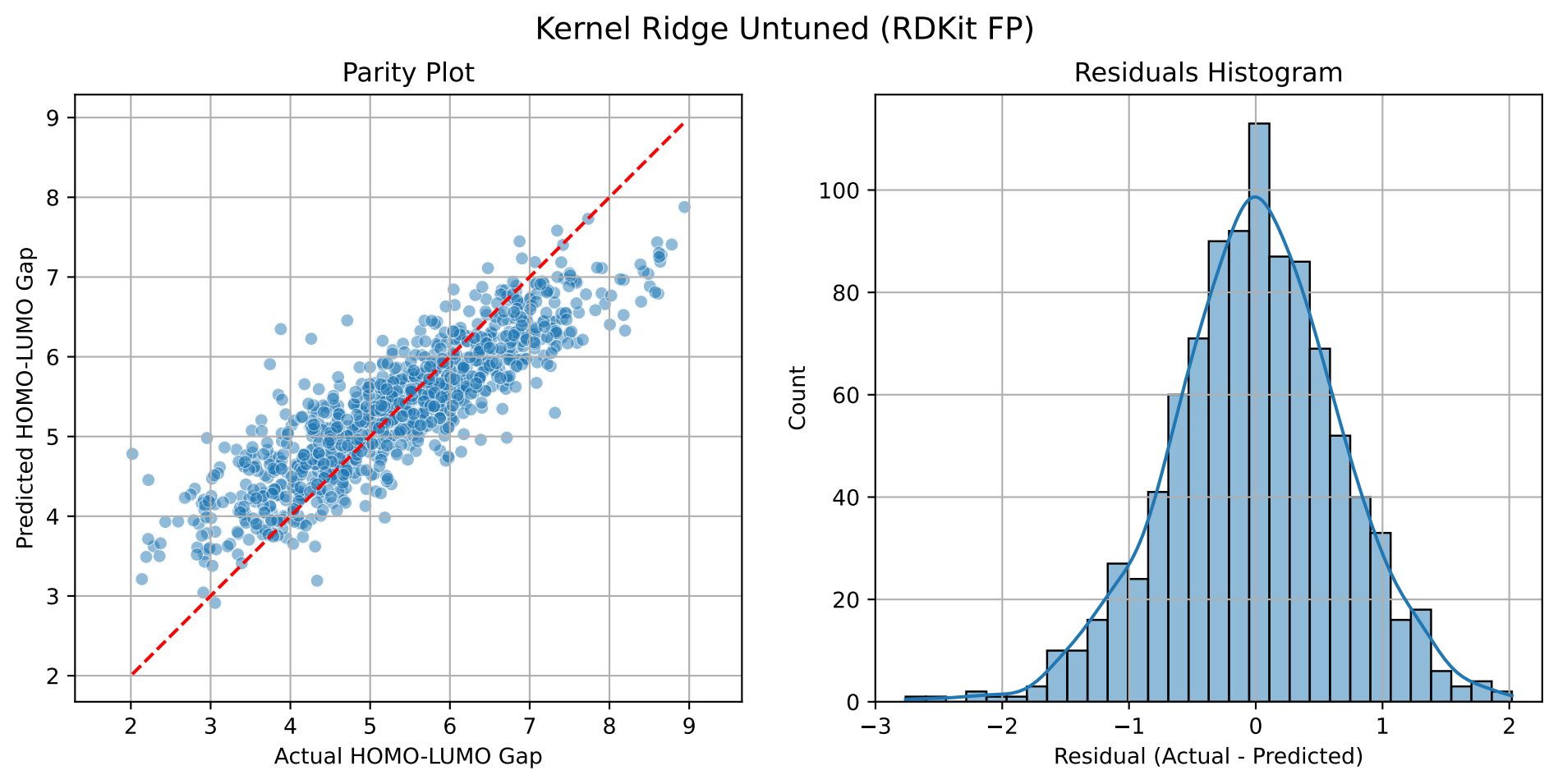
Kernel Ridge Untuned (RDKit FP)
Parity Plot
Predicted HOMO-LUMO Gap
Actual HOMO-LUMO Gap
2
3
4
5
6
7
8
9
Residuals Histogram
Count
Residual (Actual - Predicted)
0
20
40
60
80
100
−3
−2
−1
0
1
2