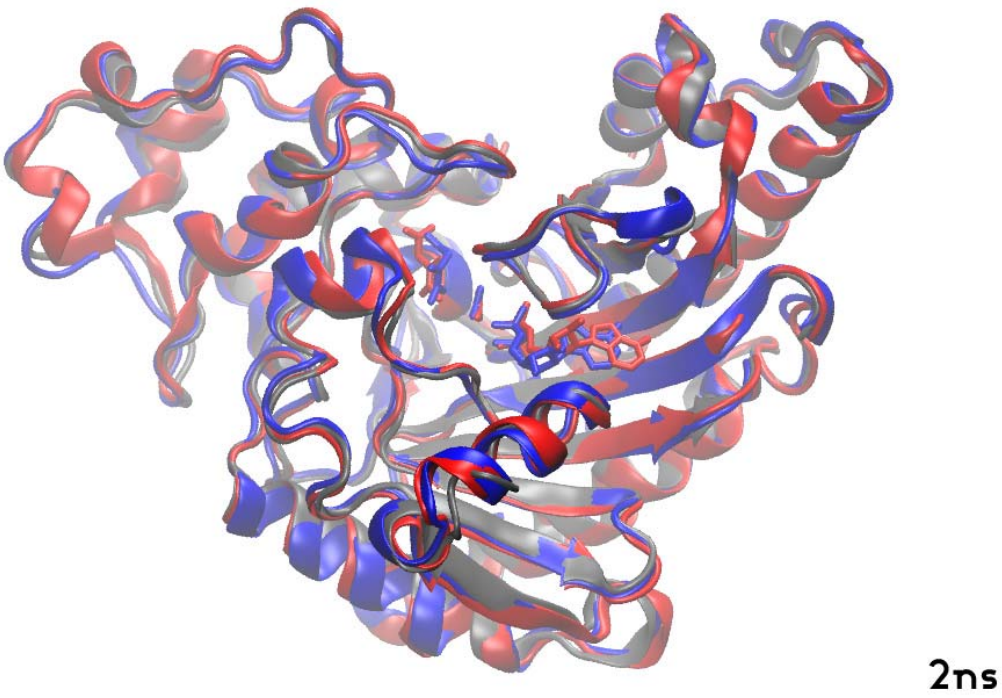
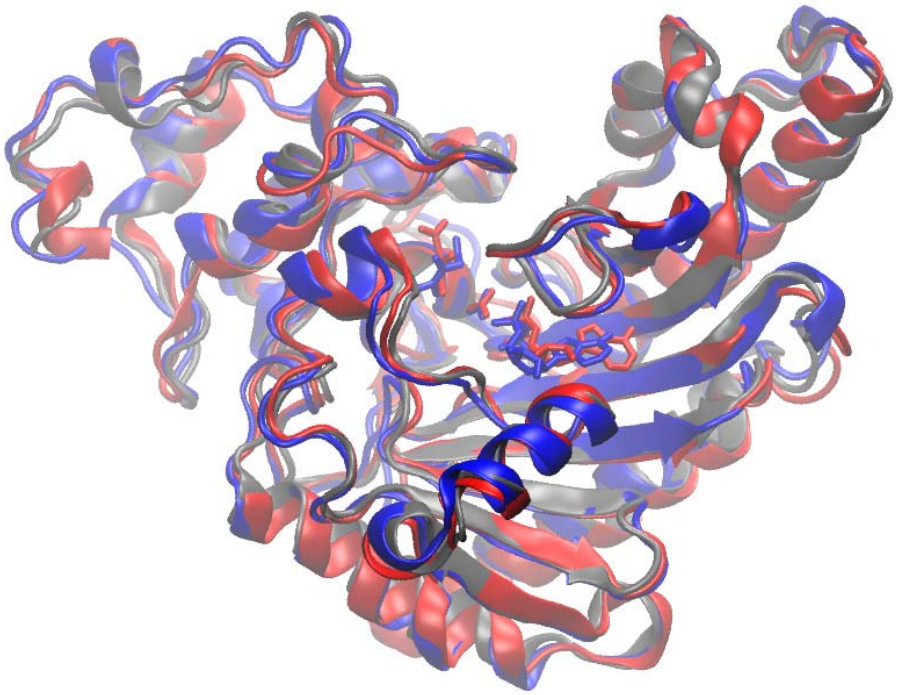
Table 1. Force Field Parameters Developed For Creatine.

