# 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 Å