Atom Type	Occurrences	Potential Contacts	Ratio
C5'_U	22	79	3.591
C2'_G	46	106	2.304
C5_U	22	50	2.273
OP2_G	47	96	2.043
O2'_G	46	90	1.957
OP1_G	47	92	1.957
C4'_G	47	91	1.936
C5'_G	47	87	1.851
C1'_G	47	86	1.830
C3'_U	22	39	1.773
O2'_U	22	36	1.636
C5_G	48	78	1.625
O4_U	22	33	1.500
C4'_U	22	28	1.273
C6_U	22	28	1.273
N2_G	48	60	1.250
O3'_U	22	24	1.091
O5'_U	21	20	0.952
O3'_G	45	40	0.889
O4'_G	47	39	0.830
OP1_U	9	7	0.778
C2'_U	22	16	0.727
N3_G	48	31	0.646
O2_U	22	14	0.636
C3'_G	46	29	0.630
C1'_U	22	13	0.591
OP2_U	9	5	0.556
C4_U	22	11	0.500
N3_U	22	11	0.500
O5'_G	47	16	0.340
N1_U	22	7	0.318
C8_G	48	15	0.312
P_G	47	10	0.213
O4'_U	22	3	0.136
C2_G	48	5	0.104
C2_U	22	2	0.091
C6_G	48	2	0.042
C4_G	48	2	0.042
N7_G	48	1	0.021
N1_G	48	1	0.021

Table 4: *Hydration index by atom type: for each atom type in structures P1A, P1B and P2C the number of occurrences of atoms of that type, the number of potential water contacts that have an atom of that type as target and the ratio of contacts to occurrences is shown. Potential contacts to modeled hydrogen atoms are credited to the atom to which the hydrogen is attached. Atoms with alternate conformations are excluded from the list of potential targets.*

Group/Atom	Occurrence:Contacts	O		Ca		Sr	
backbone	372:412(1.11)	375	3.07(0.34)	32	2.76(0.54)	5	2.78(0.43)
C5'	69 :43(0.62)	43	3.44(0.10)	-	-	-	-
O3'	67 :79(1.18)	67	3.28(0.24)	9	2.66(0.48)	3	2.85(0.59)
O5'	68 :36(0.53)	36	2.95(0.33)	-	-	-	-
OP1	56 :120(2.14)	109	2.88(0.26)	9	2.46(0.16)	2	2.66(0.04)
OP2	56 :111(1.98)	105	2.97(0.33)	6	2.32(0.07)	-	-
P	56 :23(0.41)	15	3.48(0.09)	8	3.54(0.07)	-	-
base	608:168(0.28)	163	3.21(0.30)	3	2.80(0.63)	2	2.50(0.00)
C2_G	48 :5(0.10)	5	3.55(0.03)	-	-	-	-
C2_U	22 :2(0.09)	2	3.35(0.13)	-	-	-	-
C4_G	48 :2(0.04)	2	3.52(0.09)	-	-	-	-
C4_U	22 :13(0.59)	12	3.44(0.21)	1	3.52(-)	-	-
C5_G	48 :1(0.02)	1	3.39(-)	-	-	-	-
C5_U	22 :15(0.68)	15	3.45(0.12)	-	-	-	-
C6_G	48 :2(0.04)	2	3.46(0.05)	-	-	-	-
C6_U	22 :11(0.50)	11	3.35(0.15)	-	-	-	-
C8_G	48 :2(0.04)	2	3.51(0.00)	-	-	-	-
N1_G	48 :1(0.02)	1	3.46(-)	-	-	-	-
N1_U	22 :7(0.32)	7	3.51(0.07)	-	-	-	-
N2_G	48 :20(0.42)	20	3.29(0.20)	-	-	-	-
N3_G	48 :31(0.65)	31	3.08(0.26)	-	-	-	-
N3_U	22 :2(0.09)	2	3.40(0.25)	-	-	-	-
N7_G	48 :1(0.02)	1	3.51(-)	-	-	-	-
O2_U	22 :14(0.64)	14	3.01(0.24)	-	-	-	-
O4_U	22 :39(1.77)	35	2.95(0.26)	2	2.44(0.06)	2	2.50(0.00)
furanose	411:304(0.74)	287	3.17(0.30)	14	3.21(0.38)	3	3.03(0.47)
C1'	69 :38(0.55)	38	3.36(0.09)	-	-	-	-
C2'	68 :57(0.84)	52	3.31(0.13)	5	3.59(0.01)	-	-
C3'	68 :15(0.22)	11	3.43(0.15)	3	3.33(0.23)	1	3.58(-)
C4'	69 :18(0.26)	18	3.49(0.08)	-	-	-	-
O2'	68 :134(1.97)	126	2.98(0.30)	6	2.85(0.24)	2	2.76(0.04)
O4'	69 :42(0.61)	42	3.23(0.24)	-	-	-	-
solvent	221:529(2.39)	473	2.94(0.35)	35	2.52(0.25)	21	2.59(0.10)
CA	3 :7(2.33)	7	2.50(0.19)	-	-	-	-
O	201:502(2.50)	446	2.97(0.35)	35	2.52(0.25)	21	2.59(0.10)
SR	17 :20(1.18)	20	2.62(0.22)	-	-	-	-

Table 5: *Solvent contact distances: the distribution of solvent contacts across all structures examined. Each non-bonding contact links a solvent ion/water, with full or partial occupancy, and a target atom. Target atoms are grouped into four classes, only those with full occupancy are considered. The number of occurrences of atoms of that type, the number of contacts to such atoms, and the average number of contacts per atom across all structures are shown in the first column. The three columns on the right show the number of contacts and the average and standard deviation of the contact distance for HOH, Ca, and Sr respectively.*

	α	β	γ	δ	ϵ	ζ	χ
U1			52.8(1.3)	79.2(1.2)	-155.7(3.5)	-89.5(1.7)	-145.2(2.6)
G2	-97.0(1.5)	63.8(3.0)	175.7(1.8)	82.9(1.7)	-153.1(2.4)	-71.7(2.3)	-167.2(1.8)
G3	-69.0(2.2)	-171.3(3.0)	59.5(1.2)	149.7(1.4)	-170.0(1.8)	-117.6(1.4)	-120.8(1.8)
G4	-77.0(1.6)	176.3(1.3)	45.6(1.2)	76.0(0.7)	-151.8(3.5)	-74.2(3.7)	-154.6(1.4)
G5-A	-67.1(3.5)	138.2(105.6)	50.5(1.4)	80.4(3.7)	-158.3(2.9)	59.5(5.5)	-148.7(1.9)
G5-B	-71.4	175.8	50.4	75.9	-152.5	-78.7	-148.8
G5-C	-69.2	174.4	49.0	75.8	-163.5	43.0	-148.9
U6-A	154.8(16.6)	151.8(7.3)	54.7(14.2)	141.8(2.5)			-135.2(4.2)
U6-B	-62.1	171.6	64.1	122.5			-130.8
U6-C	73.0	176.0	52.2	90.6			-159.4

Table 6: *Torsion angles. Torsion angles averaged over twelve chains from structures P1A, P1B and P2C [47]. For residues G5 and U6, angles are computed separately for conformations 3'U-A (ten chains), 3'U-B and 3'U-C (one chain each).*