

Table S1: Conformational searching through flexible models. The table presents the lower χ^2 found for each one of the 14 model constructions.

Loop interactions removed	Agreement between curves		
	pH 4	pH 6	pH 8
	<i>lowest χ^2</i>		
Shadow	6.1	11.9	3.2
1	2.5	2.9	3.2
2	8.3	10.4	3.2
3	8.1	10.5	3.2
4	7.3	9.4	3.2
1 and 2	6.8	9.2	3.2
1 and 3	5.4	7.3	3.2
1 and 4	5.5	8.5	3.2
2 and 3	8.4	9.3	3.2
2 and 4	8.1	10	3.2
3 and 4	7.8	10.3	3.2
1, 2 and 3	5.7	7.7	3.2
1, 2 and 4	5.7	7.3	3.2
1, 3 and 4	5.3	7	3.2
2, 3 and 4	7.2	9.1	3.2
1, 2, 3 and 4	5.5	6.4	3.2
Reference (PDB id: 3PZ9)	11.9	18.9	3.2