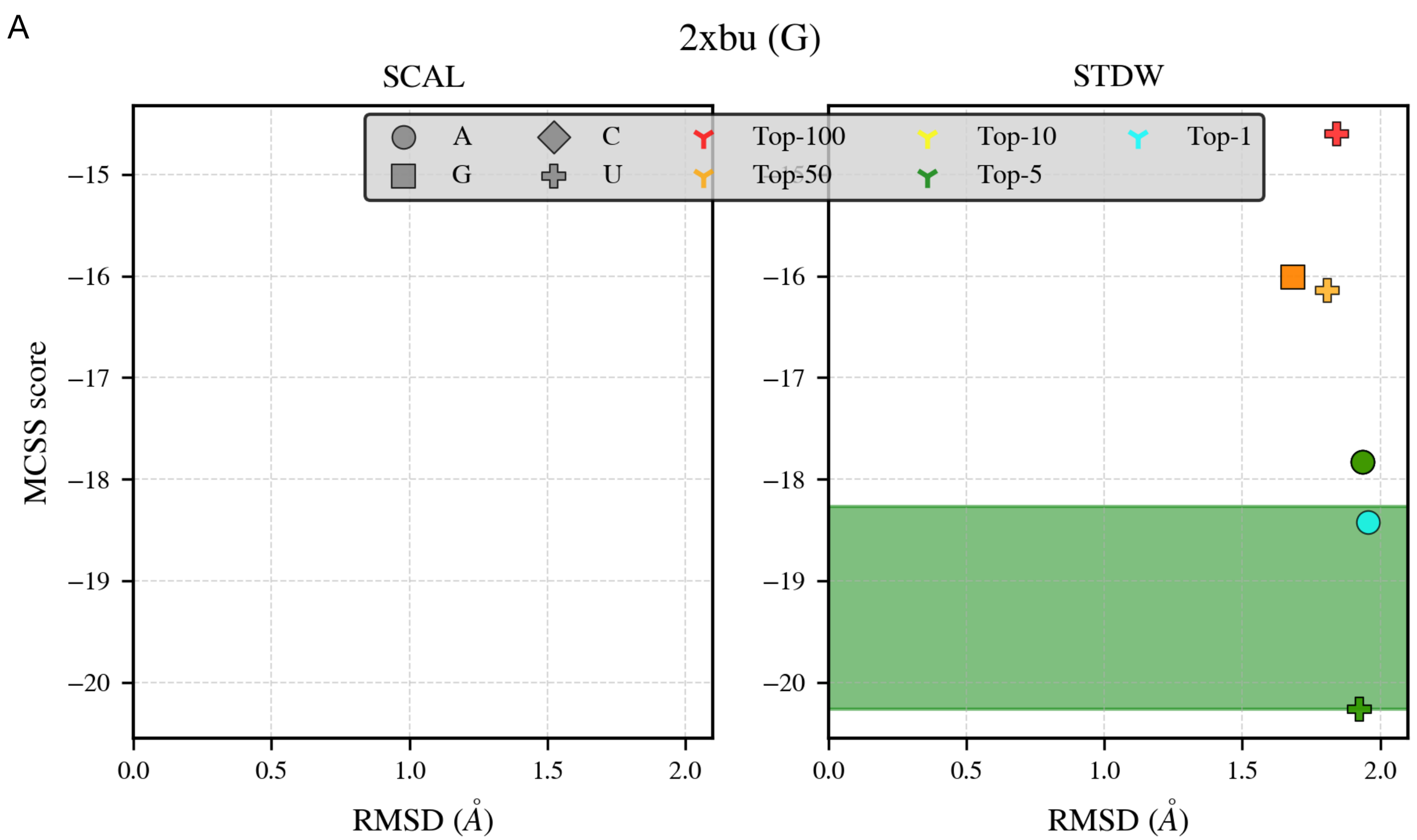
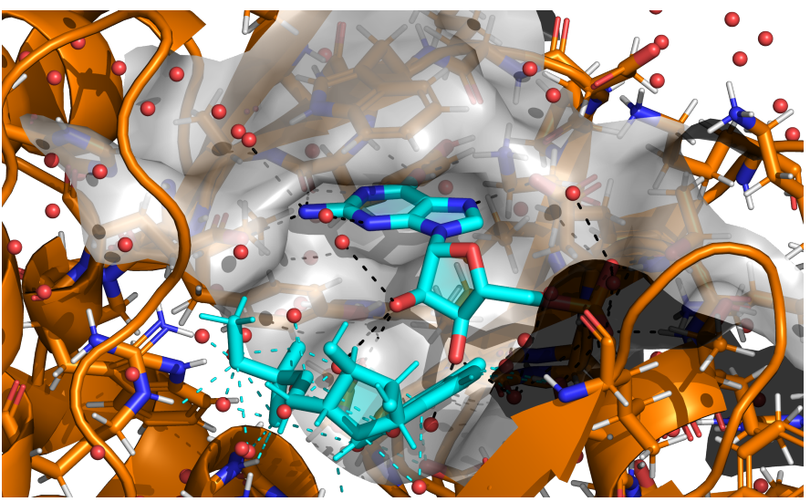
