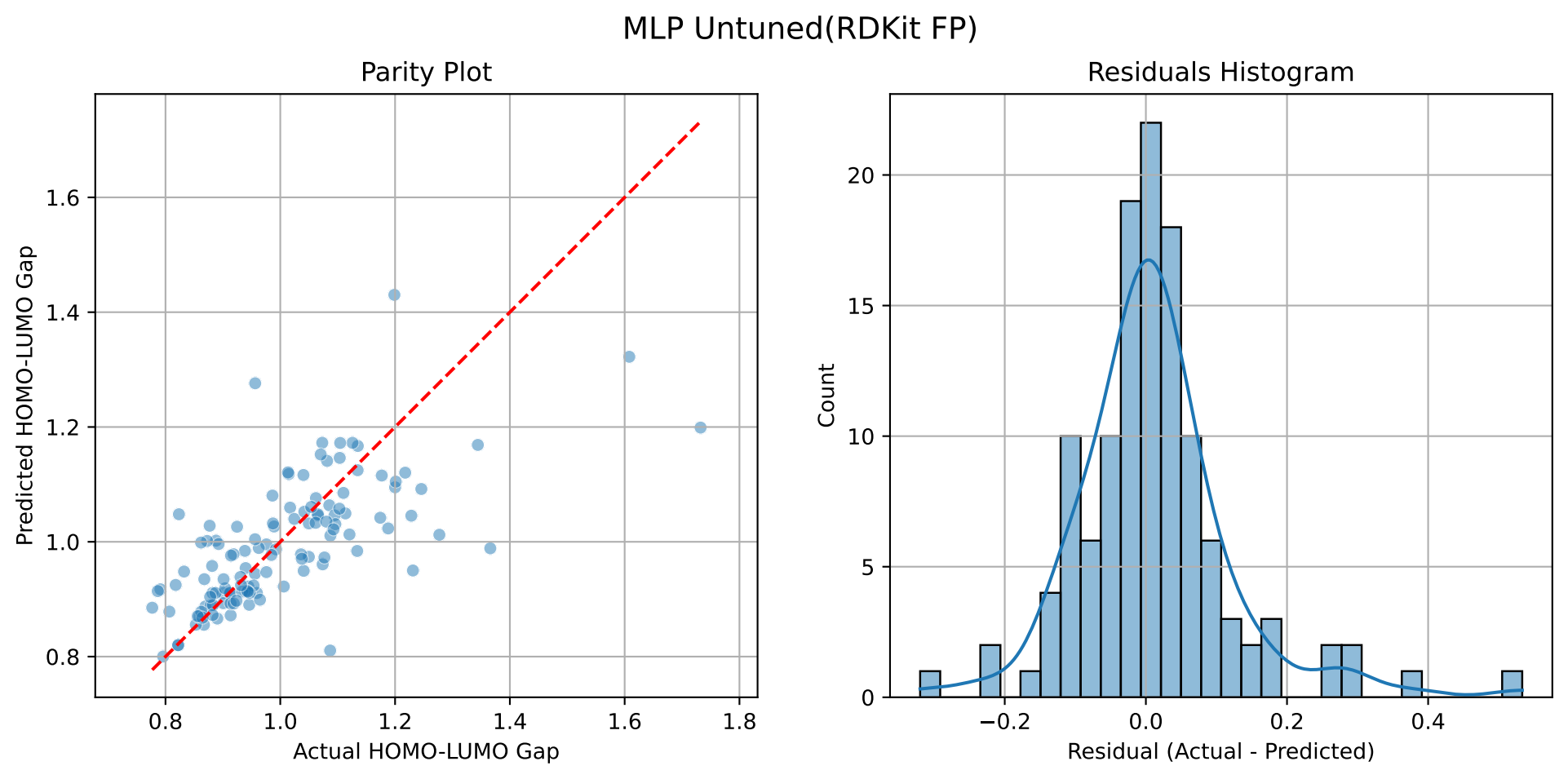
MLP Untuned(RDKit FP)
Parity Plot
Predicted HOMO-LUMO Gap
Actual HOMO-LUMO Gap
0.8
1.0
1.2
1.4
1.6
1.8
Residuals Histogram
Count
Residual (Actual - Predicted)
0
5
10
15
20
−0.2
0.0
0.2
0.4