	−8(1)	−5(1)	−3(1)
O20	20(1)	27(1)	28(1)	−13(1)	−3(1)	−5(1)
C21	20(1)	26(1)	30(1)	−7(1)	−6(1)	−1(1)
C22	22(1)	29(1)	39(1)	2(1)	−2(1)	−3(1)
C23	29(2)	24(1)	60(2)	−11(1)	−20(1)	−3(1)
C24	31(1)	23(1)	29(1)	−12(1)	−14(1)	7(1)
C25	19(1)	31(1)	26(1)	−3(1)	−4(1)	1(1)
N21	19(1)	24(1)	24(1)	−9(1)	−7(1)	0(1)
O21	21(1)	45(1)	47(1)	16(1)	−1(1)	−1(1)
C31	44(2)	33(2)	40(2)	−4(1)	−23(1)	−8(1)
C32	43(2)	32(1)	41(2)	−8(1)	−22(1)	−1(1)
C33	42(2)	35(2)	34(2)	−1(1)	−19(1)	−3(1)
C34	34(1)	28(1)	29(1)	−6(1)	−11(1)	−3(1)
C35	40(2)	33(1)	27(1)	−7(1)	−9(1)	1(1)
N31	32(1)	27(1)	31(1)	−12(1)	−13(1)	1(1)
O31	35(1)	24(1)	29(1)	−8(1)	−12(1)	5(1)
O41	28(1)	26(1)	32(1)	−9(1)	−6(1)	1(1)

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

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
H7	3498	7545	2874	31	1
H8	3694	2119	7800	41	1
H9	10939	6173	3803	34	1
H10	6043	8433	7882	41	1
H17	6228	8053	2967	36	1
H18	6192	13247	–2228	35	1
H19	–1071	9277	1931	31	1
H20	3847	6751	–2012	37	1
H21C	9684	2461	–976	31	1
H21D	10612	3072	–91	31	1
H22A	10668	5139	–2032	40	1
H22B	8969	4848	–2052	40	1
H23A	8373	6732	–692	43	1
H23B	9607	6031	189	43	1
H24	7452	5019	2040	31	1
H25A	5566	6096	892	32	1
H25B	6169	5021	–315	32	1
H21A	8415	2700	1903	26	1
H21B	7395	2633	849	26	1
H21	4157	4076	1656	68	1
H31A	2525	2286	4789	44	1
H31B	3804	1477	3524	44	1
H32A	2982	–22	6269	44	1
H32B	3097	–906	4966	44	1
H33A	522	–1316	6435	43	1
H33B	294	234	7010	43	1
H34	–198	–185	4398	36	1
H35A	–2111	1221	5969	41	1
H35B	–853	2402	5755	41	1
H31C	1969	806	2745	34	1
H31D	1201	2392	3149	34	1
H31	–1779	3474	4018	43	1
H41A	1384	4845	1933	44	1
H41B	2376	4882	403	44	1

Table 6. Torsion angles [°].

