

S4 Table. Frequency of OM-residue hydrogen bonds during OM-bound MD simulations

Residue	OMA1^a	OMA2^a	OMB1^a	OMB2^a
R712	0.18	0.47	0.61	0.31
C705	0.04	0.50	0.02	0.47
A91	0.11	0.22	0.25	0.15
N711	0.09	0.22	0.22	0.00
S118	0.06	0.12	0.00	0.10
K762	0.21	0.00	0.01	0.01
L120	0.19	0.00	0.00	0.00

^aHydrogen bonds are calculated using a threshold of 3.5 Å on the D(onor)-A(ceptor) distance and 30° on the D-H-A angle.