1. Predicted pKa values on PPD (Protein pKa Database) dataset with optimal parameters $\varepsilon_{ref} = 8, \sigma = 0.70$. The calculations are performed with AMBER, CHARMM and PARSE force fields, respectively.

PDB_NAME	RES_NAME	RES_NUM	EXP_Value	AMBER	CHARMM	PARSE
1A2P	ASP	8	3.3	3.39	3.3	3.84
1A2P	ASP	12	3.8	3.45	3.96	3.56
1A2P	ASP	22	3.3	3.61	3.59	3.83
1A2P	ASP	44	3.4	3.74	3.79	4.17
1A2P	ASP	54	2.2	2.71	2.23	2.19
1A2P	ASP	75	3.1	2.35	1.96	1.89
1A2P	ASP	86	4.2	3.39	3.45	3.69
1A2P	ASP	93	2	2.7	2.57	1.92
1A2P	ASP	101	2	2.71	2.39	0.69
1A2P	GLU	29	3.8	4.48	4.45	4.17
1A2P	GLU	60	3	3.97	3.46	3.51
1A2P	GLU	73	2.2	3.8	3.58	3.54
1A2P	HIS	18	7.7	6.8	6.81	6.87
1A2P	HIS	102	6.3	6.26	6.5	6.69
1A6K	HIS	12	6.5	6.79	7.04	6.94
1A6K	HIS	24	5	6.27	6.61	5.5
1A6K	HIS	36	8	6.83	7.11	7.16
1A6K	HIS	48	5.6	6.28	6.53	6.19
1A6K	HIS	64	5	5.86	5.55	5.86
1A6K	HIS	81	6.9	6.77	6.87	6.79
1A6K	HIS	82	5	7.15	7.8	7.02
1A6K	HIS	97	5.6	5.62	5.47	5.48
1A6K	HIS	113	5.4	6.31	6.35	5.97
1A6K	HIS	116	6.7	6.51	6.5	6.54
1A6K	HIS	119	6.2	5.49	5.93	5.21
1BEO	ASP	21	2.5	3.26	2.49	2.31
1BEO	ASP	30	2.5	3.65	3.46	3.83
1BEO	ASP	72	2.6	3.75	3.74	4.16
1BEO	LYS	61	10.4	10.06	10.08	10.07
1BEO	LYS	94	9.4	9.97	10.01	10.08
1DG9	HIS	66	8.3	7.04	7.2	7.15
1DWR	HIS	36	7.8	6.77	7	7.04
1DWR	HIS	48	5.6	6.51	6.52	6.29
1DWR	HIS	81	6.9	6.47	6.28	6.28
1DWR	HIS	113	5.9	6.1	6.05	5.91
1DWR	HIS	116	6.8	6.23	6.16	6.18
1DWR	HIS	119	6.6	6.03	6.58	6.1
1ERT	ASP	16	4	4	4.12	4.48
1ERT	ASP	20	3.8	3.61	3.61	3.83
1ERT	ASP	58	2.8	3.88	4.25	3.16
1ERT	ASP	60	4.2	3.59	3.72	3.83
1ERT	ASP	61	5.3	4.07	4.57	4.79
1ERT	ASP	64	3.2	3.41	3.42	3.2
1ERT	GLU	6	4.8	5.18	5.31	5.58
1ERT	GLU	13	4.4	4.86	4.55	4.89
1ERT	GLU	47	4.1	4.54	4.15	4.45
1ERT	GLU	56	3.1	4.64	5	4.77

1ERT	GLU	68	4.9	4.53	4.32	4.56
1ERT	GLU	70	4.6	4.8	4.55	4.81
1ERT	GLU	88	3.7	4.17	3.64	3.91
1ERT	GLU	95	4.1	4.57	4.27	4.53
1ERT	GLU	98	3.9	4.11	3.61	3.95
1ERT	GLU	103	4.4	5	4.79	5.1
1ERT	HIS	43	5.5	6.84	7.01	6.89
1ERU	ASP	16	4.2	4.02	4.3	4.58
1ERU	ASP	20	3.8	3.59	3.71	3.87
