Figure 1. Buried solvent-accessible surface (SAS) area of individual residues from both the p66 and p51 subunits of HIV-1 RT upon dimerization. For clarity only those amino acids that bury more than 60 $Å^2$ of SAS are displayed.

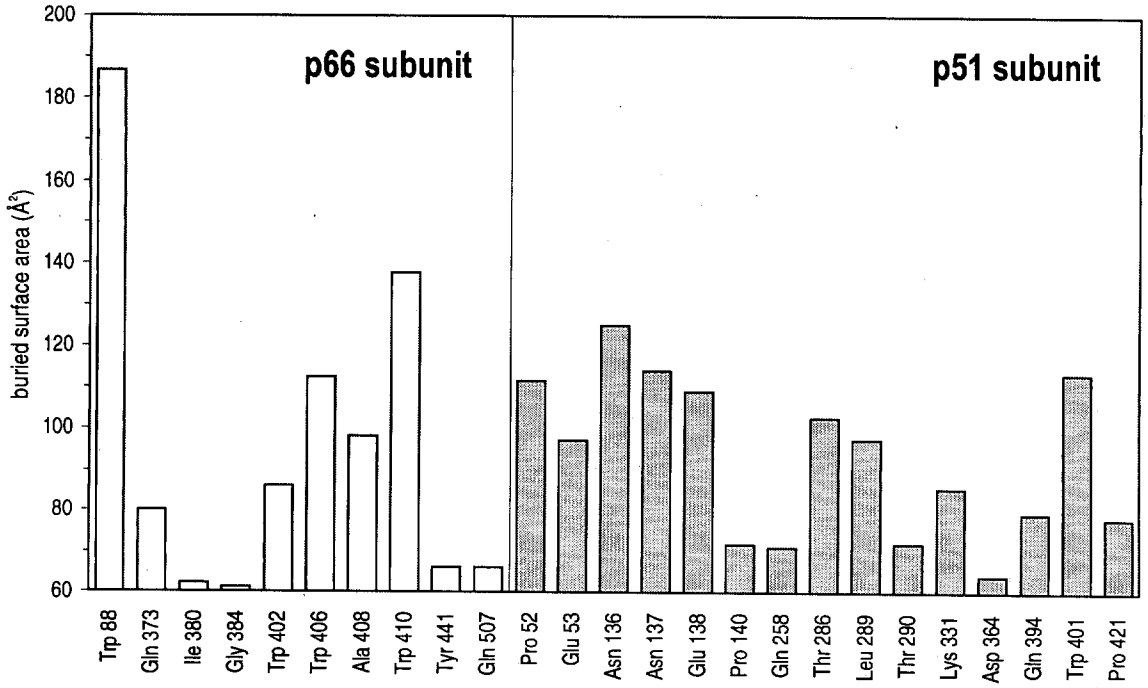


Figure 2A. van der Waals (AMBER) and electrostatic (DelPhi) contributions of the p51 subunit to the dimerization energy of wild-type and E138K HIV-1 RT of amino acid residues comprising or near the β7-β8 loop.

