Table 1. Dataset of 42 protein-RNA complexes selected from PDB. Among them, 25 structures are used for training and 17 used for testing.

Training Set			Testing Set		
PDB	Res. (Å)	Ref.	PDB	Res. (Å)	Ref.
1A1V	2.20	*Structure* 1998, **6**, p89.	1A34	1.81	*J. Mol. Biol*., 1998, **277**, p37.
1A9N	2.38	*Nature* 1998, **394**, p645.	1C9S	1.90	*Nature* 1999, **401**, p235.
1B2M	2.00	*Biochemistry* 1999, **38**, p2452.	1CX0	2.30	*Nature*, 1998, **395**, p567.
1C0A	2.40	*EMBO J.* 1999, **18**, p6532.	1DFU	1.80	*PNAS,* 2000, **97**, p2023.
1DI2	1.90	*EMBO J.* 1998, **17**, p7505.	1DUL	1.80	*Science* 2000, **287**, p1232.
1E6T	2.20	*RNA* 2001, **7**, p1616.	1FEU	2.30	*Acta.Crys.*, Sect. D, 2001, **57**, p968.
1EC6	2.40	*Cell* 2000, **100**, p323.	1HP6	2.40	*Nature* 2001, **410**, p780.
1F7U	2.20	*EMBO J.* 2000, **19**, p5599.	1M5O	2.20	*Science* 2002, **298**, p1421.
1FXL	1.80	*Nat. Stru. Biol.* 2001, **8**, p141.	1MJI	2.50	*RNA* 2002, **8**, p1548.
1G59	2.40	*Nat. Stru. Biol*. 2001, **8**, p203.	1MSW	2.10	*Science* 2002, **298**, p1387.
1GTF	1.75	*Acta. Crys.* Sect. 2002, D 58, p615.	1N35	2.50	*Cell* 2002, **111**, p733.
1H2T	2.15	*EMBO. J.* 2002, **21**, p5548.	1N78	2.10	*EMBO J.* 2003, **22**, p676.
1HQ1	1.52	*J. Mol. Biol*. 2001, **307**, p229.	1QTQ	2.40	*Structure* 1998, **6**, p439.
1J1U	1.95	*Nat. Struct. Biol.* 2003, **10**, p425	1R3E	2.10	*PNAS* 2003, **100**, p12648.
1JBS	1.97	*Nat. Stru. Biol.* 2001, **8**, p968.	1R9F	1.85	*Nature* 2003, **426**, p874.
1JID	1.80	*Science* 2001, **294**, p598.	1RPU	2.50	*Cell, 2003,* **115**, p799.

1JJ2	2.40	*EMBO J.* 2001, **20**, p4214.	1UVJ	1.90	*Structure* 2004, **12**, p307.
1K8W	1.85	*Cell* 2001, **107**, p929.			
1KNZ	2.45	*Cell* 2002, **108**, p71.			
1LNG	2.30	*Nature* 2002, **417**, p767.			
1M8W	2.20	*Cell* 2002, **110**, p501.			
1OOA	2.45	*PNAS* 2003, **100**, p9268.			
1QTQ	2.40	*Structure* 1998, **6**, p439.			
1URN	1.92	*Nature* 1994, **372**, p432.			
2A8V	2.40	*Mol. Cell* 1999, **3**, p487.			

Table 2. Distance-dependent energy parameters for the hydrogen bonds between protein and DNA/RNA. Energies are omitted for bins with zero counts (cutoff values).

