

Paired t-test (% of NOE distance restraints satisfied)

ensemble GaMD	1	0.49	0.87	0.11	0.026	1	1	0
ensemble cMD	0.005	1	0	0	0	1	1	0.21
Omega best	0.01	0	1	1	1	0.002	0.004	0
Omega LICUV 10	0.001	0	0.88	1	1	0.002	0.001	0
Omega NAMFIS 10	0	0	0.34	0.34	1	0.002	0	0
Omega low_energy 10	0.18	0.028	0	0	0	1	1	0
Omega random 10	0.3	0.015	0	0	0	0.91	1	0
Omega random 1	0	0.002	0	0	0	0	0	1

Wilcoxon signed rank test (% of NOE distance restraints satisfied)

ensemble GaMD	1	1	1	0.13	0.009	1	1	0
ensemble cMD	0.014	1	0.003	0.001	0.003	1	1	0.4
Omega best	0.014	0	1	1	1	0.001	0.002	0
Omega LICUV 10	0.001	0	0.93	1	1	0.008	0.002	0
Omega NAMFIS 10	0	0	0.28	0.41	1	0.006	0.002	0
Omega low_energy 10	0.27	0.018	0	0	0	1	1	0
Omega random 10	0.53	0.023	0	0	0	0.8	1	0
Omega random 1	0	0.004	0	0	0	0	0	1

Paired t-test (RMSD)

ensemble GaMD	1	0.01	0.92	0.028	0.002	1	1	0
ensemble cMD	0	1	0.001	0	0	0.14	0.8	0.077
Omega best	0.013	0	1	1	1	0.29	0.057	0
Omega LICUV 10	0	0	0.18	1	1	0.006	0.001	0
Omega NAMFIS 10	0	0	0.017	0.073	1	0.001	0	0
Omega low_energy 10	1	0.001	0.003	0	0	1	1	0
Omega random 10	0.54	0.011	0.001	0	0	0.21	1	0
Omega random 1	0	0.001	0	0	0	0	0	1

Wilcoxon signed rank test (RMSD)

ensemble GaMD	1	0.049	1	0.022	0.001	1	1	0
ensemble cMD	0	1	0	0	0	0.3	0.94	0.096
Omega best	0.036	0	1	1	1	0.32	0.096	0
Omega LICUV 10	0	0	0.24	1	0.88	0.001	0	0
Omega NAMFIS 10	0	0	0.016	0.012	1	0.001	0	0
Omega low_energy 10	0.87	0.003	0.004	0	0	1	1	0
Omega random 10	0.61	0.014	0.001	0	0	0.28	1	0
Omega random 1	0	0.001	0	0	0	0	0	1

ensemble GaMD

ensemble cMD

Omega best

Omega LICUV 10

Omega NAMFIS 10

Omega low_energy 10

Omega random 10

Omega random 1

ensemble GaMD

ensemble cMD

Omega best

Omega LICUV 10

Omega NAMFIS 10

Omega low_energy 10

Omega random 10

Omega random 1