Supplementary Material: Force Field of the RPSB

Atom Name	AMBER Atom Type	Charge
C1	CT	0.1249
C2	CT	-0.0625
C3	CT	-0.0625
C4	CT	-0.0625
C5	CD	0.0741
C6	CD	-0.1068
C7	CD	-0.0385
C8	CD	-0.1912
C9	CD	0.0897
C10	CD	-0.2323
C11	CD	0.0031
C12	CD	-0.3557
C13	CD	0.2952
C14	CD	-0.4220
C15	CD	0.0876
C16	CT	-0.2036
C17	CT	-0.2036
C18	CT	-0.1681
C19	CT	-0.0556
C20	CT	0.0210
N	N2	-0.3093
HN	H	0.3534
H021	HC	0.0407
H022	HC	0.0407
H031	HC	0.0407
H032	HC	0.0407
H041	HC	0.0407
H042	HC	0.0407
H071	H4	0.1400
H081	H4	0.0968
H101	H4	0.1786
H111	H4	0.1687
H121	H4	0.1576
H141	H4	0.1901
H151	H4	0.2305
H161	HC	0.0567
H162	HC	0.0567
H163	HC	0.0567
H171	HC	0.0567
H172	HC	0.0567
H173	HC	0.0567
H181	HC	0.0574
H182	HC	0.0574
H183	HC	0.0574
H191	HC	0.0502
H192	HC	0.0502
H193	HC	0.0502
H201	HC	0.0306
H202	HC	0.0306
H203	HC	0.0306

Table 1: Force field for the RPSB. The first two digits of the hydrogen names indicate the number of the carbon atoms they are bonded to (except for the Schiff base proton HN).

Supplementary Material: Inter-helical Hydrogen Bonds

Donor	Acceptor	1HZX	RHO_1 0.6-2.1 ns	RHO_2 2.5-4.0 ns	RHO_3 5.0-6.5 ns	RHOiso_1 0.6-2.1 ns	RHOiso_2 2.5-4.0 ns	RHOiso_3 5.0-6.5 ns
43	**293**	0.0	65.3	99.9	99.9	0.3	24.8	13.0
43	**297**	0.0	0.0	0.0	0.0	84.1	77.7	96.5
55	**83**	100.0	1.5	1.0	0.8	1.0	1.1	0.4
55	**299**	100.0	100.0	100.0	100.0	99.6	99.9	100.0
73	**306**	0.0	67.3	74.0	80.0	67.6	63.7	64.4
78	**127**	100.0	0.0	0.0	0.0	0.1	1.4	7.5
78	**157**	0.0	8.0	13.5	14.2	11.8	18.5	20.7
78	**160**	100.0	39.4	40.9	66.3	72.0	85.2	96.4
83	**298**	100.0	42.4	38.6	23.7	3.5	6.5	5.7
94	**113**	0.0	0.5	2.5	100.0	0.2	99.8	100.0
94	**185**	0.0	99.8	98.0	0.0	100.0	0.0	0.0
97	**185**	0.0	7.0	3.3	22.5	47.2	80.0	31.9