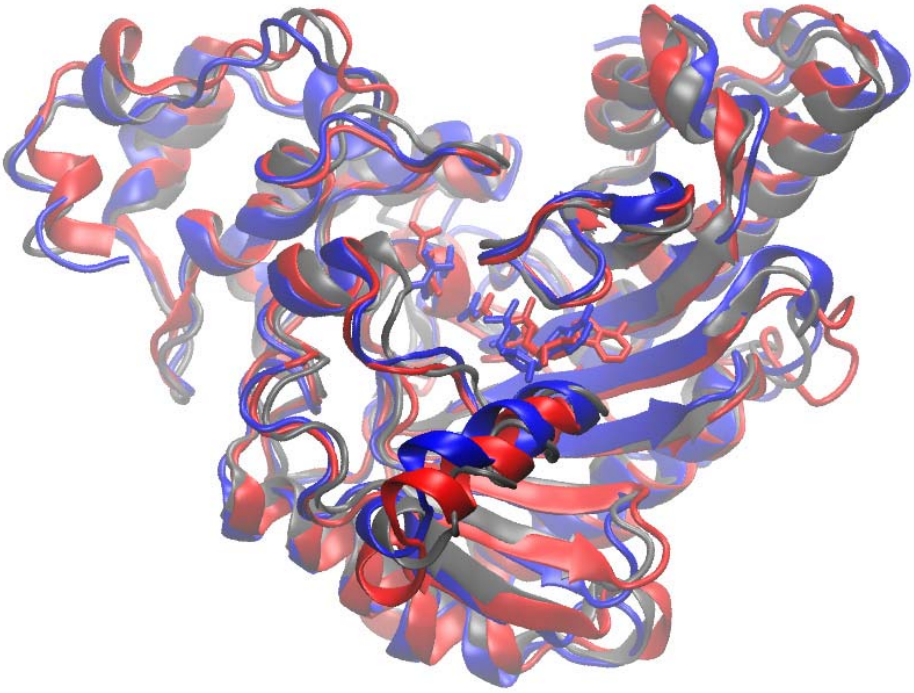
Atom Name	X	Y	Z	Atom Type	Atomic Charge
NA	2.686	0.285	0.437	na	-0.7483
CA	1.599	0.329	0.031	c2	0.5405
NB	1.603	1.675	0.018	na	-0.7483
NC	0.563	0.362	0.477	na	-0.1644
CB	0.557	1.825	0.397	c3	-0.3069
CC	0.811	0.348	0.719	c3	0.0076
CD	2.003	0.128	0.185	c	0.6312
O1	1.812	0.262	1.369	o	-0.6487
02	3.136	0.356	0.302	o	-0.6487
H1	0.317	2.407	0.772	h1	0.1437
H2	1.475	2.207	0.901	h1	0.1437
H3	0.744	2.118	0.663	h1	0.1437
H4	2.683	1.388	0.426	hn	0.3978
H5	3.551	0.291	0.808	hn	0.3978
H6	0.704	2.183	0.405	hn	0.3978
H7	2.468	2.251	0.353	h1	0.3978
H8	-0.620	1.446	0.767	h1	0.0318
H9	-1.130	-0.120	1.763	h1	0.0318

FIGURE 1: Snapshots of creatine kinase sampled during the MD simulations are shown as colored ribbon diagrams (red: Cys283-anion; blue: Cys283-neutral). These are superimposed on the crystal conformation of CK-TSAC (gray). The TSAC is shown in licorice. The time at which the snapshots were taken accompany the figures.

