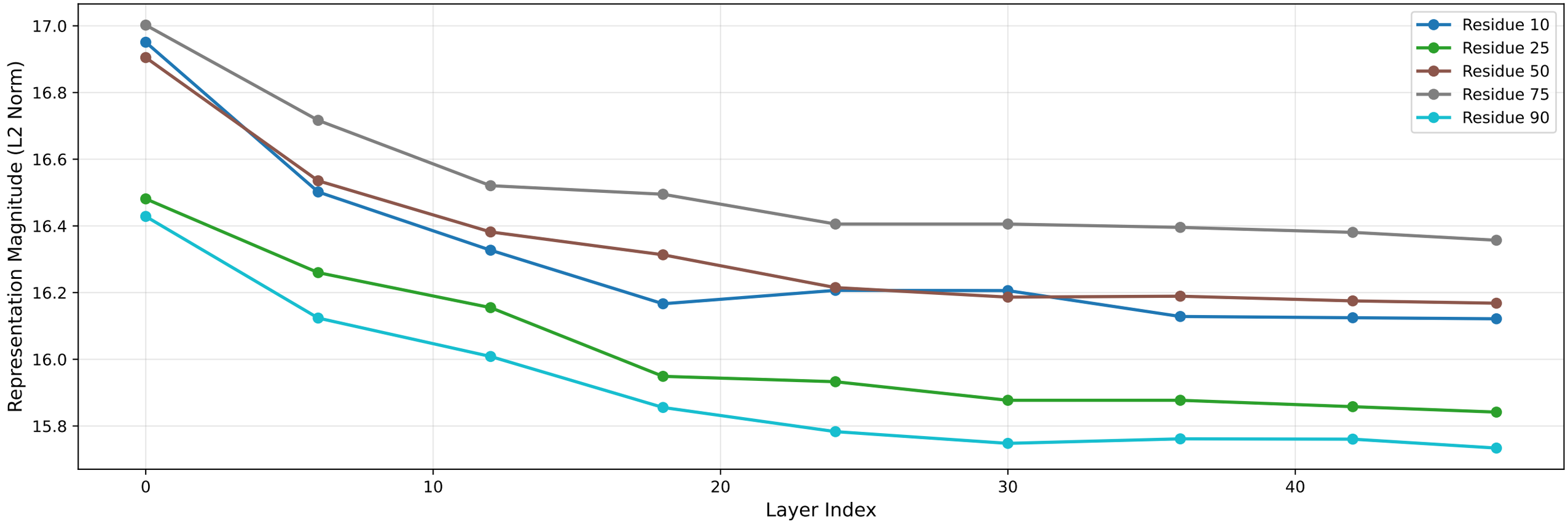
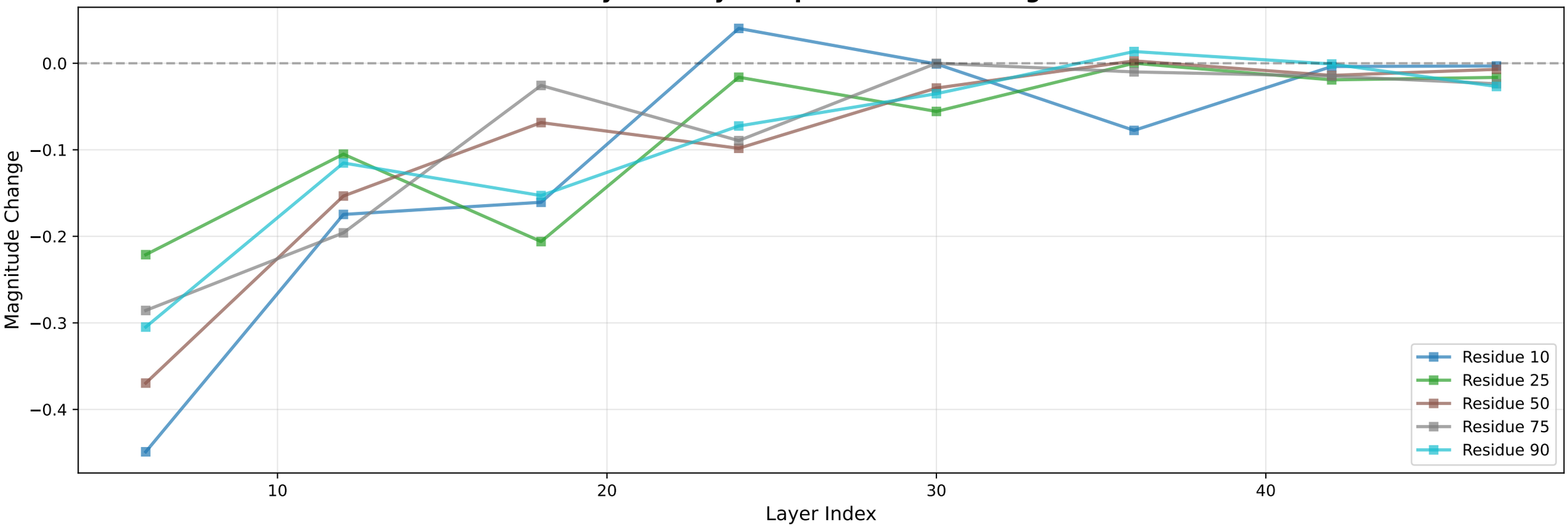
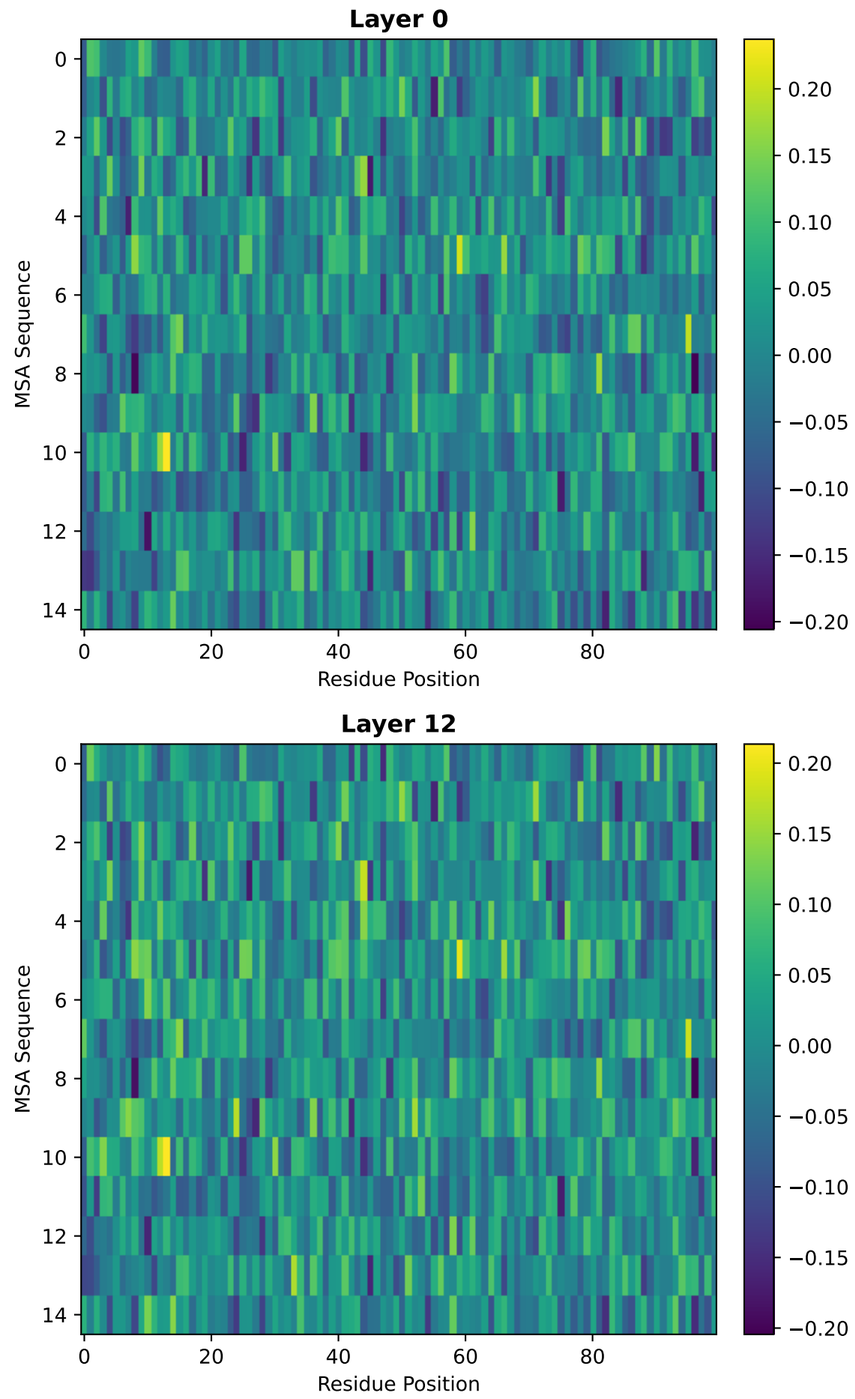
MSA Representation Evolution Across All Layers