DISTANCE BIN [Å] (1.0 Å per bin)		*ENERGY*										
		1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*
1.4	1.5	-	-	-	1.51	-	-	-	-	-	-	-
1.5	1.6	-	-	-	1.17	-	1.20	-	-	-	-	1.53
1.6	1.7	-0.10	-	0.38	0.48	1.25	0.29	1.61	-	0.29	-	0.69
1.7	1.8	-0.39	-	-0.32	-0.06	-	-0.41	0.92	-0.69	-0.41	-	-0.59
1.8	1.9	-0.88	-0.54	-0.88	-0.62	1.25	-0.30	-0.59	-	-1.10	-	-0.98
1.9	2.0	-0.61	-1.23	-0.88	-0.69	-0.13	-0.94	-0.96	-1.39	-1.10	-0.09	-1.03
2	2.1	-0.51	-0.54	-0.32	-0.41	-0.54	-0.50	-0.96	-1.39	-0.41	-1.19	-0.50
2.1	2.2	-0.51	-0.54	-0.54	-0.28	-0.69	-0.18	-0.34	-0.69	0.29	-1.19	-0.01
2.2	2.3	0.30	-	-0.03	0.13	-0.36	0.11	-0.34	-	0.29	-0.09	0.44
2.3	2.4	1.00	-	0.38	0.08	-0.54	0.29	0.51	-	0.29	-0.09	1.25
2.4	2.5	1.69	-0.54	1.07	0.48	-0.36	0.51	0.51	-	-	-0.09	1.53
2.5	2.6	0.59	-0.54	-	0.35	-0.69	0.80	0.92	-	-	-0.09	1.53

1, na_NH_aa_sc_sp2; ***2***, na_NH_aa_sc_sp3; ***3***, na_NH_aa_bb_O; ***4***, na_P_aa_sc_NH; ***5***, na_O_aa_sc_NH; ***6***, na_base_O_aa_sc_NH; ***7***, na_base_N_aa_sc_NH; ***8***, na_base_N_aa_bb_NH; ***9***, na_base_O_aa_bb_NH; ***10***, na_O_aa_bb_NH; ***11***, na_P_aa_bb_NH.

Table 3. Angle-dependent energies (not scaled) for hydrogen bonds between na_base_N and aa_bb_NH.

ANGLE BIN *(10° per bin)*	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	-1.75	-	-
-170	-2.00	-	-
-160	-1.75	-	-
-150	-0.90	-	-
-140	-1.19	-	-
-130	0.20	-	-
-120	-	-	-
-110	-	-	-
-100	-	-	-
-90	-	-	-
-80	-	-	-
-70	-	-	-
-60	-	-	-
-50	-	-	-
-40	-	-	-
-30	-	-	-
-20	-	-	-
-10	-	-	-
0	-	-	-
10	-	-	-
20	-	-	-
30	-	-	-
40	-	-	-
50	-	-	-
60	-	-	-
70	-	-	-
80	-	-	-
90	-	0.37	-
100	-	-1.24	-
110	-	-2.47	1.59
120	-	-1.71	1.59
130	-0.49	-2.40	0.90
140	-1.19	-1.24	-0.97
150	-0.49	-	-1.67
160	-0.49	-	-2.40
170	-0.90	-	-2.79

Table 4. Angle-dependent energies (not scaled) for hydrogen bonds between na_base_N and aa_sc_NH.

ANGLE BIN (10° per bin)	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	-2.12	-	-
-170	-1.53	-	-
-160	-1.05	-	-
-150	-0.69	-	-
-140	-0.22	-	-
-130	0.29	-	-
-120	0.47	-	-
-110	-	-	-
-100	-	-	-
-90	-	-	-
-80	-	-	-
-70	-	-	-
-60	-	-	-
-50	-	-	-
-40	-	-	-
-30	-	-	-
-20	-	-	-
-10	-	-	-
0	-	-	-
10	-	-	-
20	-	-	-
30	-	-	-
40	-	-	-
50	-	-	-
60	-	-	-
70	-	-	3.25
80	-	-	1.86
90	-	-0.26	3.25
100	2.08	-1.19	1.30
110	1.39	-2.29	0.42
120	0.29	-2.28	0.42
130	0.14	-1.84	-0.64
140	0.47	-1.19	-1.11
150	-0.69	-0.74	-1.70
160	-1.38	-	-2.47
170	-1.92	-	-2.48

Table 5. Angle-dependent energies (not scaled) for hydrogen bonds between na_base_O and aa_bb_NH.