1ERU	ASP	58	2.7	3.92	4.46	3.44
1ERU	ASP	60	3.9	3.38	3.02	3.36
1ERU	ASP	61	5.2	3.98	4.29	4.79
1ERU	ASP	64	3.2	3.67	3.68	3.54
1ERU	GLU	6	4.9	5.05	5.22	5.55
1ERU	GLU	13	4.4	4.86	4.64	4.88
1ERU	GLU	47	4.3	4.52	4.1	4.24
1ERU	GLU	56	3.2	4.67	4.77	4.66
1ERU	GLU	68	5.1	4.71	4.54	4.95
1ERU	GLU	70	4.8	4.59	4.54	4.58
1ERU	GLU	88	3.6	4.36	3.65	3.98
1ERU	GLU	95	4.1	4.5	4.14	4.22
1ERU	GLU	98	3.9	4.09	3.62	3.94
1ERU	GLU	103	4.5	4.95	4.73	5.04
1FKS	HIS	87	5.9	6.48	6.26	6.29
1FKS	HIS	94	5.8	6.28	6.27	6.19
1GOA	ASP	70	2.6	3.23	3.36	3.38
1GOA	ASP	95	3.2	3.26	2.97	2.88
1GOA	ASP	103	2	2.39	1.66	2.04
1GOA	ASP	109	3.2	3.2	2.71	2.92
1GOA	ASP	135	4.3	3.38	3.05	3.31
1GOA	ASP	149	2	2.51	2.35	1.79
1GOA	GLU	6	4.5	4.09	3.73	3.8
1GOA	GLU	32	3.6	3.91	3.49	3.81
1GOA	GLU	48	4.4	3.81	3.18	3.2
1GOA	GLU	57	3.2	3.51	3.39	3.27
1GOA	GLU	61	3.9	4.42	3.89	4.18
1GOA	GLU	64	4.4	4.51	4.19	4.53
1GOA	GLU	120	4.1	4.15	3.52	4.03
1GOA	GLU	130	3.6	4.28	3.67	3.66
1GOA	GLU	132	4.3	4.58	4.11	4.4
1GOA	GLU	136	4.3	4.64	4.68	4.64
1GOA	GLU	148	4.2	4.83	4.48	4.75
1GOA	GLU	155	4.4	4.55	4.12	4.55
1GOA	HIS	62	7	6.5	6.5	6.57
1GOA	HIS	84	5.5	5.98	5.95	5.85
1GOA	HIS	115	5	6.52	6.52	6.22
1GOA	HIS	125	7.1	7.12	7.57	7.26
1GOA	HIS	128	7.9	6.94	7.13	7.1
1GS9	LYS	69	10.1	10.18	10.76	10.45
1GS9	LYS	72	10	10.16	10.49	10.13
1GS9	LYS	75	10	10.77	11.22	10.88
1GS9	LYS	95	10	10.06	10.13	10.11
1GS9	LYS	143	9.4	9.79	9.86	9.62

1GS9	LYS	146	9.9	9.55	9.59	9.54
1GS9	LYS	157	10.9	10.13	10.32	10.29
1H4G	ASP	5	3.8	3.64	3.61	3.9
1H4G	ASP	15	3.4	3.08	2.71	2.93
1H4G	ASP	21	3.5	3.01	2.78	2.47
1H4G	ASP	90	3.9	3.72	3.71	4.2
1H4G	ASP	99	2.7	2.74	2.55	2.48
1H4G	ASP	118	2.7	2.48	2.26	2.12
1H4G	ASP	123	2.7	2.65	2.48	2.75
1H4G	GLU	17	4.3	4.35	4.01	3.79
1H4G	GLU	94	3.9	3.99	3.96	3.91
1H4G	GLU	126	4.5	3.99	3.44	3.51
1H4G	GLU	167	3.6	3.81	3.5	3.68
1H4G	GLU	178	4.1	3.66	3.17	3.24
1H4G	GLU	184	6.5	4.53	4.2	5.5
1H4G	HIS	11	6.5	6.21	6.24	6.17
1H4G	HIS	32	6.7	6.48	6.5	6.28
1HNG	ASP	25	3.5	3.66	3.57	4.01
1HNG	ASP	26	3.6	3.77	3.97	4.11