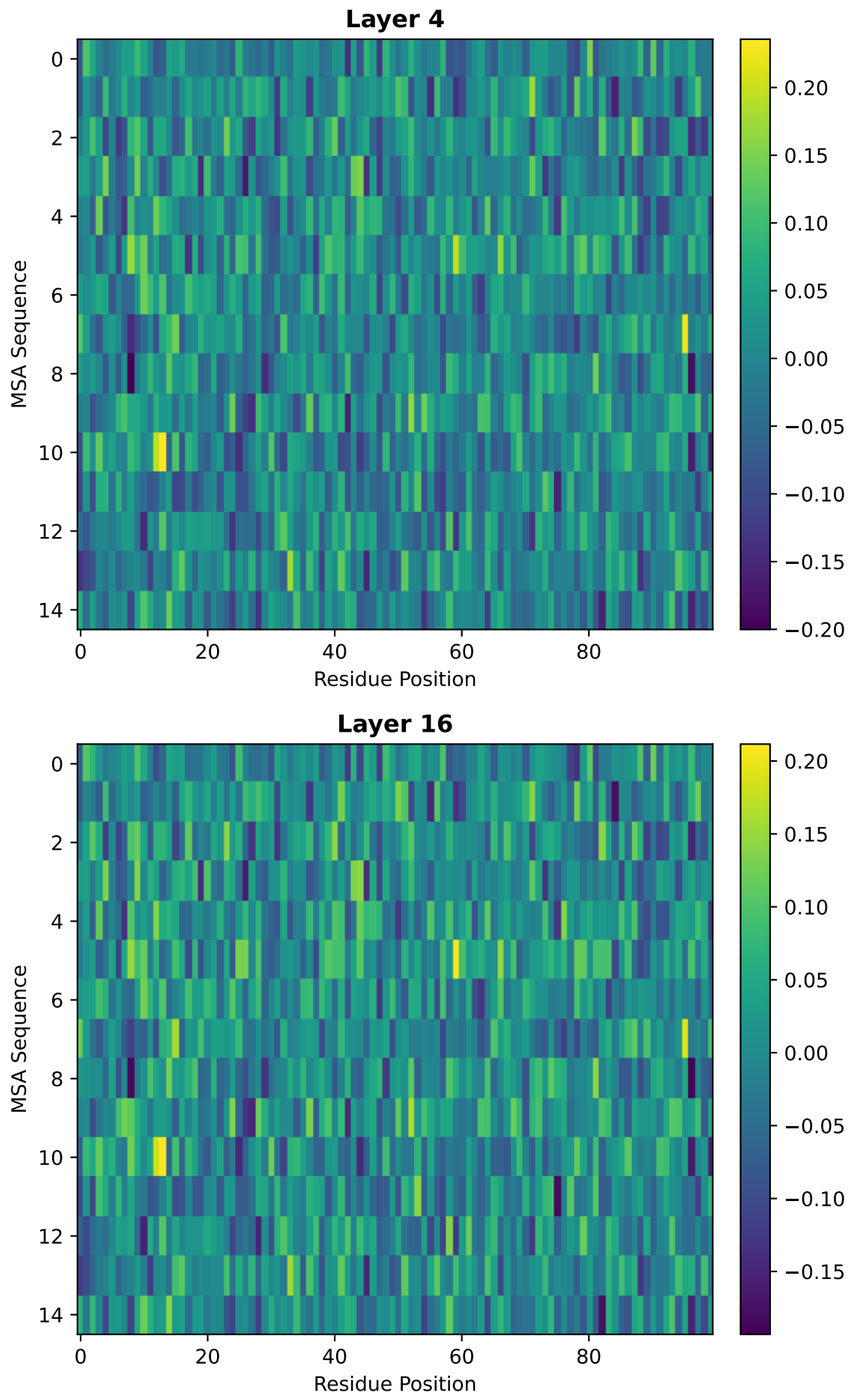


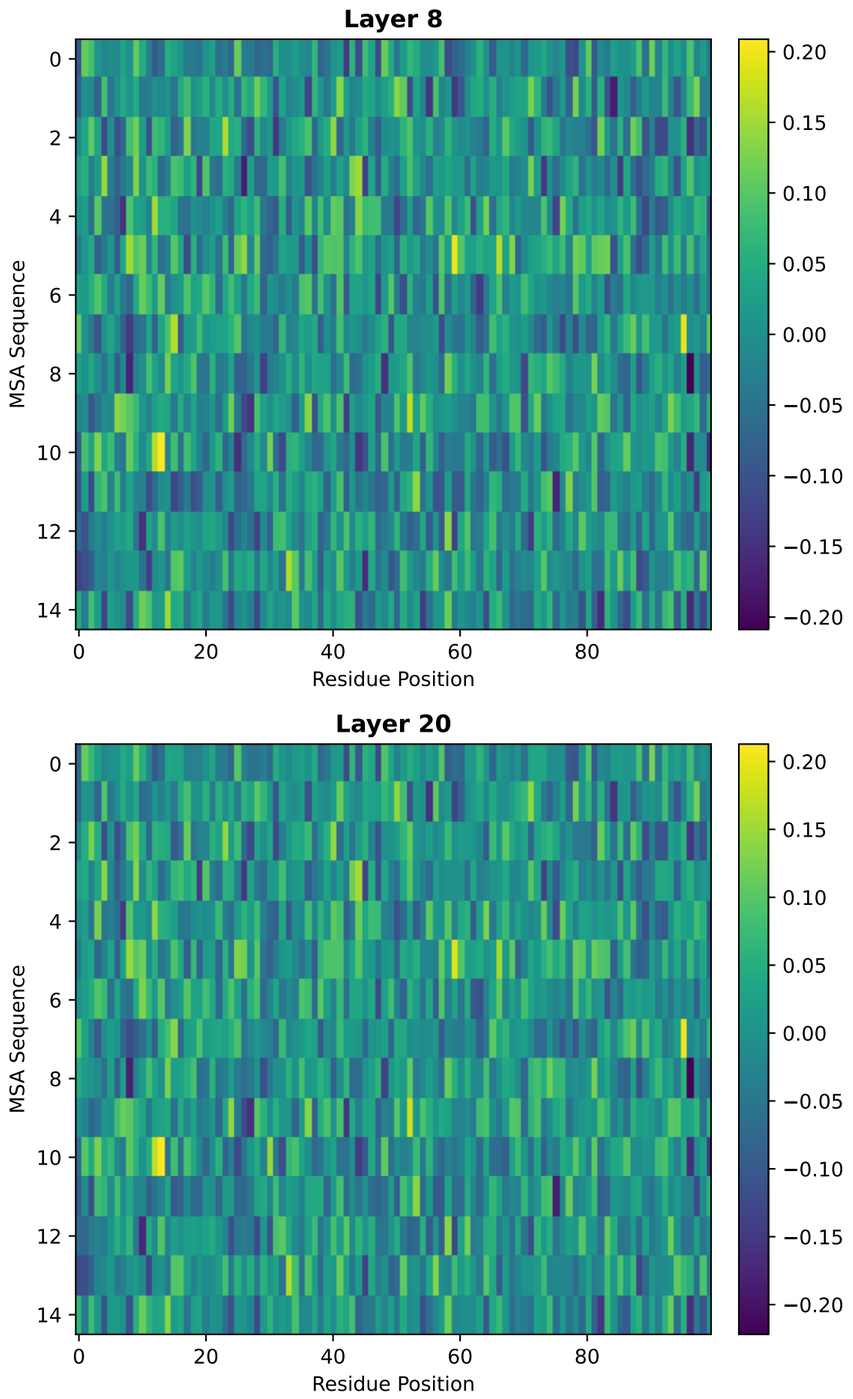
Layer-to-Layer Representation Changes

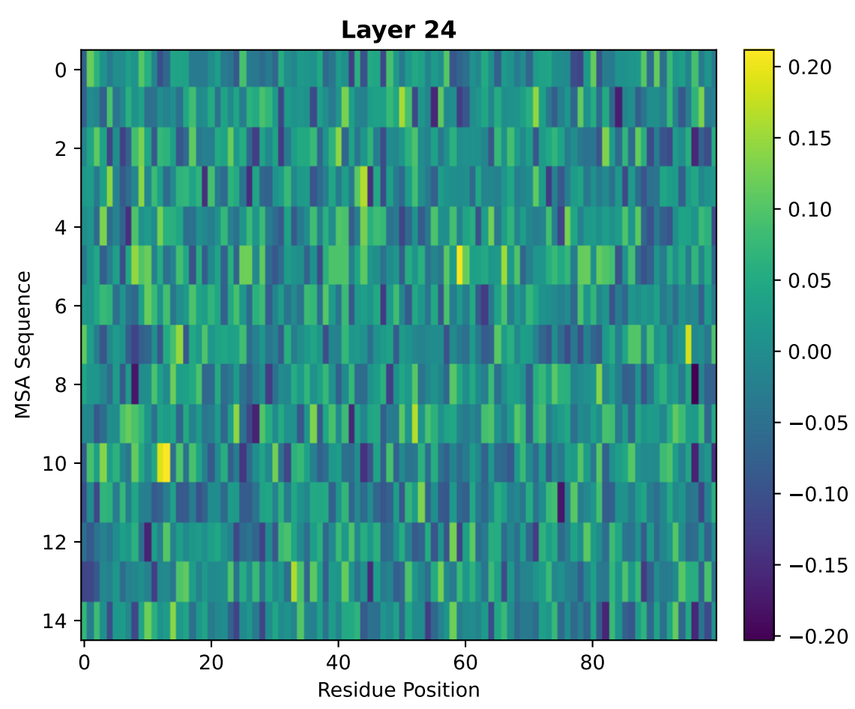


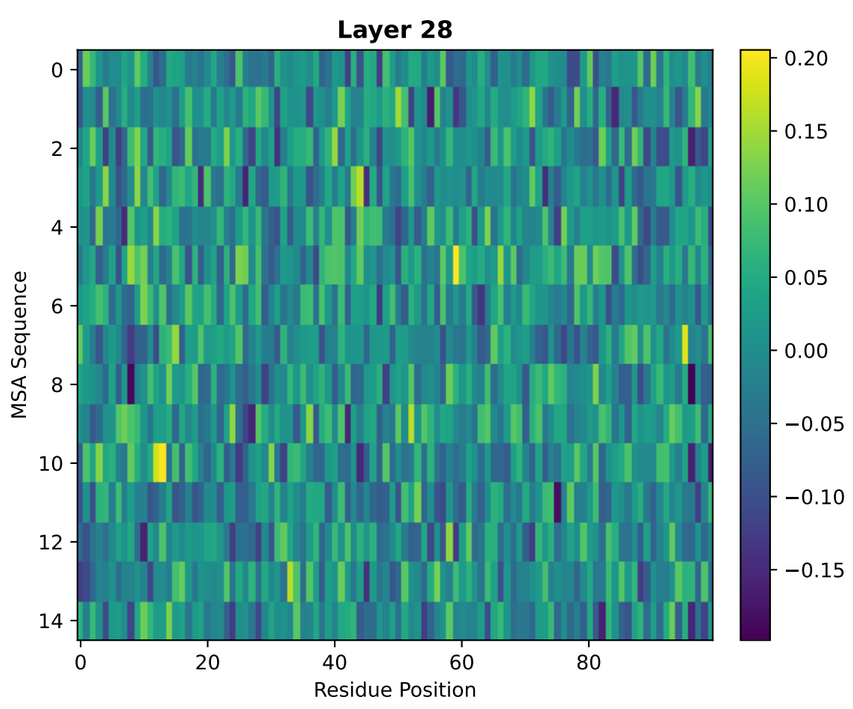
Stratified MSA Representation Comparison

