

Table S2: Residues within a 5 Å shell (of retinal with Schiff base bond formed) which interact more favorably than an interaction energy of –1 kcal/mol with the ligand are shown in order of decreasing interaction. The interaction energy values are shown in parentheses.

Ret(xtal)/closed(xtal)	Ret(HD)/closed(xtal)	Ret(HD)/closed(MS)
Glu122 (-21.9)	Glu122 (-19.8)	Glu122 (-18.2)
Glu113 (-20.3)	Glu113 (-18.0)	Thr118 (-4.0)
Glu181 (-18.0)	Glu181 (-14.9)	Tyr268 (-4.0)
Trp265 (-6.5)	Trp265 (-6.8)	Phe208 (-3.2)
Tyr268 (-4.8)	Thr118 (-5.2)	Met207 (-1.2)
Thr118 (-3.9)	Tyr268 (-5.2)	Trp265 (-1.1)
Ala292 (-2.9)	Met207 (-2.7)	Gly114 (-1.1)
Ala117 (-2.3)	Ala292 (-2.3)	Ala269 (-1.1)
Phe208 (-2.0)	Phe212 (-1.9)	Phe212 (-1.0)
His211 (-1.8)	Phe208 (-1.8)	Ile275 (-1.0)
Phe212 (-1.7)	Gly114 (-1.8)	
Gly114 (-1.6)	Cys187 (-1.3)	
Met207 (-1.6)	Phe261 (-1.2)	
Phe261 (-1.4)	Ala269 (-1.2)	
Phe293 (-1.1)		