1HNG	ASP	28	3.6	3.23	3.05	3.37
1HNG	ASP	62	4.2	3.49	3.35	3.7
1HNG	ASP	71	3.2	3.68	3.98	4.21
1HNG	ASP	72	4.1	3.47	3.51	3.8
1HNG	ASP	94	3.8	3.63	3.73	3.83
1HNG	GLU	29	4.5	4.45	4.17	3.7
1HNG	GLU	33	4.2	4.48	4.18	4.48
1HNG	GLU	41	6.5	4.53	4.36	5.35
1HNG	GLU	56	4	4.16	3.79	3.92
1HNG	GLU	99	4.1	4.15	3.78	4.03
1I0V	ASP	15	3.5	3.73	3.9	3.77
1I0V	ASP	29	4.3	4.03	4.51	4.67
1I0V	ASP	49	4.2	4.07	4.26	4.76
1I0V	ASP	66	3.9	3.96	3.92	4.2
1I0V	GLU	28	5.6	4.99	4.7	4.98
1I0V	GLU	31	5.4	4.92	4.84	5.06
1I0V	GLU	46	3.6	4.06	3.62	3.87
1I0V	GLU	58	4	3.78	3.18	3.08
1I0V	GLU	82	3.3	4.09	3.74	3.93
1I0V	GLU	102	5.3	4.89	4.59	4.91
1I0V	HIS	27	7	7.84	8.18	8.04
1I0V	HIS	40	7.9	6.88	7.27	7.06
1I0V	HIS	92	7.3	6.94	7	6.94
1IG5	ASP	47	3	3.25	3.02	3.09
1IG5	GLU	4	3.8	4.25	3.79	3.98
1IG5	GLU	5	3.4	4.44	4.08	4.02
1IG5	GLU	11	4.7	4.86	4.65	4.64
1IG5	GLU	17	3.5	5.04	5.3	5.02
1IG5	GLU	26	4.1	4.58	4.21	4.47
1IG5	GLU	48	4.6	4.57	4.37	4.55
1IG5	GLU	64	3.8	4.14	3.74	3.91
1IG5	LYS	7	11.4	10.79	10.96	10.89
1IG5	LYS	12	11.1	10.91	11.16	10.76
1IG5	LYS	16	10.1	10.54	10.74	10.8

1IG5	LYS	25	11.7	11.22	11.79	11.46
1IG5	LYS	29	11.4	10.46	10.54	10.41
1IG5	LYS	41	10.9	10.14	10.14	10.14
1IG5	LYS	55	12.1	10.96	11.32	11.06
1IG5	LYS	71	10.7	10.02	10.02	9.98
1IG5	LYS	72	11.3	10.23	10.4	10.2
1IGD	ASP	27	2.9	3.22	2.98	2.48
1IGD	ASP	41	3.9	3.95	3.74	4.16
1IGD	ASP	45	4	4.02	4.34	4.81
1IGD	ASP	51	3.6	3.55	3.49	3.12
1IGD	ASP	52	3.4	3.37	2.99	3.43
1IGD	GLU	20	4.3	4.44	3.88	4.1
1IGD	GLU	29	4.2	4.45	3.84	4.21
1IGD	GLU	32	4.6	4.47	4.08	4.17
1IGD	LYS	9	11	10.7	10.92	10.86
1IGD	LYS	15	11	10.45	10.69	10.5
1IGD	LYS	18	11	10.14	10.21	10.26
1IGD	LYS	24	11	10.1	10.11	10.01
1IGD	LYS	33	11	10.8	11.26	10.98
1JIC	ASP	15	2.9	3.41	3.03	3.14
1JIC	ASP	34	2.6	3.26	2.96	2.98
1JIC	ASP	49	3	3.35	3.23	3.3
1JIC	GLU	10	3.5	4.23	3.79	3.99
1JIC	GLU	11	3.5	4.5	4.21	4.45
1JIC	GLU	35	5.4	4.72	4.52	4.72
1JIC	GLU	47	3.5	4.2	3.91	4.42
1JIC	GLU	53	3.2	4.73	4.17	4.44
1JIC	GLU	59	4.1	4.77	4.5	4.78
1JIC	LYS	6	12	10.7	10.87	10.73
