

# of poses with estimated free energy between -8.3 and -7.8 kcal/mol= 8

# of poses with estimated free energy between -7.8 and -7.3 kcal/mol= 53

-8.3 m= 23 5669377-1 # 13254 MW= 237 HBd= 4 HBa= 6 t= 7 NO2=1 r=1

Pose 84 nHB= 5 q= 0.0 pa: HH 497 TYR 82 Rbs= 0.0 F:H4C3CA6N3O3C11

Contact: L 12 O15 - 496 OH 82 TYR|L 15 N14 - 740 OE2 107 GLU

Contact: L 20 O8 - 69 1HH1 38 ARG|

Smallest and largest contact distance= 1.9 and 2.7 A