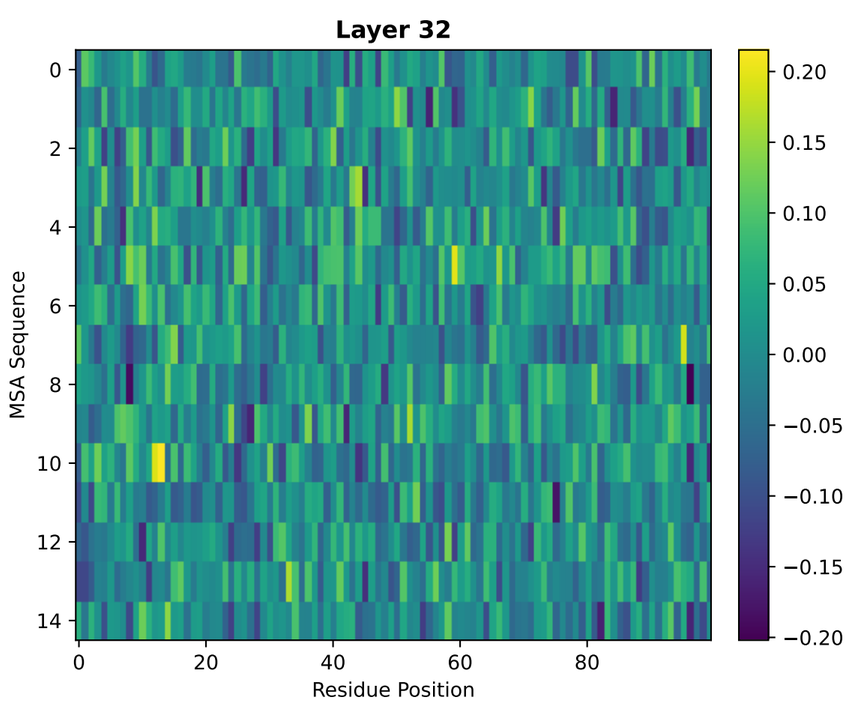


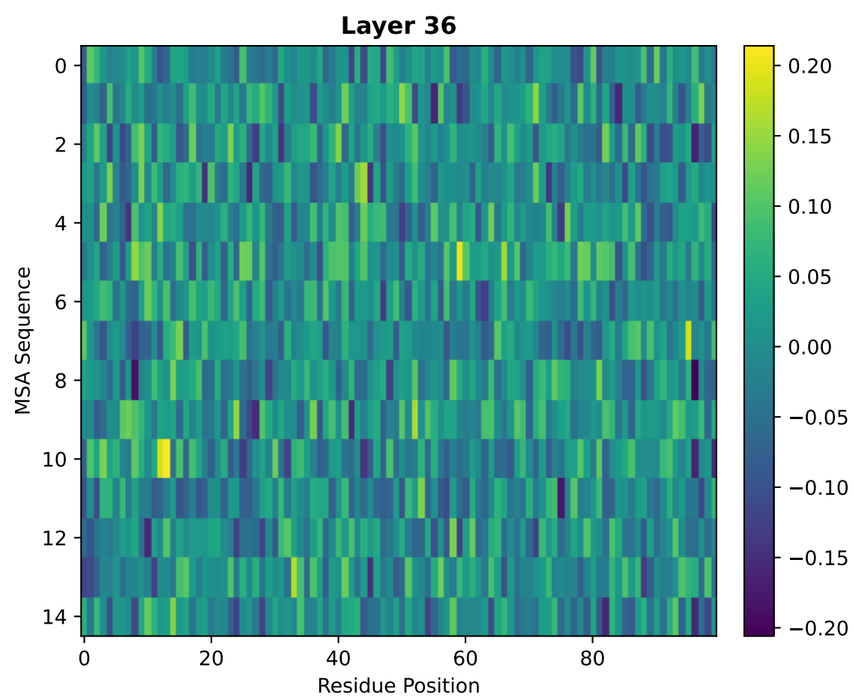


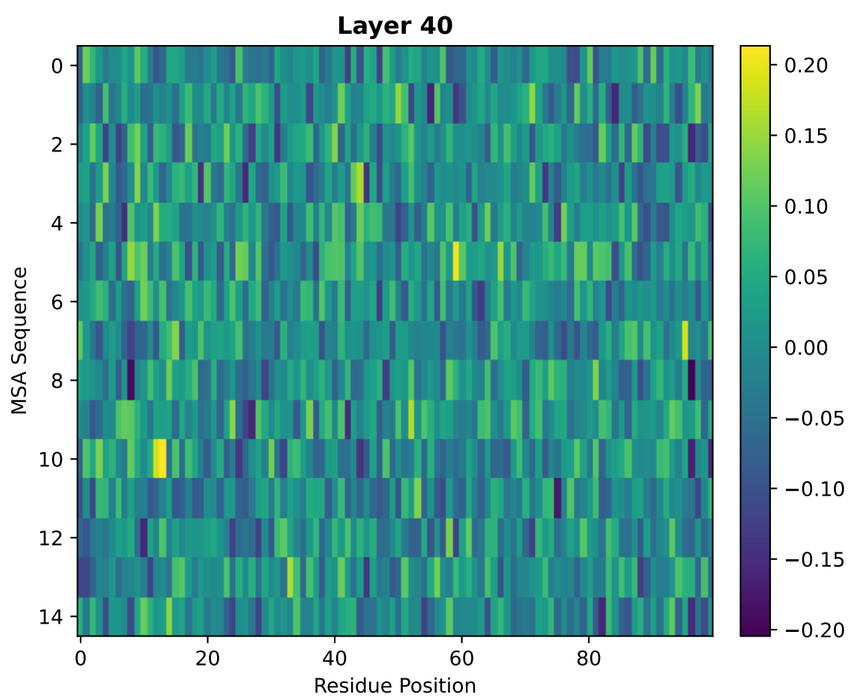


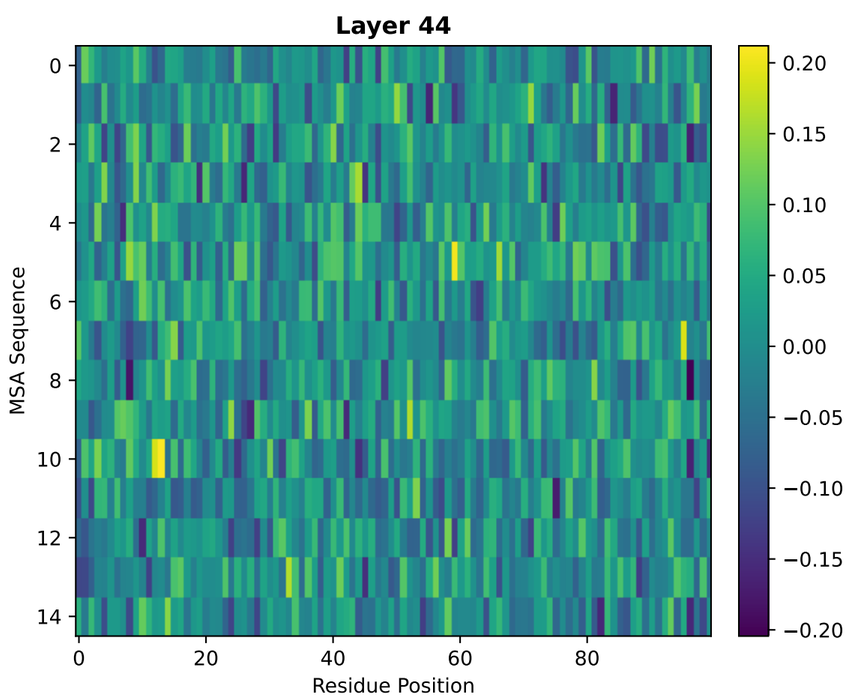