1JIC	LYS	12	10	10.54	10.95	10.81
1JIC	LYS	18	10	10.51	10.9	10.78
1KXI	ASP	42	3.2	3.28	2.63	2.7
1KXI	ASP	59	2.3	3.35	3.02	2.83
1KXI	GLU	17	4	4.74	4.2	4.53
1KXI	HIS	4	5.6	6.16	6.22	6.09
1LE2	LYS	69	10.1	10.29	10.82	10.73
1LE2	LYS	72	10	9.99	10.05	10.06
1LE2	LYS	75	10	10.5	10.84	10.58
1LE2	LYS	95	10	10.02	10.08	9.98
1LE2	LYS	143	9.4	9.45	9.59	9.42
1LE2	LYS	146	9.9	9.69	9.83	9.73
1LE2	LYS	157	10.9	10.3	10.74	10.79
1NFN	LYS	69	10.4	10.29	10.92	10.73
1NFN	LYS	72	10	10.11	10.24	10.19
1NFN	LYS	75	10.1	10.23	10.72	10.44
1NFN	LYS	95	10.1	9.98	10.06	10.04
1NFN	LYS	143	9.5	9.83	9.89	9.78
1NFN	LYS	146	9.9	9.52	9.73	9.56
1NFN	LYS	157	11.1	10.22	10.85	10.8
1PGB	ASP	22	2.9	3.05	2.58	2.15
1PGB	ASP	36	3.8	3.99	4.06	4.48
1PGB	ASP	40	4	4.05	4.48	4.94
1PGB	ASP	46	3.6	3.54	3.57	3.51

1PGB	ASP	47	3.4	3.49	3.33	3.5
1PGB	GLU	15	4.4	4.25	3.52	3.77
1PGB	GLU	19	3.7	4.88	4.67	4.83
1PGB	GLU	27	4.5	4.42	3.8	4.03
1PGB	LYS	4	11	10.88	11.54	11.18
1PGB	LYS	10	11	10.22	10.29	10.17
1PGB	LYS	13	11	10.8	10.99	10.88
1PGB	LYS	28	11	10.23	10.31	10.21
1PPF	ASP	7	2.6	3.68	3.59	3.82
1PPF	ASP	27	2.3	3.36	3.25	2.98
1PPF	GLU	10	4.2	4.19	3.87	4.09
1PPF	GLU	19	3.2	3.42	2.61	2.82
1PPF	GLU	43	3.8	4.77	4.53	4.79
1PPF	HIS	52	7.5	6.28	6.29	6.47
1PPF	LYS	13	9.9	10.26	10.77	10.57
1PPF	LYS	29	11	10.03	10.16	10.17
1PPF	LYS	34	10	10.18	10.44	10.18
1PPF	LYS	55	11	9.85	9.83	9.88
1RGG	ASP	17	3.7	3.9	3.97	4.35
1RGG	ASP	25	4.9	4.28	4.33	4.83
1RGG	ASP	33	2.4	2.65	2.52	2.09
1RGG	ASP	84	3	3.2	3	1.85
1RGG	ASP	93	3.1	3.98	4	3.98
1RGG	GLU	14	5.1	4.16	3.71	3.84
1RGG	GLU	41	4.1	4.2	3.92	4.05
1RGG	GLU	54	3.4	3.93	3.52	3.7
1RGG	GLU	74	3.5	4.94	4.7	5.01
1RGG	GLU	78	3.1	4.64	4.42	4.62
1RGG	HIS	53	8.3	7.16	7.32	7.25
1RGG	HIS	85	6.4	6.46	6.5	6.49
1RQL	LYS	53	9.3	10.07	10.22	10.07
1STY	HIS	8	6.5	6.46	6.93	6.8
1STY	HIS	46	5.9	6.14	6.15	6.03
1STY	HIS	121	5.6	6.73	6.83	6.56
1STY	HIS	124	6	5.81	6	5.79
1XNB	ASP	11	2.5	3.4	2.82	2.86
1XNB	ASP	101	2	2.95	2.77	2.75
1XNB	ASP	106	2.7	3.48	3.61	4.14
1XNB	ASP	119	3.2	3.38	3.46	3.17
