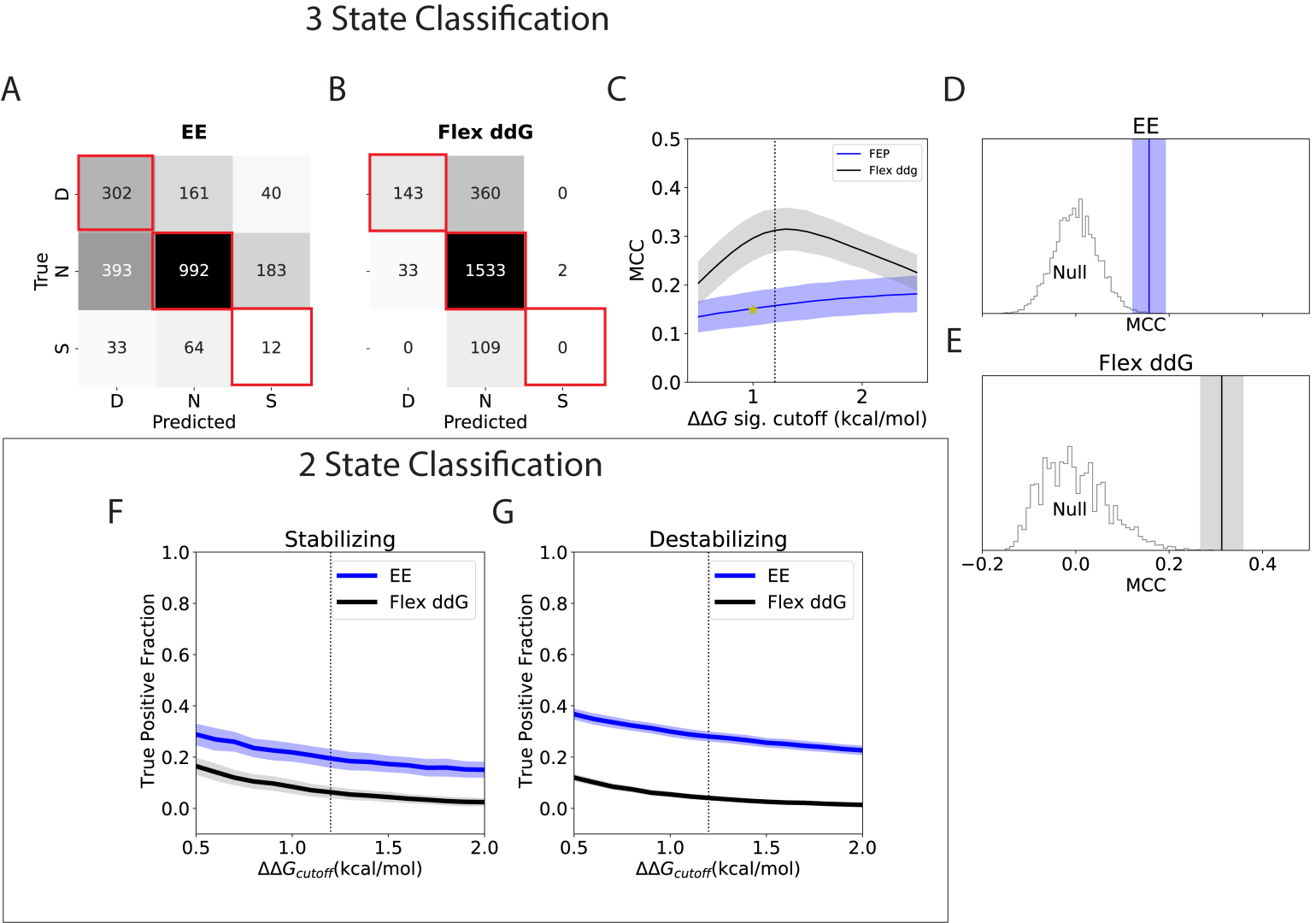
3 State Classification
A
EE
True
D
N
S
302
161
40
393
992
183
33
64
12
D
N
S
Predicted
B
Flex ddG
143
360
0
33
1533
2
0
109
0
D
N
S
Predicted
C
MCC
FEP
Flex ddg
ΔΔG sig. cutoff (kcal/mol)
D
EE
Null
MCC
E
Flex ddG
Null
MCC
2 State Classification
F
Stabilizing
True Positive Fraction
EE
Flex ddG
ΔΔG_cutoff(kcal/mol)
G
Destabilizing
True Positive Fraction
EE
Flex ddG
ΔΔG_cutoff(kcal/mol)