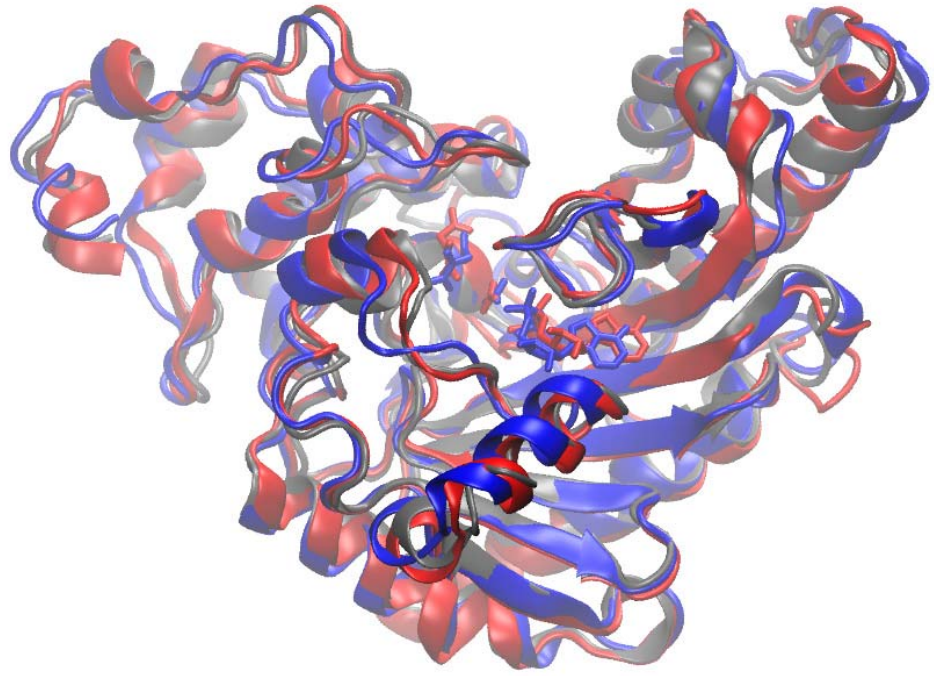




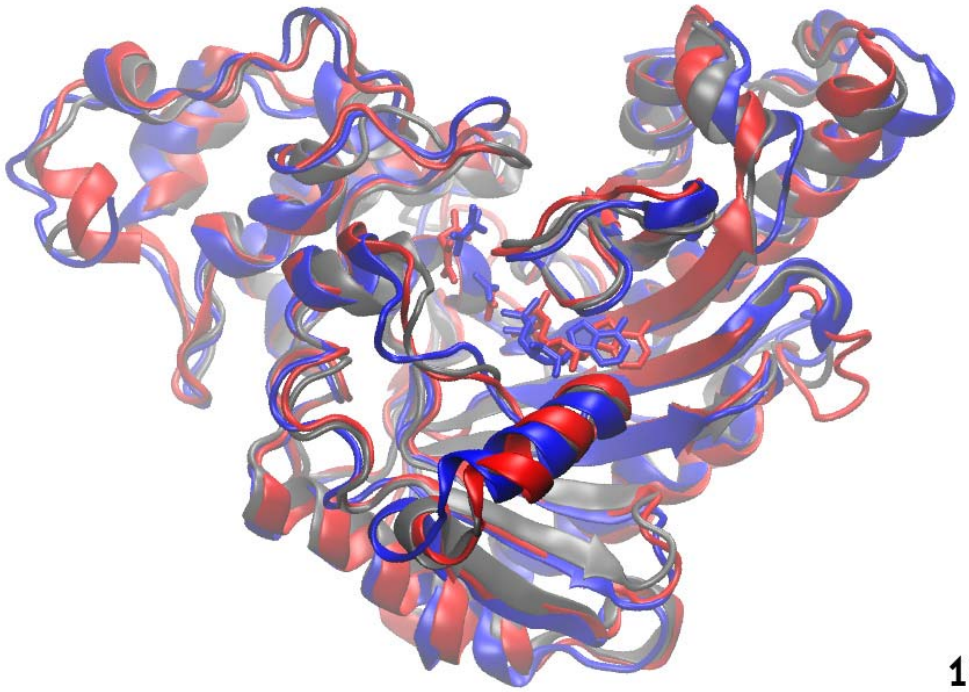
4ns