1XNB	ASP	121	3.6	3.78	3.96	4.43
1XNB	GLU	78	4.6	4.33	3.99	4.23
1XNB	HIS	156	6.5	6.26	6.45	6.23
2CI2	ASP	64	3.8	3.04	3.08	2.84
2CI2	ASP	71	2.8	3.31	2.72	2.48
2CI2	ASP	74	5	4.02	4.5	4.91
2CI2	GLU	23	3.2	4.26	3.9	4.09
2CI2	GLU	26	3.3	3.91	3.31	3.63
2CI2	GLU	33	4.2	4.52	3.64	3.29
2CI2	GLU	34	3.8	4.49	4.22	4.19
2CI2	GLU	45	3.9	4.11	3.81	4
2CI2	GLU	60	3.5	4.13	3.76	4.04
2CPL	HIS	54	4.2	6.1	6.14	5.99
2CPL	HIS	70	5.8	6.23	6.49	6.46

2CPL	HIS	92	4.2	6.53	6.57	6.15
2CPL	HIS	126	6.3	6.11	6.37	6.13
2TGA	HIS	40	4.6	7.05	7.3	5.16
2TGA	HIS	57	7.3	6.87	7.03	6.98
3EBX	HIS	6	5.8	5.91	5.96	5.78
3EBX	HIS	26	5.8	5.94	5.93	5.91
3RN3	ASP	14	1.8	3.47	3.4	3.22
3RN3	ASP	38	3.5	3.53	3.47	3.84
3RN3	ASP	53	3.7	3.91	4.03	3.97
3RN3	ASP	83	3.3	3.31	3.19	3.25
3RN3	ASP	121	3	2.7	2.23	1.96
3RN3	GLU	2	2.6	3.49	2.88	3.02
3RN3	GLU	9	4	4.46	4.17	4.41
3RN3	GLU	49	4.7	4.61	4.33	4.64
3RN3	GLU	86	4	4.45	4.25	4.48
3RN3	GLU	111	3.5	4.5	4.15	4.43
3RN3	HIS	12	6	6.03	6.09	6.22
3RN3	HIS	48	6.1	6.22	6.78	6.2
3RN3	HIS	105	6.5	6.25	6.13	6.2
3RN3	HIS	119	6.5	6.58	6.97	6.82
4LZT	ASP	18	2.7	3.25	2.78	3.16
4LZT	ASP	48	1.6	3.41	3.38	3.1
4LZT	ASP	52	3.7	3.38	3.09	3.46
4LZT	ASP	66	0.9	2.69	2.37	1.68
4LZT	ASP	87	2.1	2.82	2.48	2.29
4LZT	ASP	101	4.1	3.7	3.77	4.19
4LZT	ASP	119	3.2	3.34	3.2	3.22
4LZT	GLU	7	2.9	3.85	3	3.48
4LZT	GLU	35	6.2	4.46	4.24	4.87
4LZT	HIS	15	5.4	6.48	6.52	6.25
4LZT	LYS	13	10.5	9.83	9.92	9.99
4LZT	LYS	33	10.4	10.24	10.49	10.33
4LZT	LYS	96	10.8	10.23	10.29	10.48
4LZT	LYS	97	10.3	10.21	10.47	10.52
4LZT	LYS	116	10.2	9.88	10	9.86
4PTI	ASP	3	3.6	3.76	3.75	4.09
4PTI	ASP	50	3.2	3.48	3.46	3.25
4PTI	GLU	7	3.9	4.08	3.61	3.91
4PTI	GLU	49	3.9	4.29	3.89	4.18
4PTI	LYS	15	10.4	10.07	10.1	10.12
4PTI	LYS	26	10.4	9.99	9.98	9.96
4PTI	LYS	41	10.8	9.99	10.11	10.13
4PTI	LYS	46	10.4	9.86	9.94	9.88

2. Predicted pKa values on pKa-cooperative (SNase) dataset with optimal parameters $\varepsilon_{ref} = 8, \sigma = 0.93$. The calculations are performed with AMBER, CHARMM and PARSE force fields, respectively.