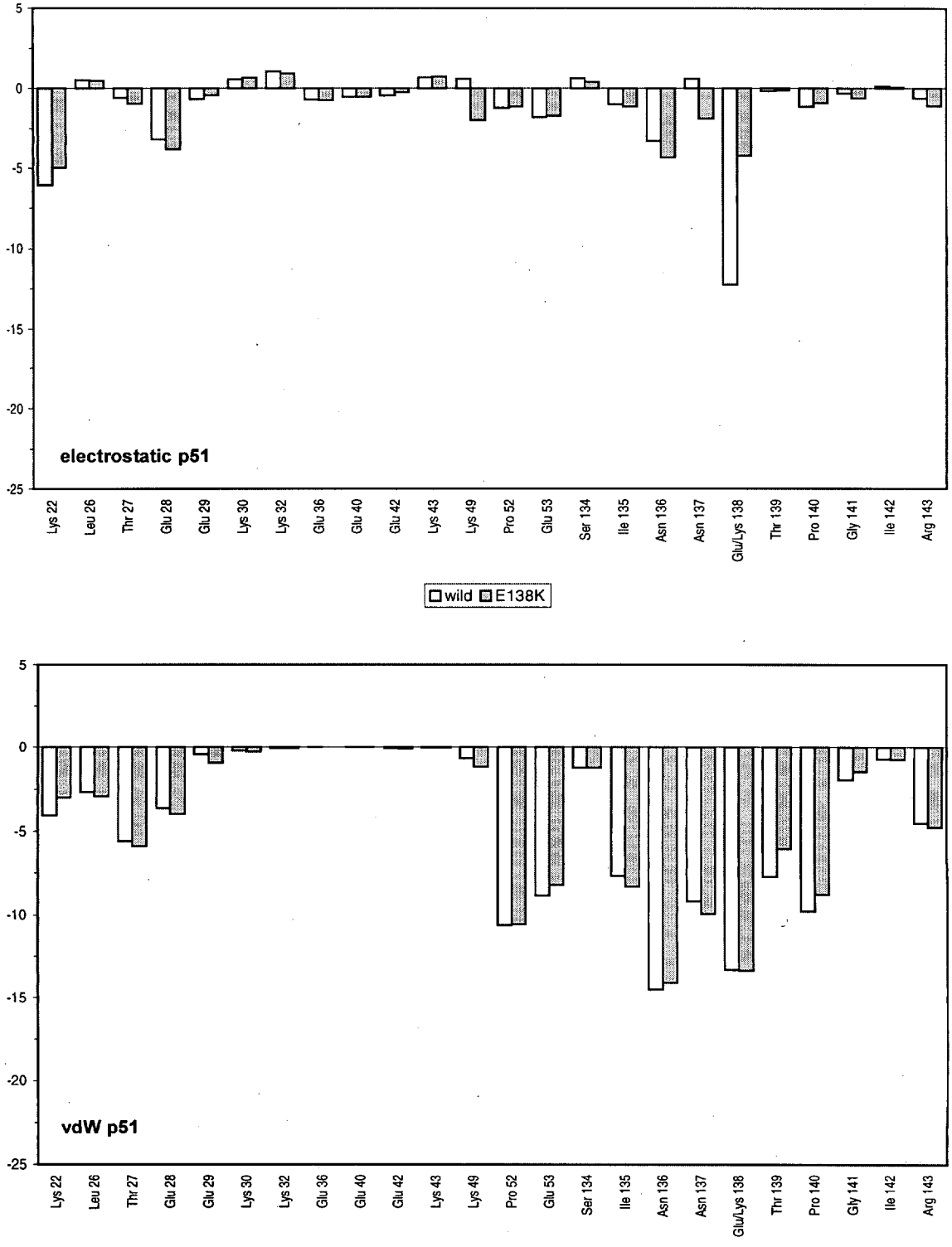


Figure 2B. van der Waals (AMBER) and electrostatic (DelPhi) contributions of the p66 subunit to the dimerization energy of wild-type and E138K HIV-1 RT of amino acid residues comprising or near the β7-β8 loop.