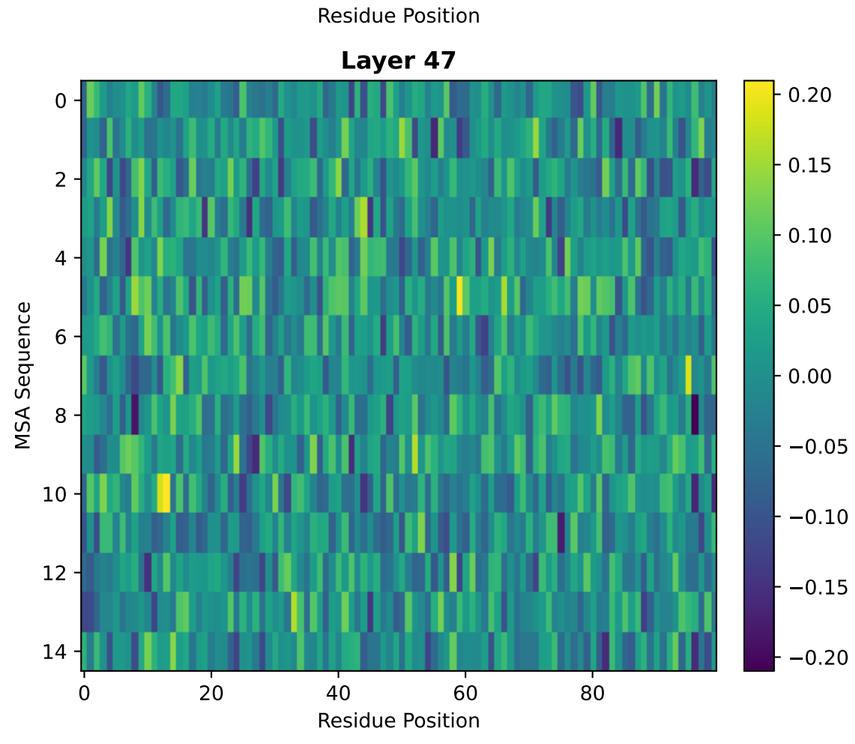




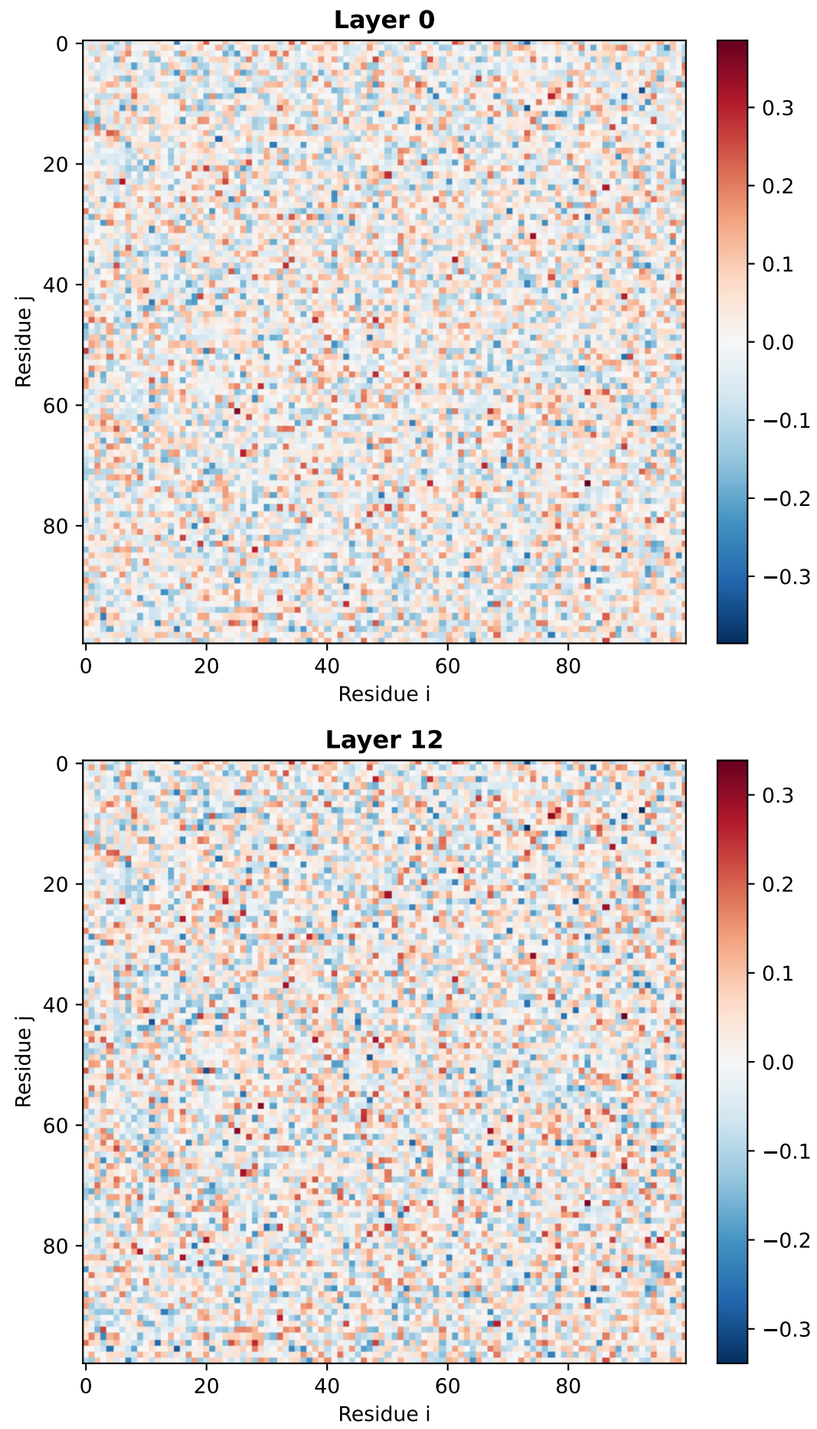


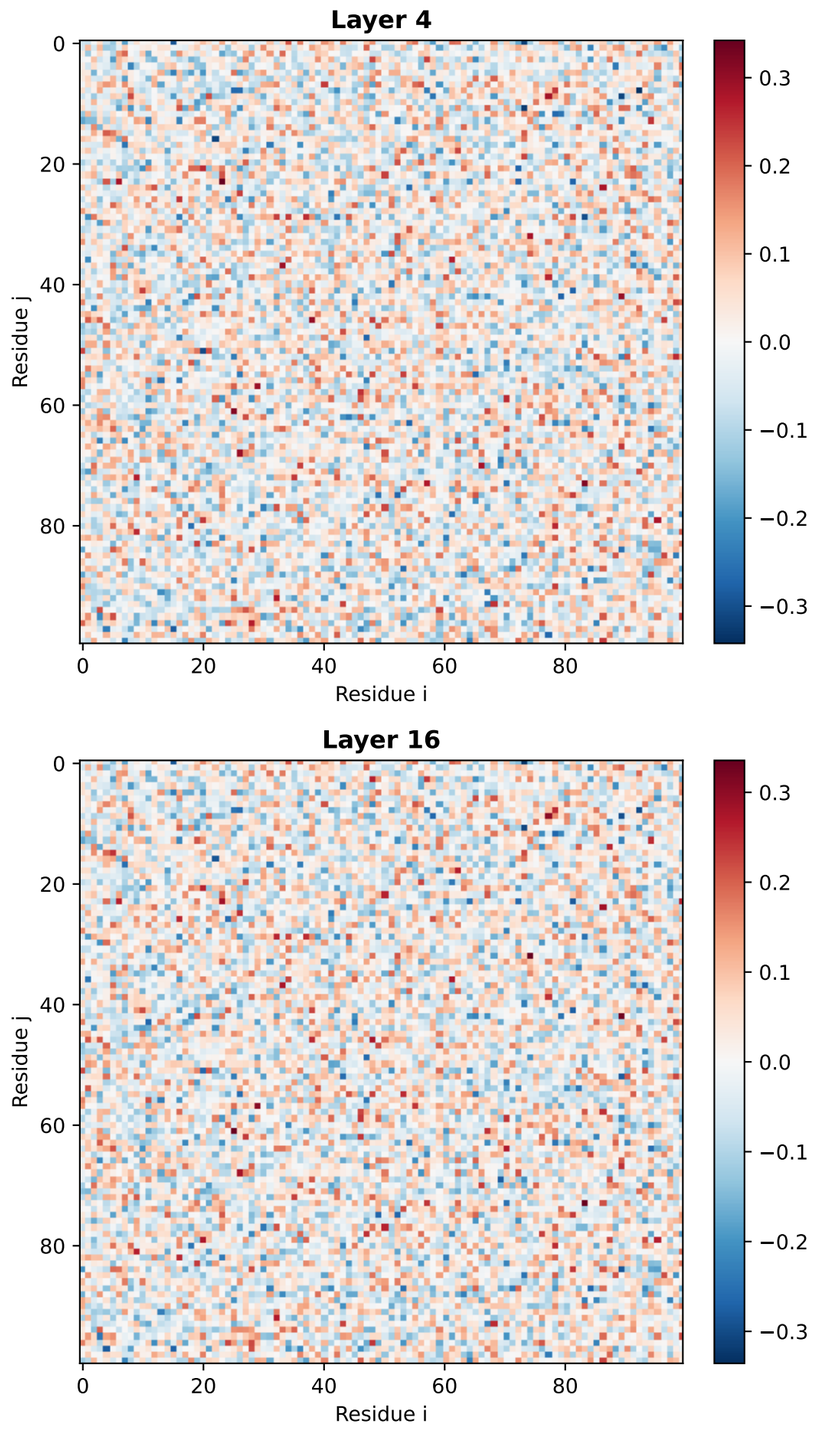


