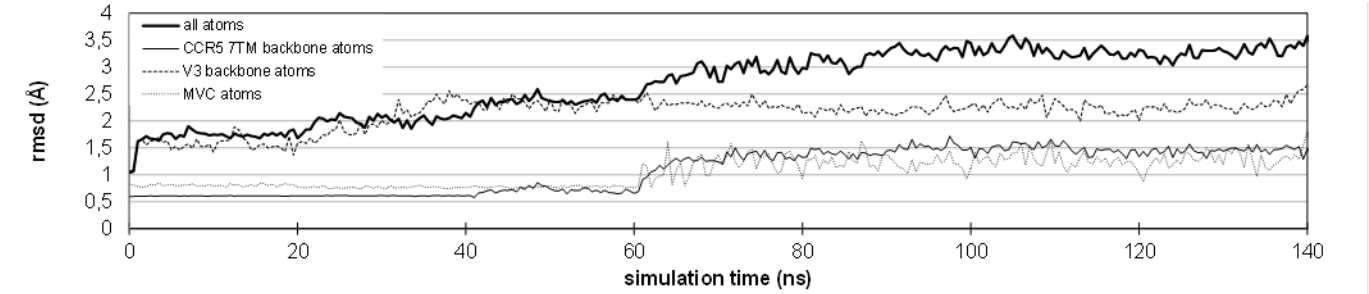
Additional file 8



Time (ns)	1-20	20-40	40-60	60-80	80-140
Contraints (10 kcal/mol.Å²)					
CCR5: ICL1-3, ECL1, ECL3, C-terminus	all	bb			
CCR5: 7TM	all	all	bb		
V3 tip: residues S308-R313					
V3 bridging sheet: C296 & C330	bb	bb	bb	bb	bb
MVC	all	all	all		
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
Intra V3 base: T297(NH) – H329(CO), T297(CO) – H329(NH)	bb	bb	bb	bb	bb
CCR5 TM7 – V3 tip: E283 (COO^-) – R313(guadinidium)					
CCR5 ECL2 – V3 tip: S180(CO) – A314(NH) F182(CO) – Y316 (NH) F182(NH) – A314(CO)	bb	bb	bb	bb	
Intra V3 tip: S308(NH) – F315(CO) S308(CO) – F315(NH)	bb	bb	bb		