PDB	RES_NAME	RES_NUM	EXP_Value	AMBER	CHARMM	PARSE
1STN	HIS	8	6.5	6.86	7.19	7.17
1STN	HIS	121	5.3	2.22	2.64	3.08
1STN	HIS	124	5.7	5.35	5.47	5.53
3BDC	ASP	19	2.3	5.57	3.41	0.25
3BDC	ASP	21	6.5	6.72	4.45	6.31
3BDC	ASP	40	3.9	5.95	5.96	6.24
3BDC	ASP	43	4	6.5	0	0
3BDC	ASP	77	1	1.77	0	0
3BDC	ASP	83	1	0.3	0	0
3BDC	ASP	95	2.2	2.14	5.32	5.58
3BDC	GLU	10	2.9	4.02	7.05	6.7
3BDC	GLU	52	4	3.58	4.15	2.5
3BDC	GLU	57	3.6	3.88	4.14	3.1
3BDC	GLU	67	3.8	3.03	2.12	2.06
3BDC	GLU	73	3.9	2.87	3.57	1.87
3BDC	GLU	75	3.3	3.1	2.02	0.8
3BDC	GLU	101	3.9	3.8	3.56	3.71
3BDC	GLU	122	3.9	4.28	4.87	3.81
3BDC	GLU	129	3.8	3.19	3.5	3.2
3BDC	GLU	135	3.8	4.63	5.03	4.44
A109D	ASP	109	7.5	5.58	8.51	7.47
A109E	GLU	109	7.9	6.61	8.02	8.5
A109K	LYS	109	>10.5	10.18	12.74	12
A109R	ARG	109	>10.5	11.42	13.17	14
A132D	ASP	132	7	6.88	9.12	8.27
A132E	GLU	132	7	7.32	8.91	8.03
A132K	LYS	132	>10.4	12.07	13.41	12.46
A132R	ARG	132	>10.4	13.19	12.96	14
A58D	ASP	58	6.8	7.46	7.08	6.82
A58E	GLU	58	7.7	7.28	7.54	8.18
A58K	LYS	58	10.4	10.15	11.39	11.62
A58R	ARG	58	>10.4	12.7	12.41	14
A90D	ASP	90	7.5	5.77	6.21	6.23
A90E	GLU	90	6.4	4.77	5.8	5.3
A90K	LYS	90	8.6	8.07	9.28	8.8
A90R	ARG	90	10.5	10.5	13.12	13.92
F34D	ASP	34	7.8	5.06	6.41	5.5
F34E	GLU	34	7.3	5.19	6.45	6.23
F34K	LYS	34	>10.4	8.53	9.45	9.13
F34R	ARG	34	>10.4	11.08	12.22	12.09
I72D	ASP	72	7.6	5.31	7.99	5.87
I72E	GLU	72	7.3	5.48	6.44	6.83
I72R	ARG	72	10.8	10.93	11.95	14
I92D	ASP	92	7.1	6.18	6.69	5.94

I92E	GLU	92	9	6.16	7.87	8.09
I92K	LYS	92	5.3	5.53	6.57	6.29
L103D	ASP	103	8.7	5.84	6.94	5.94
L103E	GLU	103	8.9	6.67	8.11	7.25
L103R	ARG	103	>10.4	9.41	10.4	13.32
L125D	ASP	125	7.6	5.53	6.43	4.25
L125E	GLU	125	9.1	6.17	6.96	7.29
L125R	ARG	125	>10.4	11.15	12.86	12.86
L25D	ASP	25	6.8	5.47	6.56	5.14
L25E	GLU	25	7.5	6.02	7.43	6.57
L25K	LYS	25	6.3	7.41	8.26	7.5
L25R	ARG	25	>10.4	9.75	11.94	11.07
L36D	ASP	36	7.9	4.42	5.81	3.76
L36E	GLU	36	8.7	5.82	7.41	5.29
L36R	ARG	36	>10.4	10.49	12.18	14
L37D	ASP	37	<4	4.39	8.03	6.52
L37E	GLU	37	5.2	5.15	7.42	4.36
L37K	LYS	37	>10.4	10.89	14	10.98
L37R	ARG	37	>10.4	9.49	11.6	11.69
L38D	ASP	38	6.8	5.93	5.81	6.36
L38E	GLU	38	7	6.45	2.77	8
L38K	LYS	38	10.6	10.75	12.32	11.06
L38R	ARG	38	10.4	8.74	11.7	12.18
N118D	ASP	118	7	5.15	7.53	7.01
N118E	GLU	118	<4.5	5.01	5.86	4.98
N118K	LYS	118	>10.4	9.46	11.22	9.47
N118R	ARG	118	>10.4	11.76	12.93	12.01
T62D	ASP	62	8.7	6.44	8.06	7.74
T62E	GLU	62	7.7	6.44	8.12	7.24
T62K	LYS	62	8.1	8.86	10.87	10.18
T62R	ARG	62	>10.4	7.47	10.89	14
V104D	ASP	104	9.7	6.9	5.39	5.86
V104E	GLU	104	9.4	6.65	7.79	7.96
V104K	LYS	104	7.7	8.89	10.56	10.94
V104R	ARG	104	>10.4	10.89	14	13.82
V23D	ASP	23	6.8	4.88	7.14	6.27
V23E	GLU	23	7.1	5.5	6.9	5.17
