Supplementary Tables

Table 1. Evaluation of the interpolation methods.

System	Feature Vectors	Resolution of Map	Rigid Body Registration		Constrained MD	Splines									IDW					
						TPS			EBS Kernel 1†			EBS Kernel 2†			Global‡			Local§		
			RMSD	CC	CC	RMSD	CC	Time	RMSD	CC	Time	RMSD	CC	Time	RMSD	CC	Time	RMSD	CC	Time
RNAP	15	15	6.65	0.86	0.88	3.17	0.88	0.3	3.83	0.87	1.0	3.26	0.88	1.0	1.81	0.88	0.2	1.79	0.88	0.3
GroEL	112	14	6.11	0.96	0.96	4.01	0.93	5.3	3.34	0.96	21.0	3.70	0.97	21.0	2.75	0.95	3.3	2.71	0.95	3.7
Myosin	10	14	5.27	0.91	0.95	2.36	0.94	0.1	1.93	0.94	0.3	2.16	0.94	0.3	1.87	0.94	0.1	1.80	0.95	0.1

Map resolution shown in Å. RMSD measures the C_α root-mean squared deviation (in Å) between interpolation-based model and constrained MD-based model. CC represents the cross-correlation coefficient to the experimental map.† elasticity coefficient $\nu = 0.5$. ‡ weighting power $c = 8$. § weighting power $c = 4$, and the radius of influence R encompassing nine feature vectors. Time represents the execution time (in seconds) on an Intel Core 2 duo, 2.4GHz, with 4GB RAM.

Table 2. Parameter robustness of IDW and effect of stereochemical idealization. C_α RMSD in Å.

System	Test 1†	Test 2‡	Test 3§	RefMac∗
RNAP	1.81	1.81	1.82	1.66
GroEL	2.82	2.73	2.75	2.49
Myosin	1.82	1.82	1.87	1.71

† Local IDW, R holding 60% vectors, c set from 3-4 in 0.2 increments (average RMSD). ‡ Local IDW, R holding 50-90% vectors in 10% increments, c = 3.5 (average RMSD). § Global IDW, c set from 7-9 in 0.4 increments (average RMSD). ∗ Local IDW, R holding 9 vectors and $c = 4$, post-processed with 20 iterations of RefMac (see text). The RMSD values are nearly identical to the values given in Supplementary Table 1.