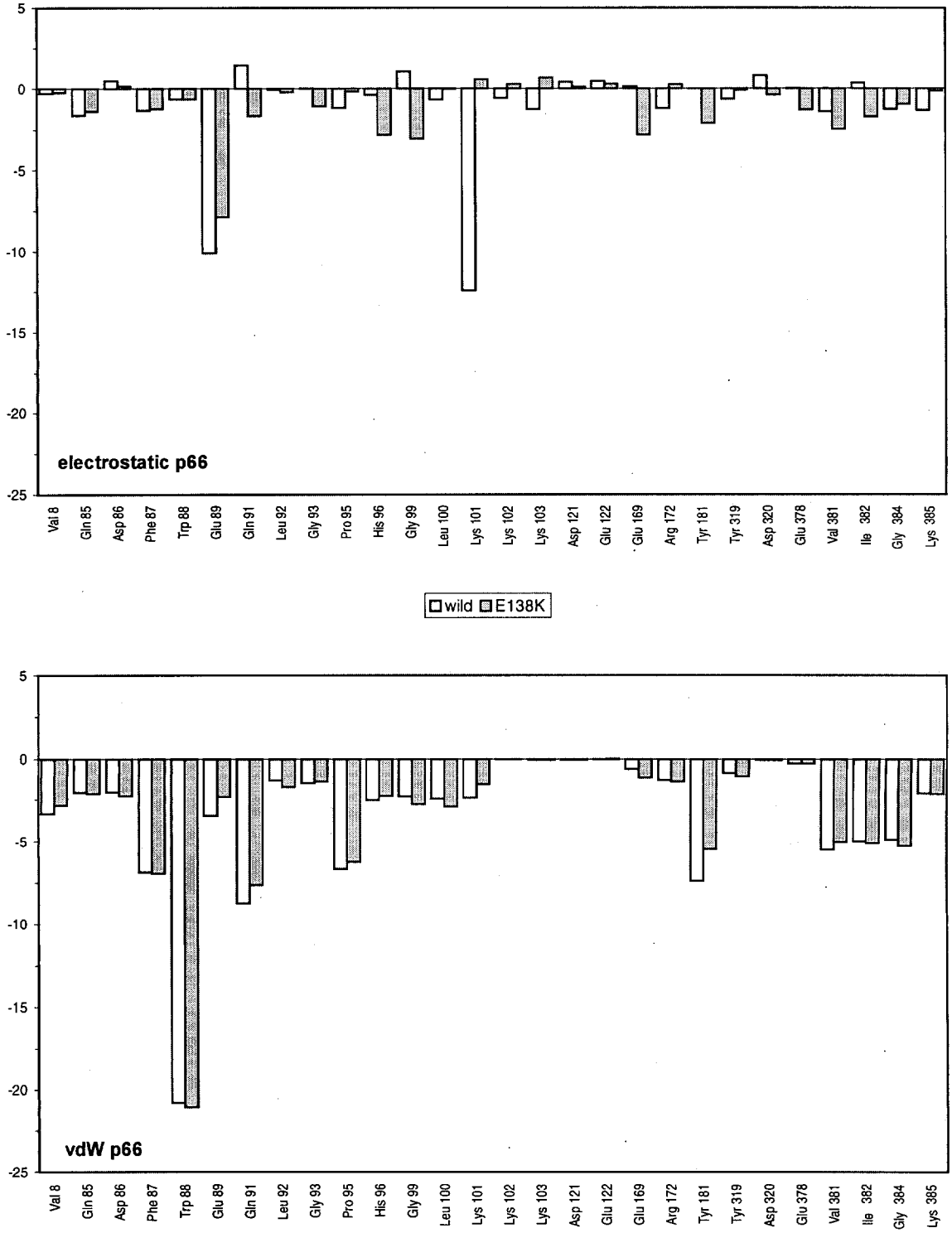


Figure 3. Time evolution of the root-mean-square deviation of peptide backbone atoms from the corresponding refined initial structure along the MD trajectories for wild-type RT with (thick line) and without (thin line) bound TSAO-m^{3}T.