V23K	LYS	23	7.3	8.01	8.83	8.04
V23R	ARG	23	>10.4	8.8	12.49	12.21
V39D	ASP	39	8.1	5.39	7.07	6.59
V39E	GLU	39	8.2	5.56	6.83	8.15
V39K	LYS	39	9	9.66	12.75	11.12
V39R	ARG	39	>10.4	8.14	13.19	14
V66D	ASP	66	8.7	6	6.53	5.69
V66E	GLU	66	8.5	6.42	7.48	7.04
V66K	LYS	66	8.5	6.03	6.99	7.54
V74D	ASP	74	8.3	5.75	6.02	5.07
V74E	GLU	74	7.8	6.79	3.86	7.57
V74K	LYS	74	7.4	7.42	7.77	8.73
V74R	ARG	74	>10.4	12.5	10.49	12.18
V99D	ASP	99	8.5	5.53	5.12	5.57
V99E	GLU	99	8.4	6.4	7.02	6.59
V99K	LYS	99	6.5	8.32	10.09	9.19

V99R	ARG	99	>10.4	8.21	11.09	13.34
Y91D	ASP	91	7.2	4.34	3.58	2.88
Y91E	GLU	91	7.1	6.28	11.19	6.89
Y91R	ARG	91	>10.4	10.93	13.34	12.6

3. Topology information of nucleic acids

```
#  res atom obtal conf batm batm batm batm
$  A   P      sp3      SD   OP1  OP2  O3'  O5'
$  A   OP1  s          SD   P
$  A   OP2  s          SD   P
$  A   O5'   sp3      SD   P    C5'
$  A   C5'   sp3      SD   O5'  C4'  H5'  H5''
$  A   C4'   sp3      SD   C5'  O4'  C3'  H4'
$  A   O4'   sp3      SD   C4'  C1'
$  A   C3'   sp3      SD   C4'  O3'  C2'  H3'
$  A   O3'   sp3      SD   C3'  P
$  A   C2'   sp3      SD   C3'  O2'  C1'  H2'
$  A   O2'   sp3      SD   C2' HO2'
$  A   C1'   sp3      SD   O4'  C2'  N9   H1'
$  A   N9    sp2      SD   C1'  C8   C4
$  A   C8    sp2      SD   N9   N7   H8
$  A   N7    sp2      SD   C8   C5
$  A   C5    sp2      SD   N7   C6   C4
$  A   C6    sp2      SD   C5   N6   N1
$  A   N6    sp2      SD   C6   H61  H62
$  A   N1    sp2      SD   C6   C2   H1
$  A   C2    sp2      SD   N1   N3   H2
$  A   N3    sp2      SD   C2   C4
$  A   C4    sp2      SD   N9   C5   N3
$  A   H5'   s        SD   C5'
$  A   H5''  s        SD   C5'
$  A   H4'   s        SD   C4'
$  A   H3'   s        SD   C3'
$  A   H2'   s        SD   C2'
$  A  HO2' s          SD   O2'
$  A   H1'   s        SD   C1'
$  A   H8    s        SD   C8
$  A   H61  s         SD   N6
$  A   H62  s         SD   N6
$  A   H2    s        SD   C2
$  A   H1    s        SD   N1
```

```
#  res atom obtal conf batm batm batm batm
$  C   P    sp3   SD   O5'  OP1  OP2  O3'
$  C   OP1  s     SD   P
$  C   OP2  s     SD   P
$  C   C5'  sp3   SD   C4'  O5'  H5'  H5''
```

```
$  C   O5'  sp3   SD   C5'  P
$  C   C4'  sp3   SD   C3'  O4'  C5'  H4'
$  C   O4'  sp3   SD   C1'  C4'
$  C   C3'  sp3   SD   C2'  C4'  O3'  H3'
$  C   O3'  sp3   SD   C3'  P
$  C   C2'  sp3   SD   C1'  O2'  C3'  H2'
$  C   O2'  sp3   SD   C2' HO2'
$  C   C1'  sp3   SD   N1   C2'  O4'  H1'
$  C   N1   sp2   SD   C2   C6   C1'
$  C   C2   sp2   SD   N1   N3   O2
$  C   N3   sp2   SD   C2   C4   H3
$  C   C4   sp2   SD   N3   C5   N4
$  C   C5   sp2   SD   C4   C6   H5
