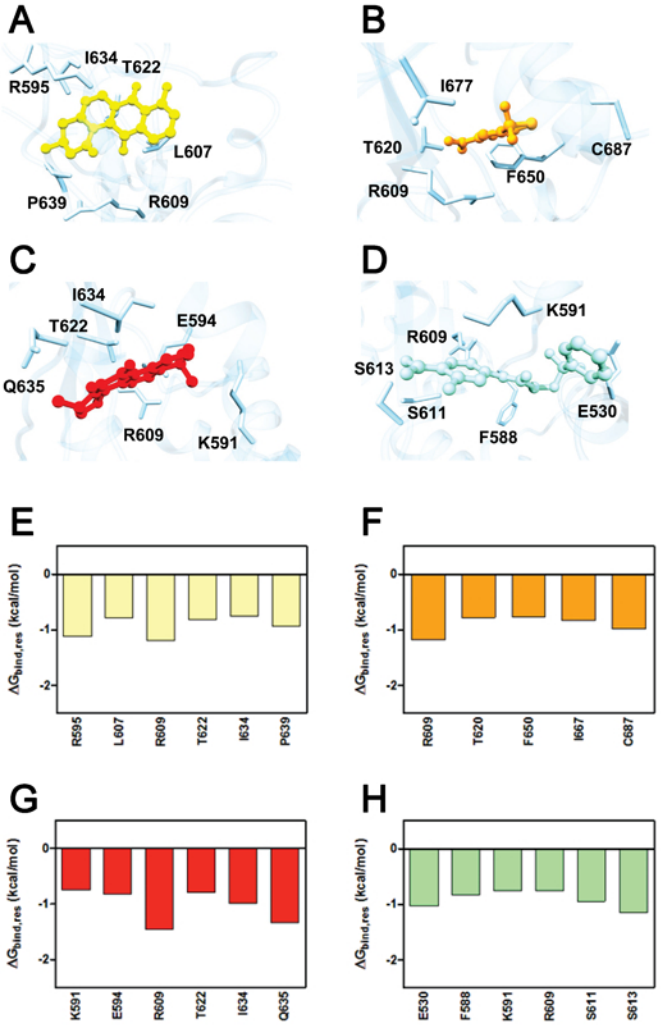
Figure S1


A
I634
T622
R595
L607
P639
R609
B
I677
T620
C687
F650
R609
C
I634
T622
E594
Q635
R609
K591
D
K591
R609
S613
S611
E530
F588
E
F
G
H
ΔG bind,res (kcal/mol)
0
-1
-2
R595
L607
R609
T622
I634
P639
R609
T620
F650
I667
C687
K591
E594
R609
T622
I634
Q635
E530
F588
K591
R609
S611
S613