122	**211**	100.0	100.0	100.0	100.0	100.0	100.0	100.0
126	**163**	100.0	29.8	31.0	26.2	50.7	42.4	30.9
135	**251**	0.0	69.0	75.7	99.0	71.8	99.1	56.5
161	**78**	100.0	100.0	100.0	100.0	100.0	100.0	102.2
167	**122**	0.0	2.1	6.4	10.9	17.4	14.3	10.5
178	**114**	0.0	30.4	42.2	38.8	41.3	44.2	20.8
178	**118**	100.0	90.7	99.9	95.9	96.9	92.8	99.7
183	**289**	100.0	100.0	100.0	100.0	96.8	94.8	99.9
185	**98**	0.0	20.4	3.5	6.0	50.3	17.4	9.8
187	**113**	100.0	100.0	100.0	100.0	100.0	100.0	100.0
191	**268**	100.0	72.2	7.0	0.6	12.0	1.5	11.5
206	**166**	0.0	43.0	90.0	99.8	69.9	36.0	7.1
211	**122**	100.0	87.5	0.0	0.0	99.6	95.5	67.5
211	**163**	0.0	54.1	0.0	0.0	73.5	79.9	82.3
211	**167**	0.0	0.6	0.7	0.1	1.6	12.1	20.7
222	**132**	100.0	1.7	0.5	2.5	0.7	1.8	0.9
223	**255**	0.0	22.6	90.2	96.8	0.0	0.0	0.0
252	**309**	0.0	6.0	19.0	47.6	1.8	0.0	0.0
264	**294**	0.0	14.3	12.0	1.1	14.3	6.8	20.9
264	**297**	0.0	31.9	47.6	31.8	0.7	0.0	0.0
265	**295**	0.0	10.3	0.1	0.1	11.8	13.4	25.6
265	**298**	0.0	68.4	18.2	33.9	94.2	63.7	95.7
268	**181**	200.0	165.2	174.3	164.2	198.9	124.0	194.7
289	**181**	0.0	42.2	55.0	57.1	15.8	4.8	29.0
296	**113**	0.0	123.4	129.4	128.9	193.1	180.7	197.1
301	**257**	0.0	6.0	2.5	26.3	2.0	57.1	21.4
302	**76**	0.0	0.1	0.0	12.8	8.8	54.0	98.8
302	**257**	0.0	44.7	34.2	5.3	0.3	0.0	0.0
306	**73**	100.0	0.3	0.0	0.2	0.0	0.0	0.0
W3	**94**	0.0	0.0	0.0	84.5	0.0	58.9	62.5
W3	**113**	300.0	205.8	213.0	222.4	189.4	243.9	213.3
W4	**181**	100.0	100.0	100.0	100.0	100.1	97.2	100.0
W4	**187**	0.0	56.6	79.9	85.1	99.4	97.9	99.1
W4	**268**	0.0	62.2	73.9	72.5	9.0	74.7	33.0
268	**W4**	0.0	59.3	68.9	70.3	8.1	14.6	27.9
186	**W4**	100.0	100.0	100.0	100.0	100.0	100.0	100.0
W5	**298**	0.0	89.8	94.1	76.7	0.1	0.0	0.0
W5	**302**	100.0	2.2	0.9	0.2	7.1	59.4	0.0

