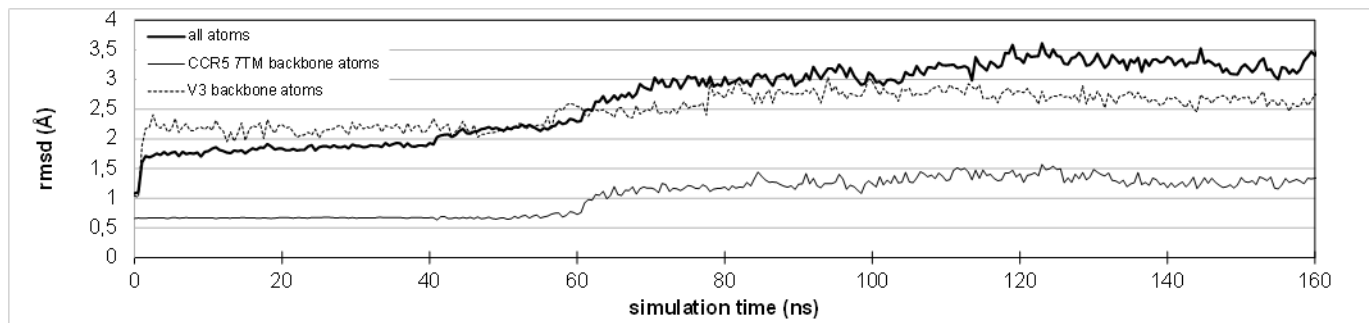


Additional file 7



Time (ns)	1-20	20-40	40-60	60-80	80-100	100-160
Constraints (10 kcal/mol.Å²)						
CCR5: ECL2 & N-terminus						
CCR5: ICL1-3, ECL1, ECL3, C-terminus	all	bb				
CCR5: 7TM	all	all	bb			
V3 tip: residues P308-R313	all					
V3 bridging sheet: C296 & C330	bb	bb	bb	bb	bb	bb
Restraints (distances and angles)						
CCR5 N-terminus – V3 base: Y10(OSO ₃ ⁻) – R326(guanidinium), Y14(OSO ₃ ⁻) – R298(guanidinium), N302(CONH ₂), T303(OH)	sc	sc	sc	sc	sc	sc
Intra V3 base: T297(NH) – H329(CO), T297(CO) – H329(NH)	bb	bb	bb	bb	bb	bb
CCR5 TM7 – V3 tip: E283 (COO ⁻) – R313(guanidinium)	sc	sc	sc	sc	sc	
CCR5 ECL2 – V3 tip: S180(CO) – A314(NH) F182(CO) – Y316 (NH) F182(NH) – A314(CO)	bb	bb	bb	bb	bb	
Intra V3 tip: P308(CO) – F315(NH)	bb	bb	bb	bb		