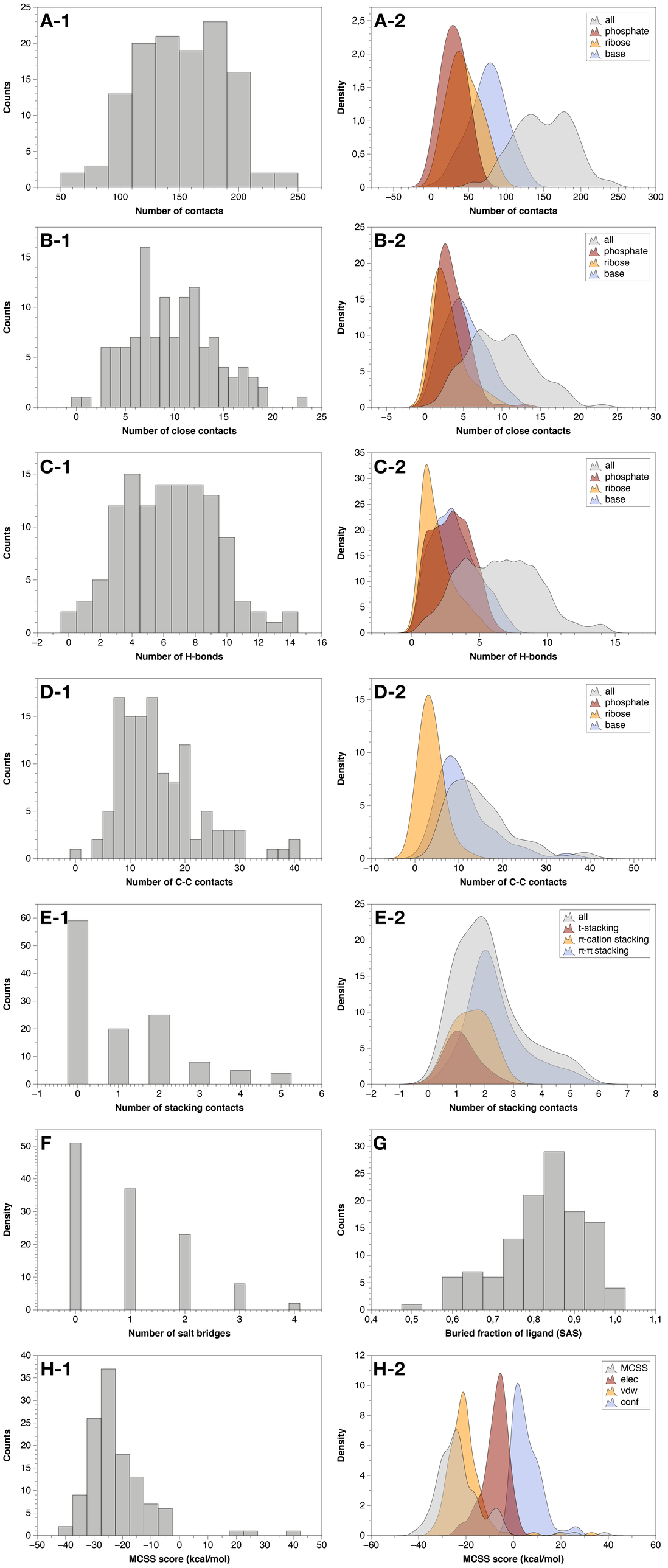
A-1
Counts
Number of contacts
A-2
Density
Number of contacts
all
phosphate
ribose
base
B-1
Counts
Number of close contacts
B-2
Density
Number of close contacts
all
phosphate
ribose
base
C-1
Counts
Number of H-bonds
C-2
Density
Number of H-bonds
all
phosphate
ribose
base
D-1
Counts
Number of C-C contacts
D-2
Density
Number of C-C contacts
all
phosphate
ribose
base
E-1
Counts
Number of stacking contacts
E-2
Density
Number of stacking contacts
all
t-stacking
π-cation stacking
π-π stacking
F
Density
Number of salt bridges
G
Counts
Buried fraction of ligand (SAS)
H-1
Counts
MCSS score (kcal/mol)
H-2
Density
MCSS score (kcal/mol)
MCSS
elec
vdw
conf