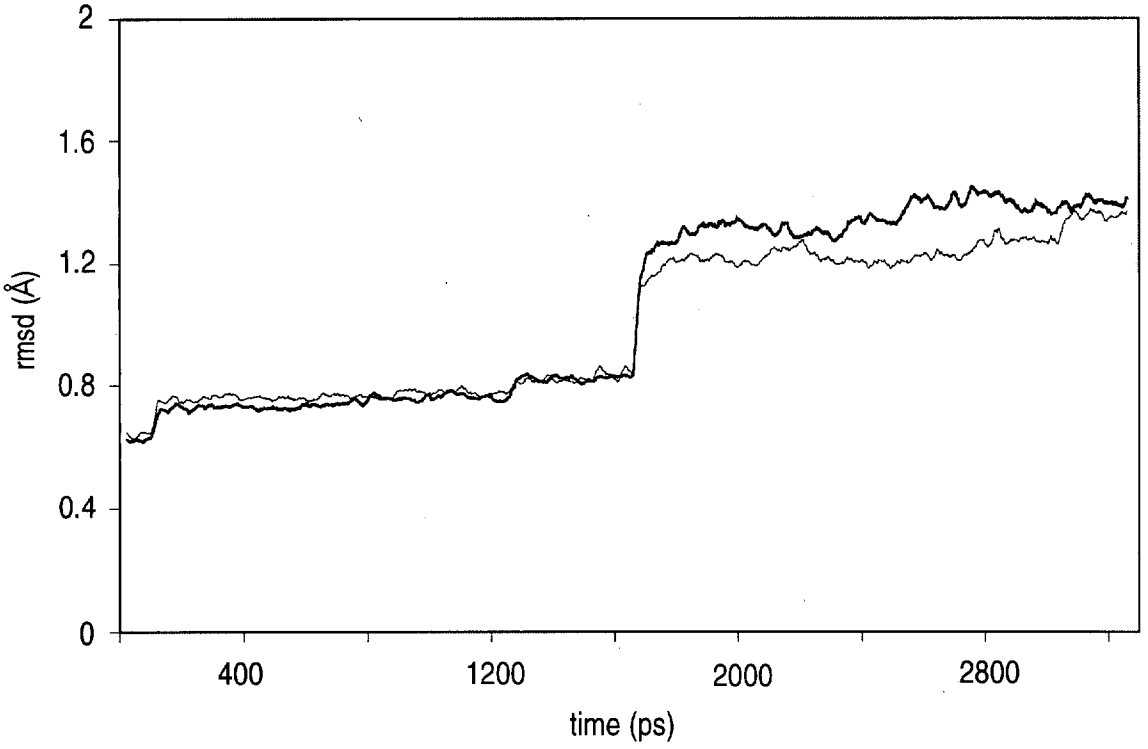


Figure 4. MEP difference map calculated between wild-type and R172A RT enzymes in aqueous solution at physiological pH. The MEP calculated for the R172A mutant was subtracted from that obtained for the wild-type enzyme to determine regions where the electrostatic potential differs between the two molecules. The region where this difference was equal to or greater than 2.5 kcal mol^{-1} appears delineated by a blue contour map. For reference, the GluB138 residue is displayed as sticks.