ANGLE BIN *(10° per bin)*	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	0.96	-	-
-170	0.96	-	-
-160	0.27	-	-
-150	-0.14	-	-
-140	-0.43	-	-
-130	-0.14	-	-
-120	-0.99	-	-
-110	0.96	-	-
-100	0.27	-	-
-90	0.27	-	-
-80	0.27	-	-
-70	-0.14	-	-
-60	-0.14	-	-
-50	0.27	-	-
-40	-0.65	-	-
-30	-0.99	-	-
-20	-0.65	-	-
-10	0.27	-	-
0	0.27	-	-
10	-1.53	-	-
20	-1.12	-	-
30	-0.14	-	-
40	-0.65	-	-
50	0.27	-	-
60	-	-	-
70	-	1.33	-
80	-	-0.46	-
90	-	-0.46	-
100	0.27	0.23	-
110	-	-1.24	0.58
120	-0.14	-1.67	0.80
130	0.96	-2.00	0.25
140	-	-2.04	-1.10
150	-	-1.81	-1.76
160	-	-0.62	-2.62
170	0.96	-	-2.44

Table 6. Angle-dependent energies (not scaled) for hydrogen bonds between na_base_O and aa_sc_NH.

ANGLE BIN *(10° per bin)*	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	2.28	-	-
-170	-0.02	-	-
-160	0.20	-	-
-150	0.20	-	-
-140	0.20	-	-
-130	0.20	-	-
-120	0.67	-	-
-110	0.49	-	-
-100	0.20	-	-
-90	0.08	-	-
-80	0.20	-	-
-70	0.89	-	-
-60	0.33	-	-
-50	-0.20	-	-
-40	0.20	-	-
-30	0.08	-	-
-20	-0.49	-	-
-10	-0.55	-	-
0	-1.33	-	-
10	-1.25	-	-
20	-0.66	-	-
30	-0.12	-	-
40	-0.61	-	-
50	-0.28	-	-
60	0.20	-	2.42
70	0.33	2.84	1.72
80	0.49	2.84	1.72
90	0.89	0.20	0.91
100	0.49	-0.45	0.62
110	0.89	-1.43	-0.39
120	0.33	-1.60	-0.80
130	0.89	-1.66	-1.36
140	2.28	-1.49	-1.52
150	0.20	-1.68	-1.95
160	0.08	-1.39	-2.11
170	0.89	-1.67	-1.97

Table 7. Angle-dependent energies (not scaled) for hydrogen bonds between na_NH and aa_bb_O.

ANGLE BIN (10° per bin)	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	1.58	-	-
-170	0.88	-	-
-160	0.88	-	-
-150	1.58	-	-
-140	1.58	-	-
-130	1.58	-	-
-120	0.19	-	-
-110	-0.62	-	-
-100	-0.22	-	-
-90	0.88	-	-
-80	-0.62	-	-
-70	0.19	-	-
-60	0.48	-	-
-50	-0.37	-	-
-40	-0.50	-	-
-30	0.19	-	-
-20	0.19	-	-
-10	-0.50	-	-
0	-0.22	-	-
10	0.88	-	-
20	-0.37	-	-
30	-0.37	-	-
40	0.48	-	-
50	0.48	-	-
60	-0.03	-	-
70	-0.37	-	-
80	0.48	-	-
90	-0.73	0.22	2.14
100	0.19	0.40	1.73
110	-0.73	-1.32	0.64
120	-0.62	-1.86	0.75
130	-0.62	-2.07	-0.34
140	0.48	-1.98	-0.93
150	-0.03	-1.84	-2.00
160	0.48	-0.39	-2.07
170	0.88	-0.39	-2.74

Table 8. Angle-dependent energies (not scaled) for hydrogen bonds between na_NH and aa_sc_sp2.

