



Difference of RMSD ( $\Delta\text{RMSD}$ ) between holo and apo D130V-Eg5 backbone atoms, **b**) difference of RMSF ( $\Delta\text{RMSF}$ ) between holo and apo D130V-Eg5 C $\alpha$  atoms, **c**) difference of radius of gyration ( $\Delta\text{Rg}$ ) between holo and apo D130V-Eg5 backbone atoms and **d**) difference in number of intramolecular H-bonds ( $\Delta\text{N}$ ) between holo and apo D130V-Eg5 structures; (*R*)-2/D130V-Eg5 (Blue), (*R*)-4/D130V-Eg5 (violet), (*R*)-5/D130V-Eg5 (green) and monastrol/D130V (red)