



**Fig. S1** Sequence alignment of Cpn60α, β1 and β2 and their homolog GroEL and residue number

αα				β1β1				β2β2			
Chain A	Chain B	Distance (Å)	Occupancy (%)	Chain A	Chain B	Distance (Å)	Occupancy (%)	Chain A	Chain B	Distance (Å)	Occupancy (%)
I6 (N)d	E63 (O)	2.0	94	E5 (OE1)	S65 (OG)d	1.8	35	L6 (O)	E63 (N)d	2.0	83
I6 (O)	K65 (N)d	2.0	55	E5 (OE1)	S65 (N)d	2.1	13	K74 (NZ)d	S44 (O)	2.3	11
Q74 (NE2)d	E43 (OE1)	1.9	100	Q78 (OE1)	A48 (N)d	2.9	5	K74 (NZ)d	G47 (O)	2.4	56
Q74 (NE2)d	G47 (O)	2.2	95	Q117 (OE1)	K36 (NZ)d	2.1	22	Q78 (OE1)	S48 (OG)d	2.2	55
E78 (OE2)	V48 (N)d	2.2	57	Q127 (OE1)	K392 (NZ)	1.7	25	R82 (NH1)	Q386 (O)	2.1	18
N114 (ND2)d	D489 (OD1)	2.1	14	R233 (NH2)	N246 (OD1)	2.0	12	R82 (NH2)	Q386 (O)	2.1	18
N114 (ND2)d	D489 (OD2)	2.8	22	E257 (OE2)	K274 (NZ)d	2.3	43	K228 (NZ)d	E218 (OE2)	2.9	7
D226 (O)	N183 (ND2)d	2.0	92	E259 (OE2)	T217 (OH)d	1.7	98	K228 (O)	N246 (ND2)d	2.3	1
D226 (OD2)	N183 (ND2)d	2.5	83	T263 (N)d	R270 (O)	3.5	3	A232 (N)d	T272 (OG1)	1.9	39
K228 (NZ)d	E180 (OE1)	2.0	55	L521 (O)	R38 (NH1)d	2.2	16	S515 (OG)d	Q386 (OE1)	1.8	41
E254 (OE2)	T181 (OG1)d	1.8	95	L522 (O)	N39 (N)d	2.2	97	L522 (O)	N39 (N)d	1.7	93
E254 (OE1)	S182 (OG)d	1.7	100	A523 (O)	R38 (NH1)d	2.4	8	D524 (N)d	N39 (O)	2.2	92
D255 (OD2)	R212 (NH2)d	2.6	57	D524 (N)d	N39 (O)	2.2	95	V525 (O)	V41 (N)d	1.7	85
V256 (O)	R212 (NH2)d	3.3	13	V525 (O)	V41 (N)d	2.0	92	V527 (N)d	V41 (O)	1.5	99
G258 (N)d	E216 (OE2)	1.9	23	V527 (N)d	V41 (O)	2.1	98	V527 (O)	E43 (N)d	2.0	94
E259 (O)	N274 (ND2)d	3.2	19	V527 (O)	E43 (N)d	2.2	54	E529 (OE1)	K45 (NZ)d	2.9	64
E259 (OE2)	N274 (ND2)d	1.8	60	E529 (N)d	E43 (OE1)	2.3	100				
T263 (OG1)	N274 (ND2)d	2.1	31								
F283 (N)d	A386 (O)	2.2	85								
R287 (NH1)d	N183 (OD1)	2.3	19								
D306 (OD2)	N183 (N)d	1.9	86								
D306 (OD1)	K382 (NZ)d	2.2	14								
D306 (OD2)	K382 (NZ)d	2.3	12								
T522 (O)	N39 (N)d	1.9	85								
T522 (OG1)d	N39 (OD1)	1.5	44								
Q524 (N)d	N39 (O)	2.2	93								
M527 (N)d	V41 (O)	1.8	98								
M527 (O)	E43 (N)d	2.1	94								

**Fig. S2** Residues forming H-bond at time 100 ns of MD simulation and %occupancy in last 20 ns