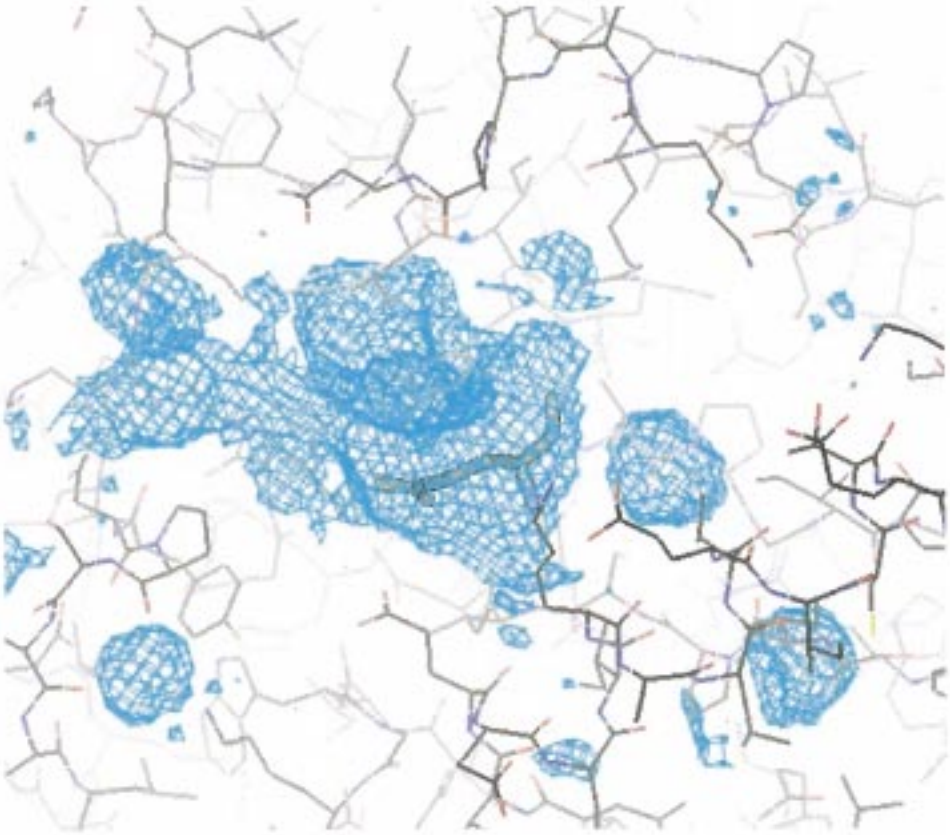
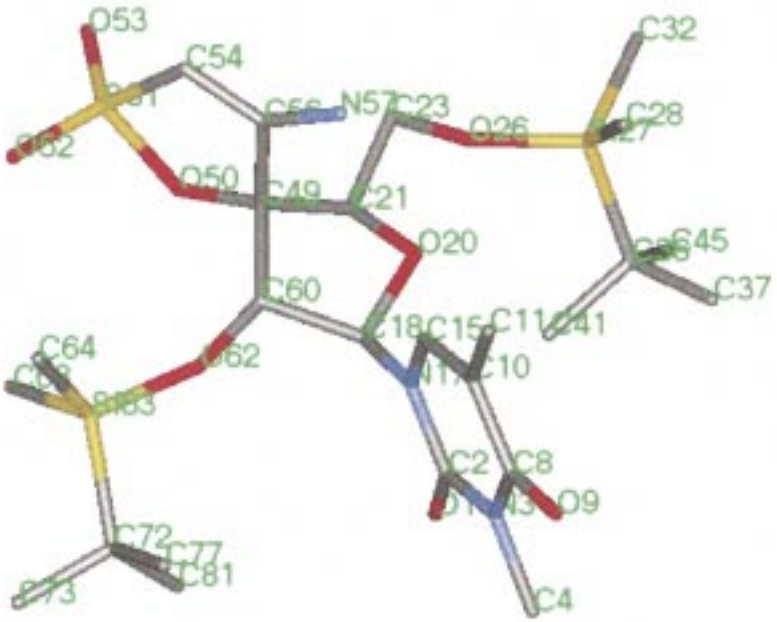


Table 1. Atomic charges for TSAO-m^{3}T.



O1	-0.470	H22	0.158	H43	0.023	C64	-0.053
C2	0.348	C23	0.047	H44	0.023	H65	0.004
N3	-0.037	H24	0.106	C45	-0.119	H66	0.004
C4	-0.081	H25	0.106	H46	0.023	H67	0.004
H5	0.074	O26	-0.454	H47	0.023	C68	-0.053
H6	0.074	SI27	0.613	H48	0.023	H69	0.004
H7	0.074	C28	-0.197	C49	0.012	H70	0.004
C8	0.435	H29	0.021	O50	-0.184	H71	0.004
O9	-0.485	H30	0.021	S51	0.826	C72	0.204
C10	0.003	H31	0.021	O52	-0.451	C73	-0.096
C11	-0.154	C32	-0.197	O53	-0.451	H74	0.008
H12	0.066	H33	0.021	C54	-0.308	H75	0.008
H13	0.066	H34	0.021	H55	0.233	H76	0.008
H14	0.066	H35	0.021	C56	0.060	C77	-0.096
C15	-0.276	C36	0.064	N57	-0.627	H78	0.008
H16	0.201	C37	-0.119	H58	0.379	H79	0.008
N17	0.032	H38	0.023	H59	0.312	H80	0.008
C18	-0.007	H39	0.023	C60	0.010	C81	-0.096
H19	0.168	H40	0.023	H61	0.178	H82	0.008
O20	-0.194	C41	-0.119	O62	-0.308	H83	0.008
C21	-0.019	H42	0.023	SI63	0.301	H84	0.008