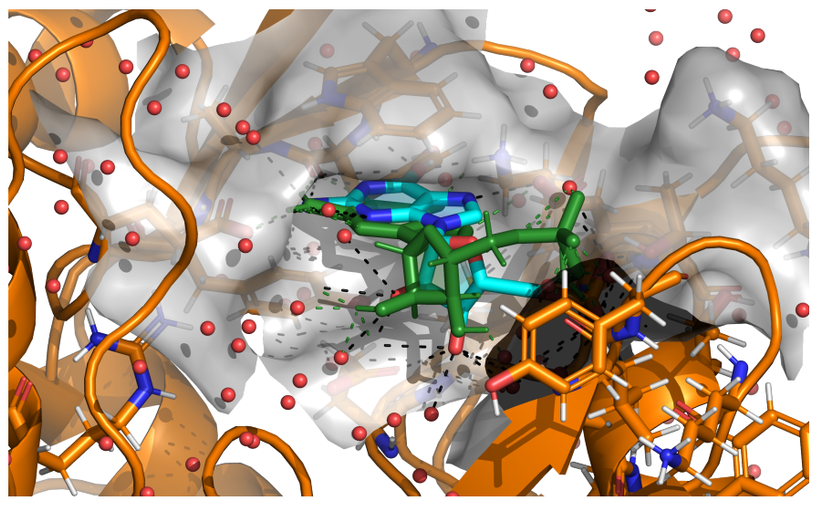
A