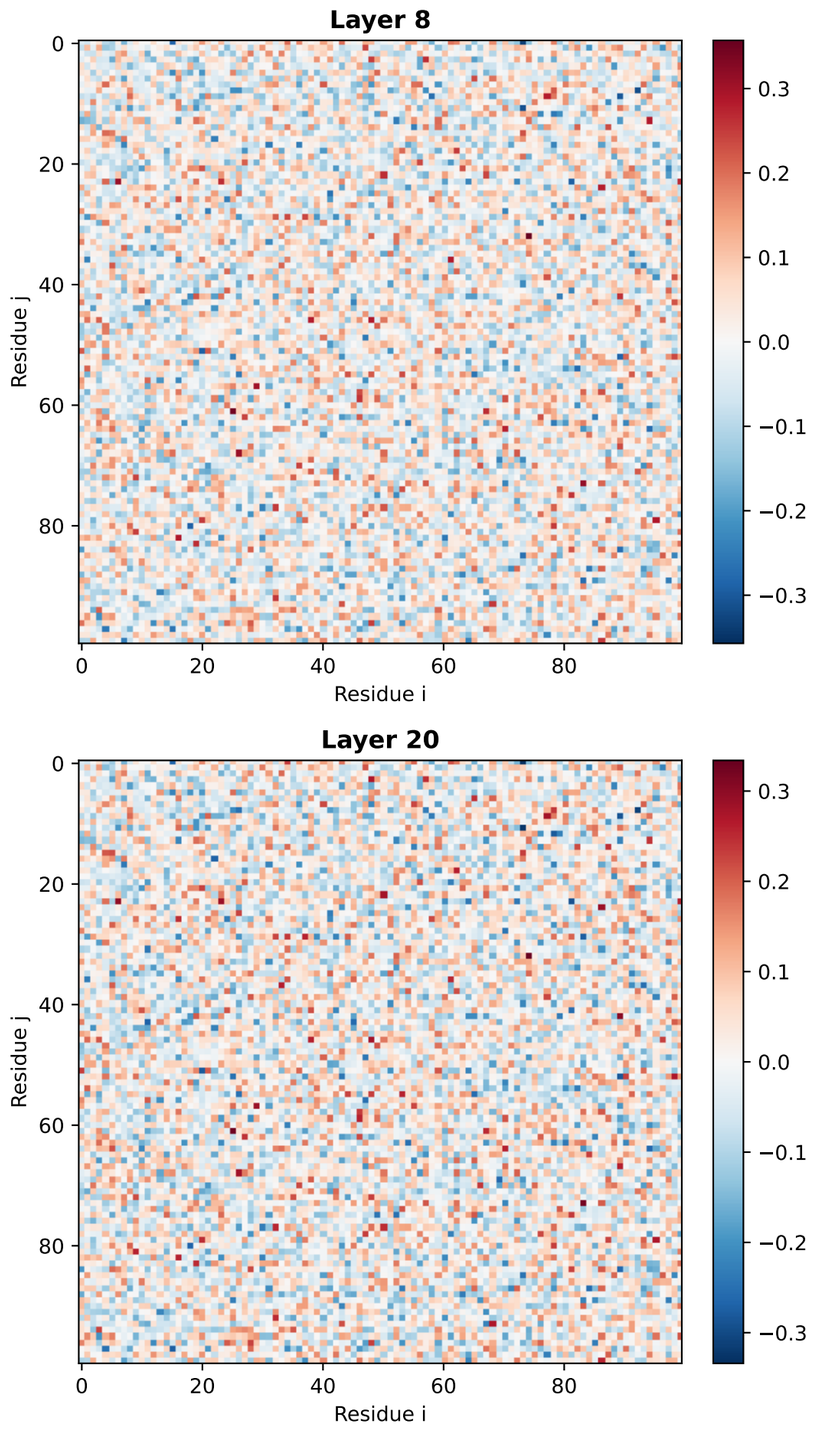


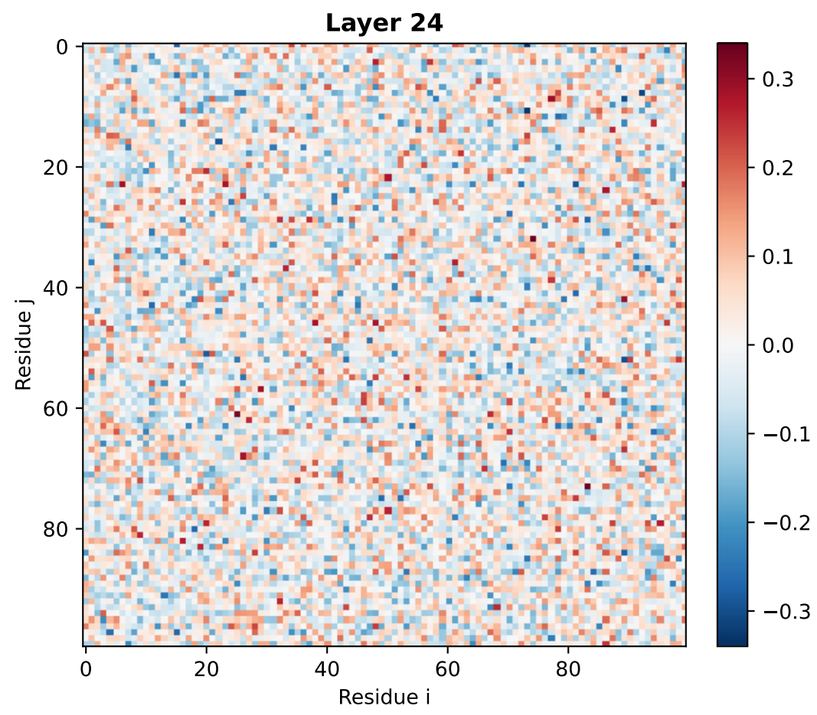


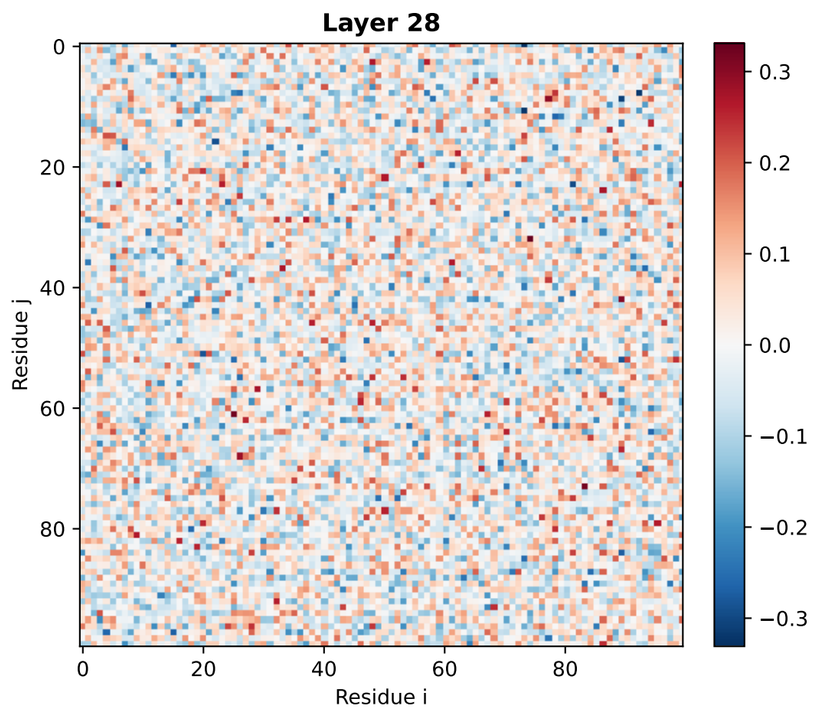
Stratified PAIR Representation Comparison

