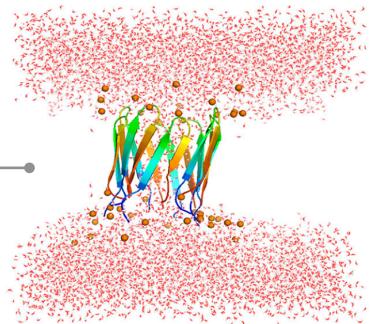


Description Representative force fields
(and limitations) Examples

ACCURACY

QM/MM

various } up to 100 QM atoms
 < 10 ns



POLARISABLE
ALL-ATOMS

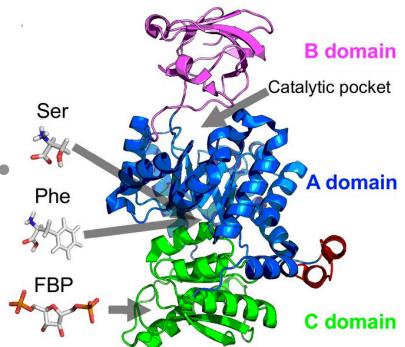
AMOEBA
AMBER ff02
Drude -CHARMM

Sizes as in All-atoms
< 100 ns
up to 100 ns
up to 100-500 ns

ALL-ATOMS

CHARMM
AMBER
OPLS

} 20 nm side
up to 1 μs



UNITED
ATOMS

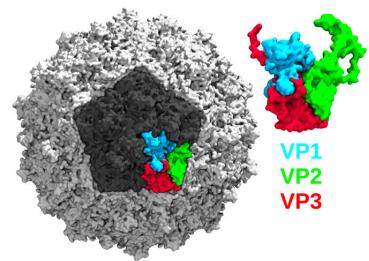
GROMOS
OPLS

} 20 nm side
up to 1 μs

POLARISABLE
COARSE GRAIN

ELBA

} 20-30 nm side
up to 1-5 μs



COARSE GRAIN

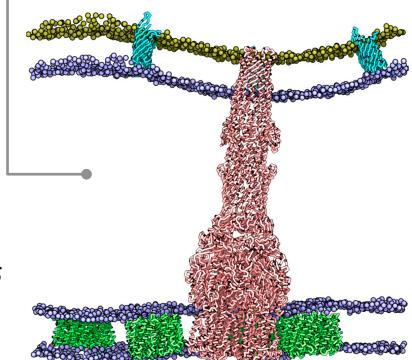
SIRAH
MARTINI

20-30 nm - 10 μs
50 nm - 1-10 μs

COARSE GRAIN
+
MEAN FIELD

OCCAM

} 20-30 nm side
up to 10 μs



IMPLICIT
SOLVENT

SASA approach
GB approach

} various sizes
up to 100 nm and 10 μs