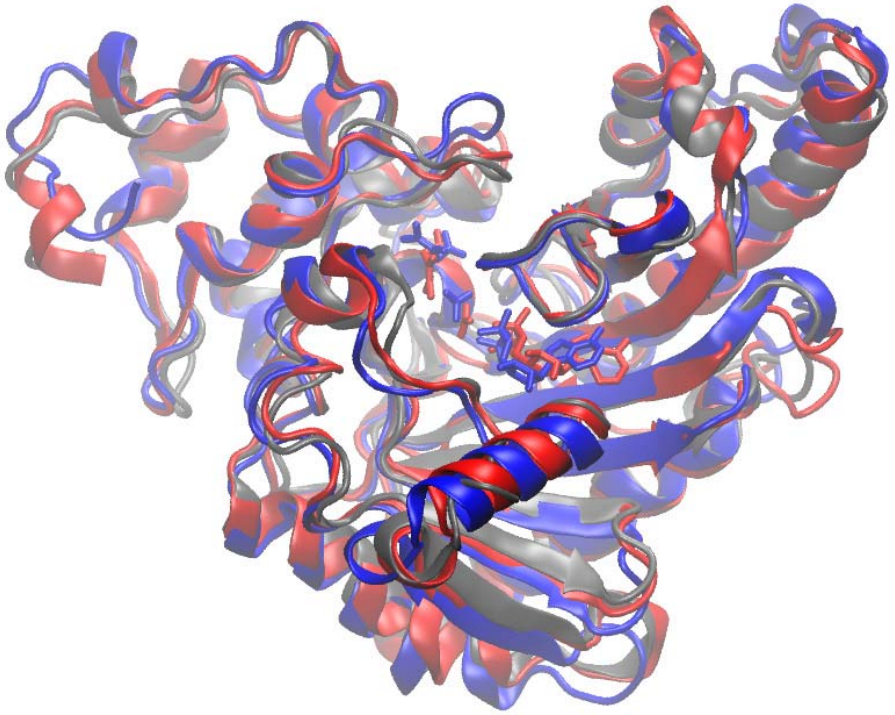
6ns



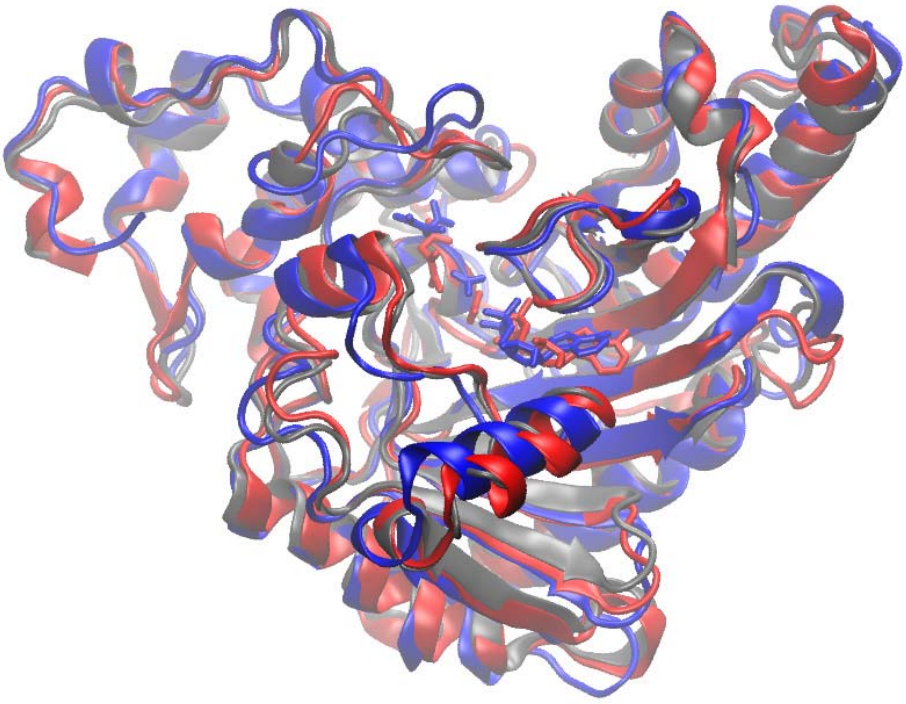
8ns



10ns



12ns



14ns