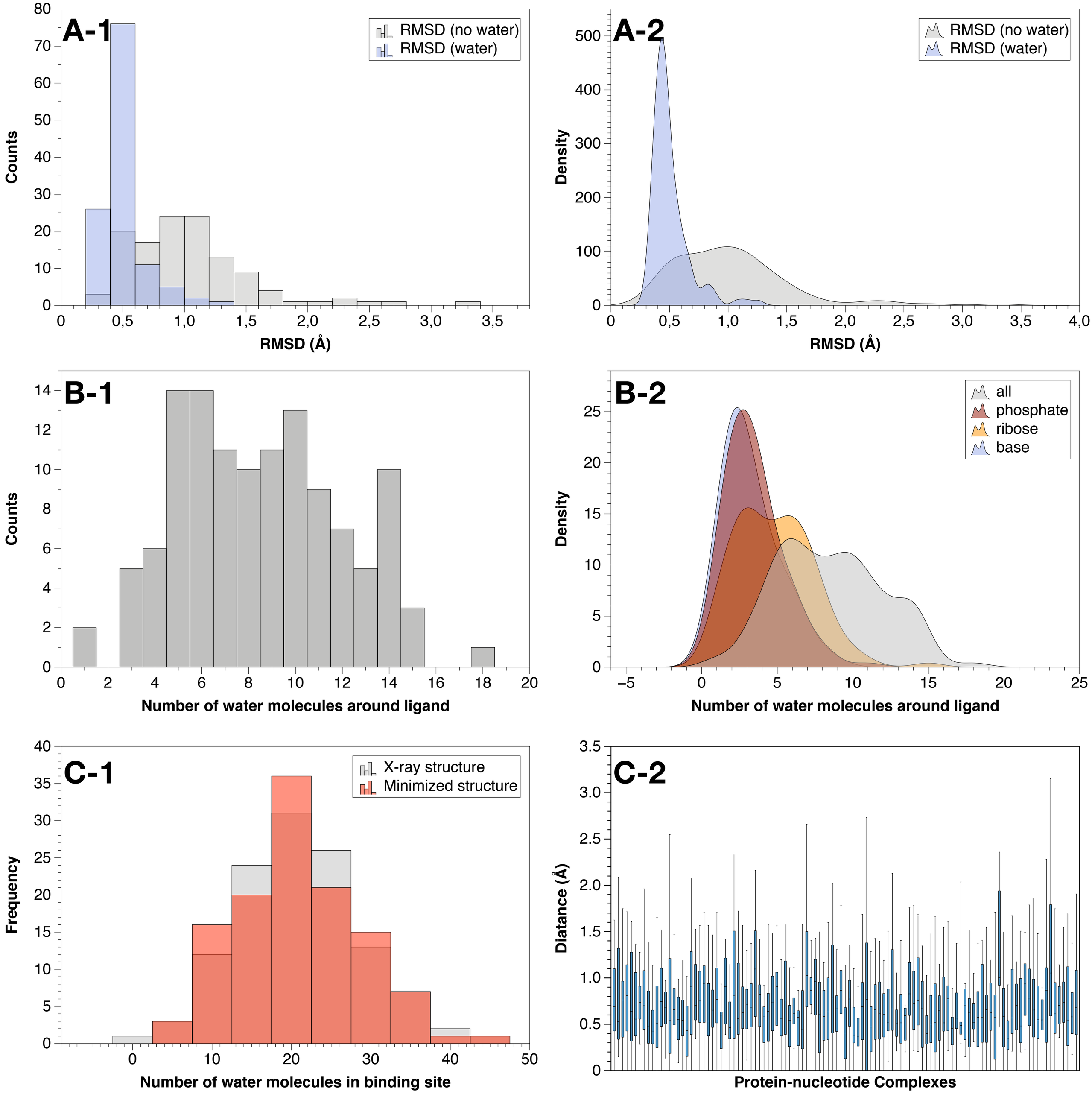
A-1
RMSD (no water)
RMSD (water)
Counts
RMSD (Å)
A-2
RMSD (no water)
RMSD (water)
Density
RMSD (Å)
B-1
Counts
Number of water molecules around ligand
B-2
all
phosphate
ribose
base
Density
Number of water molecules around ligand
C-1
X-ray structure
Minimized structure
Frequency
Number of water molecules in binding site
C-2
Diatance (Å)
Protein-nucleotide Complexes