ANGLE BIN (10° per bin)	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	-1.23	-	-
-170	-0.82	-	-
-160	-0.42	-	-
-150	-0.88	-	-
-140	-0.98	-	-
-130	-0.42	-	-
-120	0.12	-	-
-110	-0.24	-	-
-100	0.97	-	-
-90	-0.01	-	-
-80	0.68	-	-
-70	0.68	-	-
-60	0.27	-	-
-50	1.37	-	-
-40	0.46	-	-
-30	2.07	-	-
-20	1.37	-	-
-10	0.27	-	-
0	1.37	-	-
10	1.37	-	-
20	0.46	-	-
30	0.46	-	-
40	0.68	-	-
50	0.12	-	-
60	1.37	0.43	-
70	2.07	-0.03	-
80	0.68	-0.03	-
90	0.46	-0.19	3.33
100	0.27	-1.46	2.23
110	0.97	-1.64	1.94
120	-0.13	-2.09	0.69
130	-0.24	-1.58	-0.50
140	-0.13	-1.12	-1.19
150	0.12	-0.89	-1.64
160	-0.93	-0.76	-2.45
170	-0.71	-0.72	-2.60

Table 9. Angle-dependent energies (not scaled) for hydrogen bonds between na_NH and aa_sc_sp3.

ANGLE BIN (10° per bin)	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	-0.75	-	-
-170	-0.34	-	-
-160	-	-	-
-150	-0.34	-	-
-140	0.35	-	-
-130	0.35	-	-
-120	-	-	-
-110	0.35	-	-
-100	0.35	-	-
-90	-	-	-
-80	-	-	-
-70	-	-	-
-60	0.35	-	-
-50	-0.75	-	-
-40	0.35	-	-
-30	0.35	-	-
-20	0.35	-	-
-10	-0.34	-	-
0	-	-	-
10	0.35	-	-
20	0.35	-	-
30	0.35	-	-
40	-0.34	-	-
50	-	-	-
60	-	-	-
70	-0.34	-	1.15
80	-0.34	-0.10	1.15
90	-	-1.36	0.46
100	0.35	-1.81	-0.23
110	-1.26	-1.36	1.15
120	-0.75	-1.71	-0.23
130	-1.04	-1.36	-1.62
140	0.35	-0.51	-1.15
150	-0.34	-1.61	-2.11
160	0.35	-1.36	-2.14
170	-1.26	-	-1.94

Table 10. Angle-dependent energies (not scaled) for hydrogen bonds between na_O and aa_bb_NH.

ANGLE BIN (10° per bin)	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	0.80	-	-
-170	-0.59	-	-
-160	-0.99	-	-
-150	-0.81	-	-
-140	-0.30	-	-
-130	0.11	-	-
-120	0.11	-	-
-110	0.80	-	-
-100	0.80	-	-
-90	0.11	-	-
-80	-0.30	-	-
-70	-0.30	-	-
-60	0.11	-	-
-50	-	-	-
-40	0.11	-	-
-30	0.11	-	-
-20	0.80	-	-
-10	0.11	-	-
0	0.80	-	-
10	0.11	-	-
20	-	-	-
30	-0.59	-	-
40	-0.59	-	-
50	0.11	-	-
60	-0.3	-	-
70	0.11	-	-
80	0.11	1.20	-
90	0.80	0.50	-
100	0.80	-0.19	-
110	-0.59	-1.44	0.44
120	-0.59	-1.80	-0.47
130	0.80	-1.75	-0.94
140	-0.30	-1.98	-1.47
150	-	-2.06	-1.43
160	-0.30	-0.75	-2.16
170	0.80	-	-2.55

Table 11. Angle-dependent energies (not scaled) for hydrogen bonds between na_O and aa_sc_NH.