O7–B2–O1–B1	172.0(2)
O2–B2–O1–B1	–6.4(3)
O3–B1–O1–B2	12.1(3)
O4–B1–O1–B2	131.8(2)
O6–B1–O1–B2	–107.7(2)
O1–B2–O2–B3	–2.4(3)
O7–B2–O2–B3	179.1(2)
O8–B3–O2–B2	–176.0(2)
O3–B3–O2–B2	4.0(3)
O8–B3–O3–B1	–176.8(2)
O2–B3–O3–B1	3.2(3)
O4–B1–O3–B3	–129.5(2)
O6–B1–O3–B3	109.4(2)
O1–B1–O3–B3	–10.6(3)
O9–B4–O4–B1	–177.1(2)
O5–B4–O4–B1	4.1(3)
O3–B1–O4–B4	–131.3(2)
O6–B1–O4–B4	–11.4(3)
O1–B1–O4–B4	108.2(2)
O9–B4–O5–B5	–174.2(2)
O4–B4–O5–B5	4.6(3)
O6–B5–O5–B4	–4.5(3)
O10–B5–O5–B4	175.2(2)
O10–B5–O6–B1	176.1(2)
O5–B5–O6–B1	–4.2(3)
O3–B1–O6–B5	131.7(2)
O4–B1–O6–B5	11.5(3)
O1–B1–O6–B5	–107.5(2)
O17–B12–O11–B11	–173.8(2)
O12–B12–O11–B11	6.4(3)
O14–B11–O11–B12	–127.1(2)
O13–B11–O11–B12	–6.5(3)
O16–B11–O11–B12	112.3(2)
O11–B12–O12–B13	–2.4(3)
O17–B12–O12–B13	177.8(2)
O18–B13–O12–B12	178.9(2)
O13–B13–O12–B12	–0.8(3)
O18–B13–O13–B11	–179.6(2)
O12–B13–O13–B11	0.1(3)
O14–B11–O13–B13	122.5(2)
O16–B11–O13–B13	–115.6(2)
O11–B11–O13–B13	3.2(3)
O19–B14–O14–B11	–179.2(2)
O15–B14–O14–B11	1.2(3)
O13–B11–O14–B14	126.4(2)
O16–B11–O14–B14	6.0(3)
O11–B11–O14–B14	–113.0(2)
O16–B15–O15–B14	–0.3(3)
O20–B15–O15–B14	179.0(2)
O19–B14–O15–B15	175.9(2)
O14–B14–O15–B15	–4.5(3)
O20–B15–O16–B11	–170.8(2)
O15–B15–O16–B11	8.5(3)
O14–B11–O16–B15	–10.8(3)
O13–B11–O16–B15	–132.2(2)
O11–B11–O16–B15	107.9(2)
N21–C21–C22–C23	34.7(3)
C21–C22–C23–C24	–39.3(3)
C22–C23–C24–C25	–91.0(3)