W5	**W6**	0.0	13.3	18.1	29.5	99.1	2.1	0.0
W5	**W7**	0.0	80.7	87.0	88.8	0.0	0.0	0.0
83	**W5**	0.0	89.9	98.3	100.0	0.0	0.0	0.0
301	**W5**	100.0	10.0	0.0	0.0	99.8	0.0	0.0
W1	**118**	0.0	12.0	1.4	4.6	96.7	0.0	0.0
W1	**167**	100.0	103.7	94.3	98.0	0.3	0.0	0.0
W1	**181**	0.0	0.0	0.0	0.0	0.0	132.6	182.9
W1	**191**	0.0	0.0	0.0	0.0	0.0	92.1	12.6
W1	**268**	0.0	0.0	0.0	0.0	0.0	41.7	87.3
W1	**W2**	0.0	22.2	71.4	43.6	93.2	0.0	0.0
191	**W1**	0.0	0.0	0.0	0.0	0.0	7.2	88.8
189	**W1**	0.0	0.0	0.0	0.0	0.0	91.0	52.7
211	**W1**	0.0	0.0	39.1	15.8	0.0	0.0	0.0
178	**W1**	0.0	15.6	1.0	4.1	58.1	0.0	0.0
167	**W1**	100.0	42.8	56.5	41.4	0.2	0.0	0.0
W2	**122**	0.0	3.9	24.0	4.8	0.0	0.0	0.0
W2	**167**	100.0	56.5	85.0	83.4	112.2	99.4	0.0
W2	**178**	100.0	2.1	2.1	8.6	45.0	79.1	0.0
W2	**207**	0.0	59.4	38.7	31.1	22.1	0.0	0.0
W2	**W1**	0.0	75.4	27.6	56.4	7.3	0.0	0.0
167	**W2**	0.0	43.9	25.1	24.1	10.9	0.0	0.0
W6	**120**	0.0	0.0	7.5	30.3	0.0	0.0	0.0
W6	**121**	0.0	0.0	1.3	18.5	0.0	0.0	0.0
W6	**250**	0.0	0.0	0.0	0.0	0.0	43.0	93.3
W6	**257**	0.0	60.4	26.4	0.0	89.4	0.5	0.0
W6	**298**	0.0	0.1	5.9	38.1	0.0	0.0	0.0
W6	**301**	0.0	2.3	24.6	23.8	0.0	0.0	0.0
W6	**302**	100.0	98.0	67.0	0.0	98.8	0.0	0.0
W6	**W5**	100.0	4.7	19.9	22.2	0.6	10.5	0.0
W6	**W7**	0.0	0.0	32.7	84.5	0.0	0.0	0.0
265	**W6**	0.0	0.0	32.3	85.9	0.0	0.0	0.0
301	**W6**	0.0	85.5	66.6	0.0	0.0	0.0	0.0
W7	**83**	200.0	116.4	110.4	115.9	78.7	62.2	25.0
W7	**120**	0.0	99.3	93.5	98.2	61.8	35.8	5.7
W7	**298**	0.0	4.8	5.1	13.7	61.7	55.0	82.8
W7	**W9**	0.0	0.0	0.0	0.0	1.8	50.4	81.1
298	**W7**	0.0	63.5	0.5	0.0	0.0	0.7	0.0
83	**W7**	100.0	21.2	23.3	19.7	35.9	50.5	84.1
W8	**75**	0.0	64.0	59.3	88.7	95.4	97.1	97.7
W8	**127**	100.0	100.7	100.3	100.1	100.1	100.0	99.9
W8	**160**	0.0	42.1	45.2	12.5	5.6	2.1	1.2
78	**W8**	100.0	100.0	100.0	100.0	100.0	100.0	99.9
W9	**55**	0.0	98.3	100.2	27.7	7.1	0.0	0.0
W9	**83**	0.0	97.5	99.1	94.4	30.3	53.0	59.7
W9	**120**	0.0	0.0	0.0	0.0	0.0	25.8	72.0
W9	**298**	0.0	0.1	0.0	63.3	87.1	71.8	64.1
W9	**299**	0.0	1.3	0.4	50.6	4.1	0.2	0.0
W9	**W5**	0.0	1.4	2.0	55.3	2.0	0.0	0.0
W9	**W7**	0.0	0.0	0.0	0.0	85.3	48.2	7.1
83	**W9**	0.0	0.0	0.0	6.9	84.5	69.9	24.2
302	**W9**	0.0	6.4	17.0	75.9	15.8	1.2	0.0
W10	**181**	0.0	99.9	100.0	99.9	100.0	100.0	100.0
W10	**186**	100.0	119.7	110.7	130.7	108.3	113.6	115.2
185	**W10**	0.0	45.9	31.0	50.8	65.3	77.0	54.9
186	**W10**	0.0	75.3	48.1	79.5	78.9	92.1	73.2
289	**W10**	0.0	90.8	100.0	99.9	48.0	13.3	71.6

W11	**306**	100.0	71.7	83.8	56.2	76.6	39.4	47.8
73	**W11**	100.0	98.0	99.3	99.1	99.8	41.6	64.2
W12	**76**	0.0	57.0	72.5	22.4	6.6	0.0	0.0
W12	**79**	0.0	0.0	0.0	31.5	35.4	34.5	32.4
W12	**83**	0.0	1.5	0.3	71.5	91.6	99.0	93.8
W12	**W9**	0.0	99.9	99.6	38.0	8.4	0.1	0.7
302	**W12**	0.0	97.5	97.3	99.7	99.9	99.8	98.2

Table 2: Selected inter-helical hydrogen bonds in the crystal structure (**1HZX**, chain A), in the **RHO**, and in the **RHOiso** simulation. A cutoff distance between heavy atoms of 4 Å was used, and a cutoff angle of 1 radian. Values higher than 100 % are occur if two residues are connected by more than one hydrogen bond. Twelve internal water molecules (W1 to W12) are included.