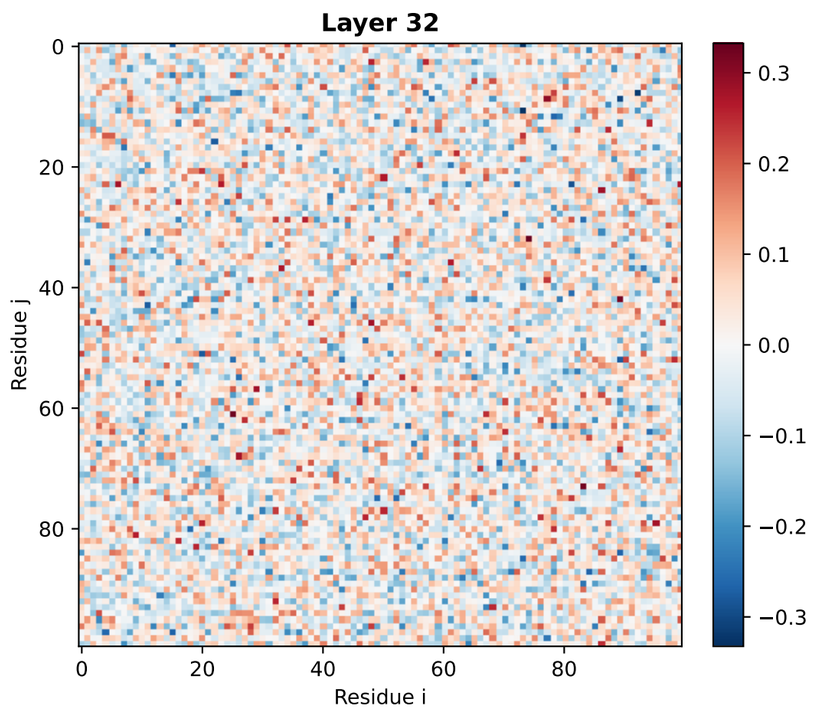


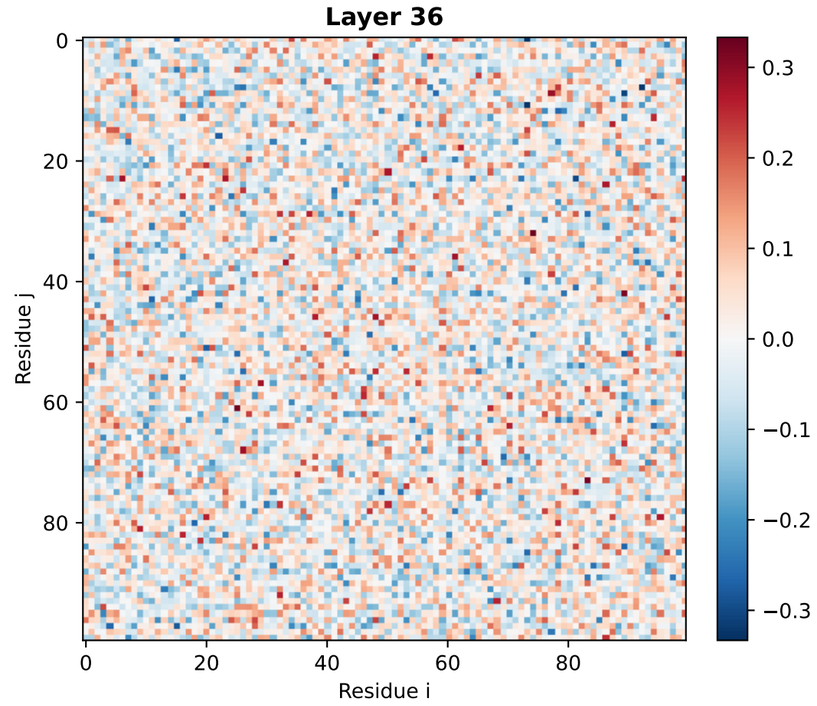


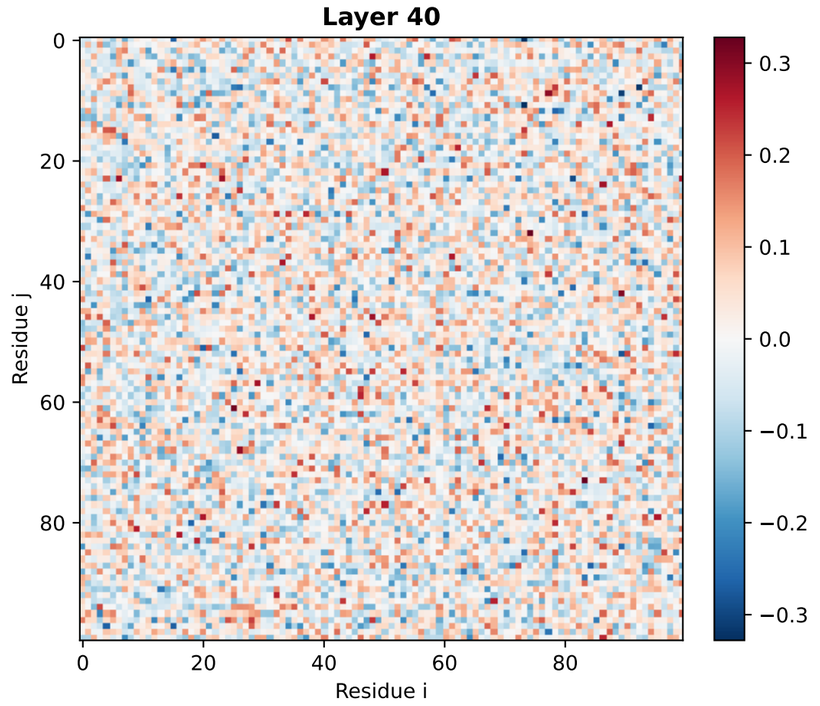


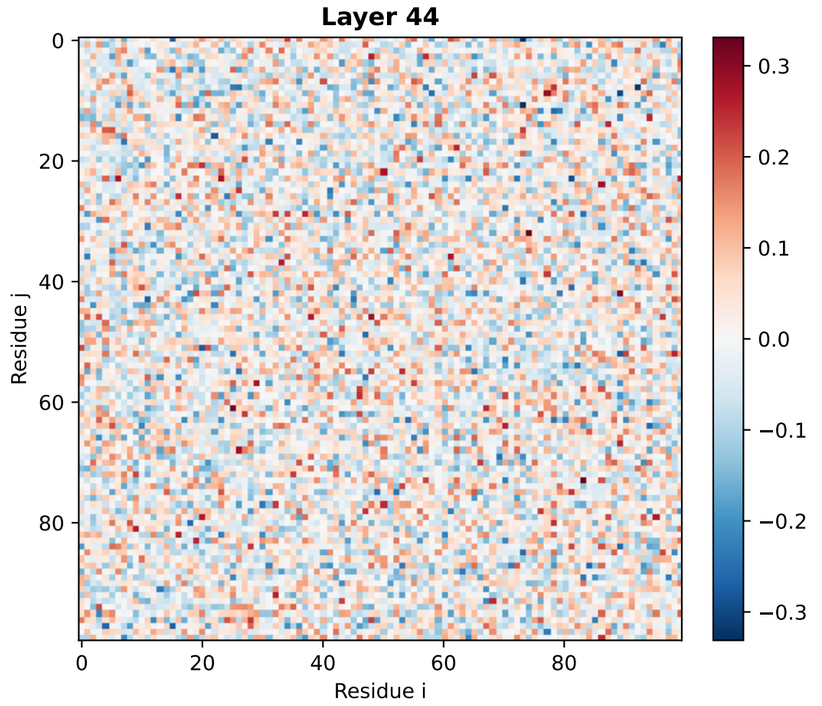


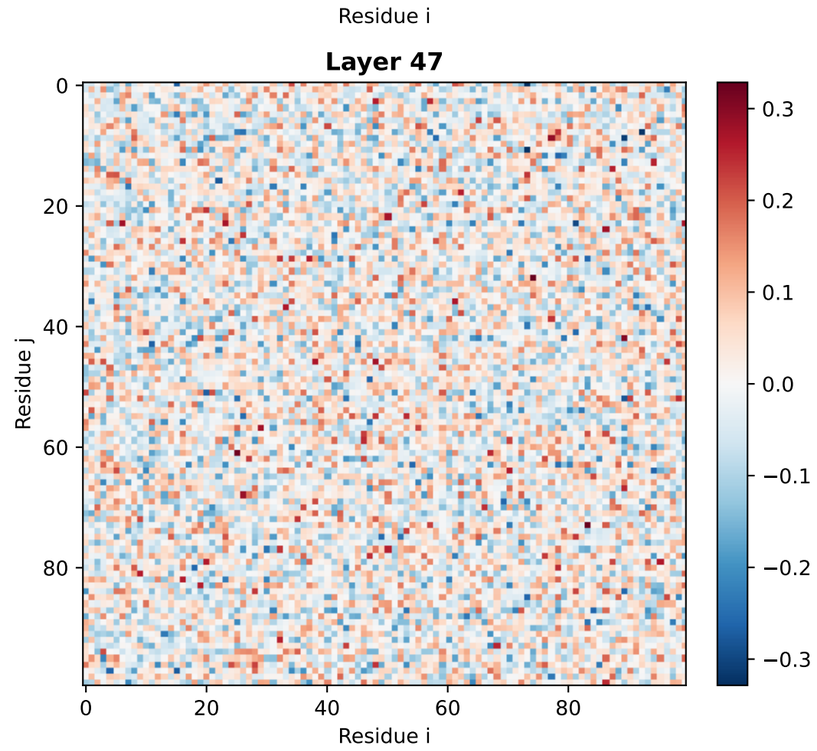


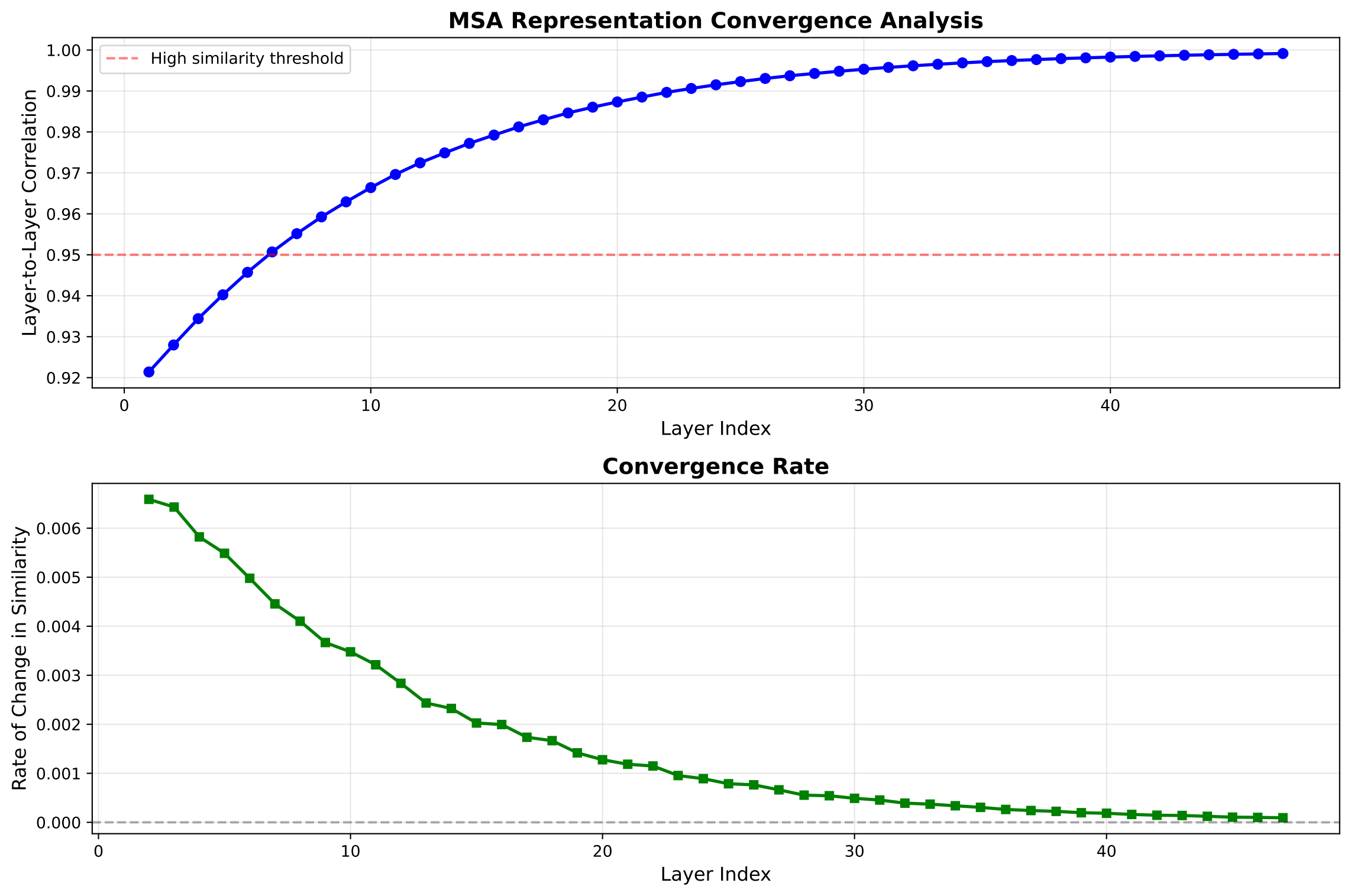


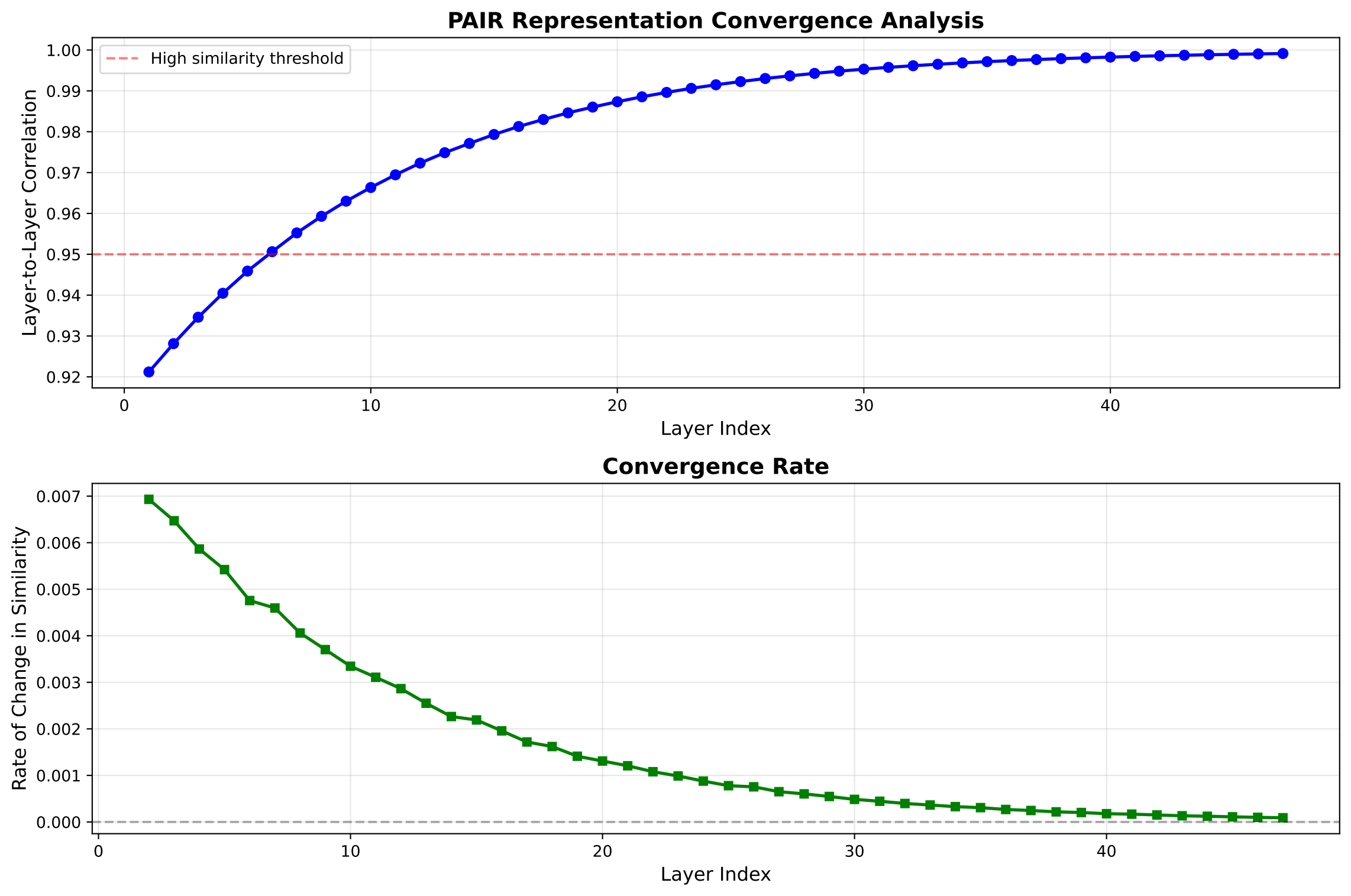


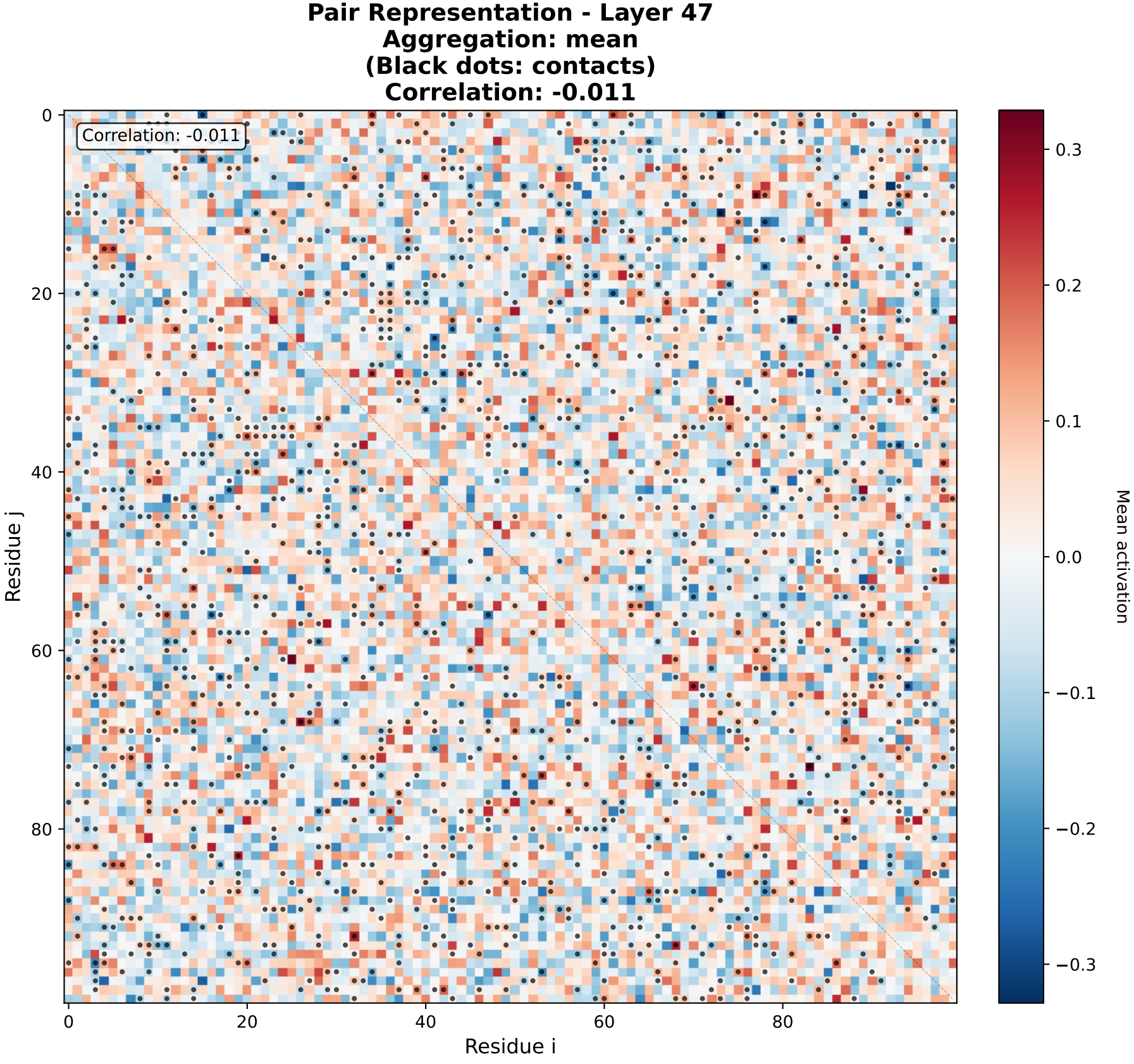







MSA Representation Convergence Analysis
High similarity threshold
Layer-to-Layer Correlation
1.00
0.99
0.98
0.97
0.96
0.95
0.94
0.93
0.92
0
10
20
30
40
Layer Index
Convergence Rate
Rate of Change in Similarity
0.006
0.005
0.004
0.003
0.002
0.001
0.000
0
10
20
30
40
Layer Index


PAIR Representation Convergence Analysis
High similarity threshold
Layer-to-Layer Correlation
1.00
0.99
0.98
0.97
0.96
0.95
0.94
0.93
0.92
0
10
20
30
40
Layer Index
Convergence Rate
Rate of Change in Similarity
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0.000
0
10
20
30
40
Layer Index


Pair Representation - Layer 47
Aggregation: mean
(Black dots: contacts)
Correlation: -0.011
Correlation: -0.011
Residue j
Residue i
Mean activation
0
20
40
60
80
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3