$  C   C6   sp2   SD   N1   C5   H6
$  C   O2   s    SD   C2
$  C   N4   sp2   SD   C4   H41  H42
$  C   H1'  s    SD   C1'
$  C   H2'  s    SD   C2'
$  C   H3'  s    SD   C3'
$  C   H4'  s    SD   C4'
$  C  HO2'  s    SD   O2'
$  C   H5'  s    SD   C5'
$  C  H5''  s    SD   C5'
$  C   H41  s    SD   N4
$  C   H42  s    SD   N4
$  C   H3   s    SD   N3
$  C   H5   s    SD   C5
$  C   H6   s    SD   C6


#  res atom obtal conf batm batm batm batm
$  G   P    sp3  SD   OP1  OP2  O3'  O5'
$  G   OP1  s    SD   P
$  G   OP2  s    SD   P
$  G   O5'  sp3   SD   P    C5'
$  G   C5'  sp3   SD   O5'  C4'  H5'  H5''
$  G   C4'  sp3   SD   C5'  O4'  C3'  H4'
$  G   O4'  sp3   SD   C4'  C1'
$  G   C3'  sp3   SD   C4'  O3'  C2'  H3'
$  G   O3'  sp3   SD   C3'  P
$  G   C2'  sp3   SD   C3'  O2'  C1'  H2'
$  G   O2'  sp3   SD   C2' HO2'
$  G   C1'  sp3   SD   O4'  C2'  N9   H1'
$  G   N9   sp2   SD   C1'  C8   C4
```

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$  G   C8   sp2   SD   N9   N7   H8
$  G   N7   sp2   SD   C8   C5
$  G   C5   sp2   SD   N7   C6   C4
$  G   C6   sp2   SD   C5   O6   N1
$  G   O6   s     SD   C6
$  G   N1   sp2   SD   C6   C2   H1
$  G   C2   sp2   SD   N1   N3   N3
$  G   N2   sp2   SD   C2   H21  H22
$  G   N3   sp2   SD   C2   C4
$  G   C4   sp2   SD   N9   C5   N3
$  G   H1'  s     SD   C1'
$  G   H2'  s     SD   C2'
$  G   H3'  s     SD   C3'
$  G   H4'  s     SD   C4'
$  G  HO2'  s     SD   O2'
$  G   H5'  s     SD   C5'
$  G  H5''  s     SD   C5'
$  G   H8   s     SD   C8
$  G   H1   s     SD   N1
$  G   H21  s     SD   N2
$  G   H22  s     SD   N2


#  res atom obtal conf batm batm batm batm
$  U   P    sp3   SD   O5'  OP1  OP2  O3'
$  U   OP1  s     SD   P
$  U   OP2  s     SD   P
$  U   O5'  sp3   SD   C5'  P
$  U   C5'  sp3   SD   C4'  O5'  H5'  H5''
$  U   C4'  sp3   SD   C3'  O4'  C5'  H4'
$  U   O4'  sp3   SD   C1'  C4'
$  U   C3'  sp3   SD   C2'  C4'  O3'  H3'
$  U   O3'  sp3   SD   C3'  P
$  U   C2'  sp3   SD   C1'  C3'  O2'  H2'
$  U   O2'  sp3   SD   C2' HO2'
$  U   C1'  sp3   SD   N1   C2'  O4'  H1'
$  U   N1   sp2   SD   C2   C6   C1'
$  U   C2   sp2   SD   N1   N3   O2
$  U   N3   sp2   SD   C2   C4   H3
$  U   C4   sp2   SD   N3   C5   O4
$  U   C5   sp2   SD   C4   C6   H5
$  U   C6   sp2   SD   N1   C5   H6
$  U   O2   s     SD   C2
$  U   O4   s     SD   C4
```

```
$  U   H1'  s    SD   C1'
$  U   H2'  s    SD   C2'
$  U  HO2'  s    SD   O2'
$  U   H3'  s    SD   C3'
$  U   H4'  s    SD   C4'
$  U   H5'  s    SD   C5'
$  U  H5''  s    SD   C5'
$  U   H3   s    SD   N3
$  U   H5   s    SD   C5
$  U   H6   s    SD   C6
```