ANGLE BIN *(10° per bin)*	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	-0.06	-	-
-170	0.10	-	-
-160	0.28	-	-
-150	0.10	-	-
-140	-0.31	-	-
-130	-0.31	-	-
-120	-0.19	-	-
-110	0.50	-	-
-100	-0.06	-	-
-90	0.50	-	-
-80	-0.06	-	-
-70	0.28	-	-
-60	-0.19	-	-
-50	-0.68	-	-
-40	-0.19	-	-
-30	0.50	-	-
-20	-0.51	-	-
-10	0.50	-	-
0	0.28	-	-
10	0.79	-	-
20	0.79	-	-
30	0.28	-	-
40	-0.06	-	-
50	-0.31	2.16	-
60	0.28	2.16	2.59
70	-0.06	2.16	1.50
80	1.89	0.77	0.80
90	-0.31	-0.14	0.80
100	-0.31	-1.5	0.03
110	0.50	-1.83	-0.62
120	-0.06	-1.97	-1.28
130	0.10	-1.87	-1.55
140	-0.19	-1.71	-1.48
150	-0.41	-1.34	-1.81
160	-0.31	1.06	-1.97
170	0.10	-	-1.79

Table 12. Angle-dependent energies (not scaled) for hydrogen bonds between na_P and aa_bb_NH.

ANGLE BIN *(10° per bin)*	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	0.22	-	-
-170	1.54	-	-
-160	0.62	-	-
-150	0.62	-	-
-140	1.13	-	-
-130	1.83	-	-
-120	0.85	-	-
-110	0.36	-	-
-100	0.85	-	-
-90	0.98	-	-
-80	0.44	-	-
-70	0.73	-	-
-60	0.36	-	-
-50	0.15	-	-
-40	-0.37	-	-
-30	-0.44	-	-
-20	-0.66	-	-
-10	-0.71	-	-
0	-0.99	-	-
10	-0.44	-	-
20	-0.47	-	-
30	-0.41	-	-
40	0.04	-	-
50	-0.29	-	-
60	-0.02	-	-
70	1.54	2.61	-
80	0.98	0.66	-
90	-0.29	-0.06	4.25
100	-0.47	-1.13	3.56
110	-0.37	-1.71	2.30
120	-0.47	-1.96	0.59
130	-0.29	-1.69	-0.08
140	0.22	-1.67	-0.93
150	0.44	-1.22	-1.89
160	-0.16	-0.87	-2.33
170	0.44	-0.74	-2.69

Table 13. Angle-dependent energies (not scaled) for hydrogen bonds between na_P and aa_sc_NH.

ANGLE BIN *(10° per bin)*	*ENERGY*		
	E (X)	*E (Ψ)*	*E (Θ)*
-180	0.84	-	-
-170	0.91	-	-
-160	0.65	-	-
-150	0.99	-	-
-140	0.48	-	-
-130	0.99	-	-
-120	0.48	-	-
-110	0.30	-	-
-100	0.15	-	-
-90	-0.16	-	-
-80	0.15	-	-
-70	-0.10	-	-
-60	-0.47	-	-
-50	-0.16	-	-
-40	-0.33	-	-
-30	-0.16	-	-
-20	-0.51	-	-
-10	-0.28	-	-
0	-0.31	-	-
10	-0.47	-	-
20	-0.02	-	-
30	-0.23	-	-
40	-0.31	-	-
50	0.11	3.82	4.42
60	-0.16	2.72	4.42
70	0.01	0.52	2.22
80	-0.10	-0.44	1.86
90	-0.02	-0.89	1.05
100	-0.23	-1.27	0.92
110	-0.08	-1.56	0.59
120	-0.10	-1.73	-0.18
130	-0.18	-1.71	-1.20
140	0.43	-1.27	-1.59
150	-0.02	-1.42	-2.07
160	0.30	-0.86	-2.18
170	0.30	-0.56	-2.11