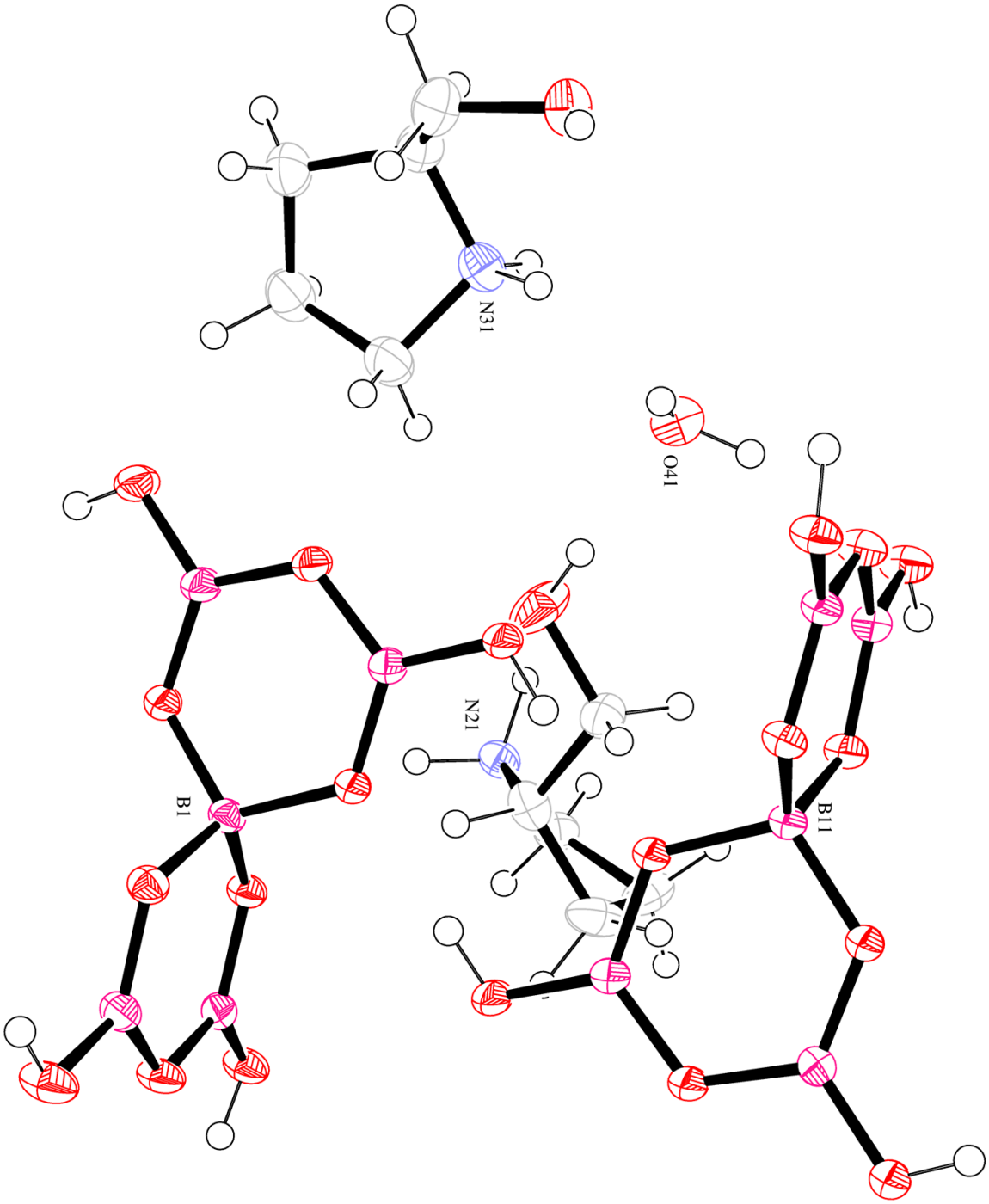
C22–C23–C24–N21	27.8(3)
C23–C24–C25–O21	169.8(2)
N21–C24–C25–O21	54.0(3)
C22–C21–N21–C24	−17.5(2)
C25–C24–N21–C21	114.4(2)
C23–C24–N21–C21	−6.3(2)
N31–C31–C32–C33	−39.3(3)
C31–C32–C33–C34	29.9(3)
C32–C33–C34–N31	−8.8(3)
C32–C33–C34–C35	−127.2(3)
N31–C34–C35–O31	53.9(3)
C33–C34–C35–O31	170.3(2)
C32–C31–N31–C34	34.9(3)
C35–C34–N31–C31	105.4(2)
C33–C34–N31–C31	−16.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds [Å and °].

D–H···*A*	*d*(*D*–H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*D*H*A*)
O7–H7···O11	0.84	1.86	2.688(2)	171.1
O8–H8···O13^{i}	0.84	1.88	2.712(2)	169.2
O9–H9···O7^{ii}	0.84	1.91	2.701(2)	156.4
O10–H10···O16^{iii}	0.84	1.88	2.717(2)	175.0
O17–H17···O1	0.84	1.84	2.680(2)	172.2
O18–H18···O3^{iv}	0.84	1.86	2.698(2)	175.0
O19–H19···O17^{v}	0.84	1.96	2.736(2)	153.4
O20–H20···O6^{vi}	0.84	1.91	2.750(2)	174.1
N21–H21A···O31^{ii}	0.99	1.93	2.853(3)	154.7
N21–H21B···O12^{vii}	0.99	2.11	3.018(3)	152.3
O21–H21···O41	0.84	1.97	2.807(3)	179.5
N31–H31C···O14^{vii}	0.99	1.83	2.791(3)	162.7
N31–H31D···O41	0.99	2.18	3.018(3)	140.8
O31–H31···O4^{v}	0.84	1.87	2.704(2)	170.0
O41–H41A···O9^{v}	0.87	1.92	2.748(2)	159.0
O41–H41B···O20	0.87	2.11	2.940(3)	158.8

Symmetry transformations used to generate equivalent atoms:
(i) x,y−1,z+1 (ii) x+1,y,z (iii) x,y,z+1 (iv) x,y+1,z−1
(v) x−1,y,z (vi) x,y,z−1 (vii) x,y−1,z


N31
O41
N21
B1
B11