2xbu (G)
SCAL
STDW
A
C
G
U
Top-100
Top-50
Top-10
Top-5
Top-1
MCSS score
−15
−16
−17
−18
−19
−20
0.0
0.5
1.0
1.5
2.0
RMSD (Å)

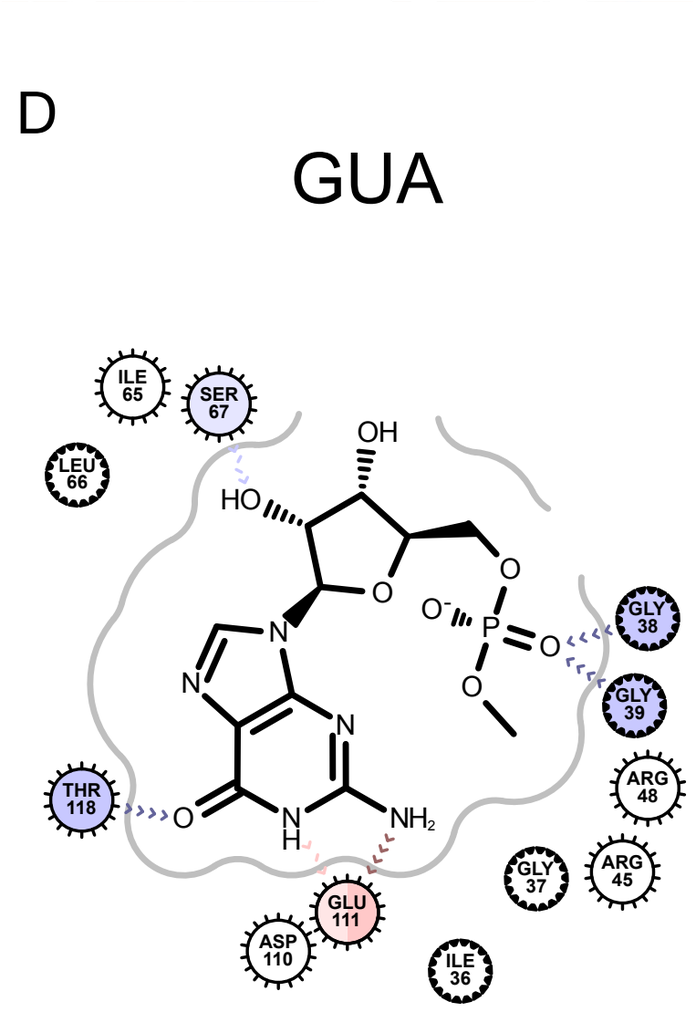
B



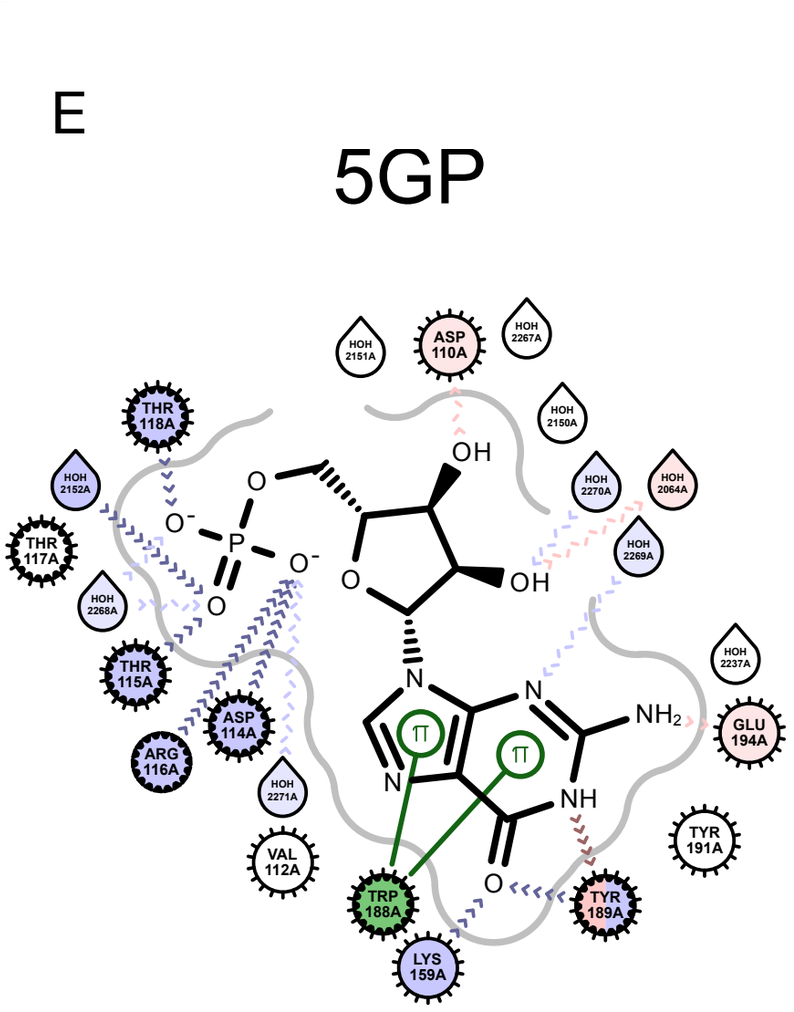
C



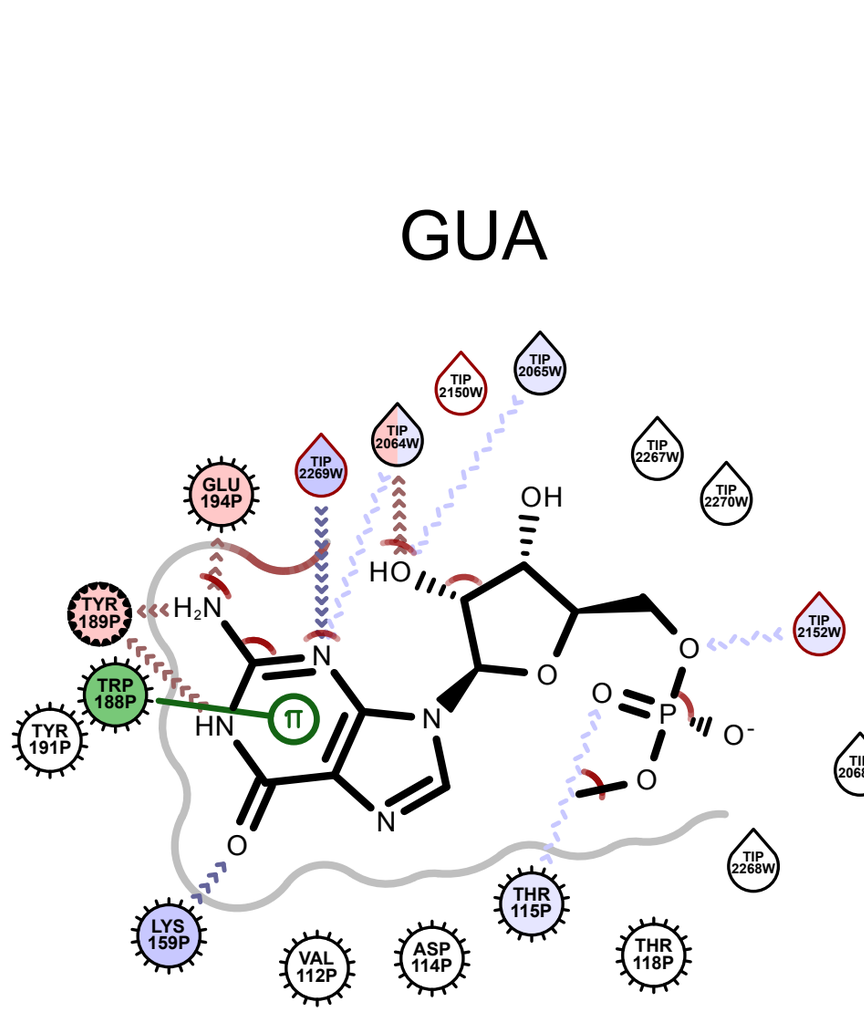
D


GUA
ILE 65
SER 67
LEU 66
THR 118
GLY 38
GLY 39
ARG 48
ARG 45
GLY 37
GLU 111
ASP 110
ILE 36

E


5GP
HOH 2151A
ASP 110A
HOH 2267A
THR 118A
HOH 2150A
HOH 2152A
HOH 2270A
HOH 2064A
THR 117A
HOH 2269A
HOH 2268A
HOH 2237A
THR 115A
GLU 194A
ASP 114A
ARG 116A
HOH 2271A
TYR 191A
VAL 112A
TRP 188A
TYR 189A
LYS 159A

F


GUA
TIP 2065W
TIP 2150W
TIP 2064W
TIP 2269W
TIP 2267W
GLU 194P
TIP 2270W
TYR 189P
TIP 2152W
TRP 188P
TYR 191P
TIP 2068W
TIP 2268W
LYS 159P
THR 115P
VAL 112P
ASP 114P
THR 118P