

GroEL 1 10 20 30 40 50 60 70 80 90 100
 α - - - E I V F - - D Q E S R R R L Q A G I N K V A D A V G V T L G P K G R N V V L E Q K F G P Q V I N D G V S I A R A I E L K D P V E N A G Q L I K E V A G R T N D A A G D G T T T A S V L A R E
 β1 - - - E L H F N K D M O A L K R M Q A G V D K L A T V V G V T I G P K G R N V V L E S K F G A P K I V N D G V T I A R E V E L S D P V E N I G A T L V R Q A A R T N D T A G D G T T T A T V L S A A
 β2 - - - E L H F N R N M E A L K K M Q A G V D K L A T V V G V T I G P K G R N V V L E S K F G S P K I V N D G V T I A R E V E L E D P V E N I G A K L V R Q A A R T N D T A G D G T T T A T V L S A A

GroEL 101 110 120 130 140 150 160 170 180 190 200
 α I I T E G L A A V A A G M N P M D L K R G I D K A V T A A V E E L K A L S V P C S D S K A I A Q V G T I S A N S D E T V G K L I A E A M D K V G K E G V I T V E D G T G L Q D E L D V V E G M Q F D R G
 β1 F I A E G M K I V S A G T N P V Q L V R G M E K T V Q E L V K E L R K M S S V Q T D K D L A N V A C V S A G G N T D I G S L I S D A M A K V G R T G V V T M E E G K T A E D Q L V F V E G M Q F E R G
 β2 F I A E G M K I V A A G T N P V Q L T R G M E K T V N A L V K E L K A A S S Q V H S D K L S N V A S V S A G G N P D V G K L I S D A M A K V G R Q G V V T M E E S K T A E D A L I F V E G M Q F D R G

GroEL 201 210 220 230 240 250 260 270 280 290 300
 α Y I S P Q F V T N Q E R L L V E Y D N C R V L V T D Q K I D A I R D I I P I L E Q V T R L N A P L L I I A E D V E G E A L A T L V V N T M R G I V K V A A V K A P G F G D R R K A M L Q D I A T L T G G
 β1 Y T S P Y F V T D P E R M I C E Y E N C K I L L V D K K I S T A R D I I T I L E S A I R G N Y P L L I M A E E V E Q E A L A T L V V N K L R G T L K V V A I K A P G F G E R R S S Y L E D I A I L T G G
 β2 Y Y S P Y F V T D P E R M L A E Y E N C R I L L V D K K I S T A R D I I G I L E A A I R G N Y P L L I M A E D V E Q E A L A T L V V N K L R G T L K V V A V K A P G F G E R K S S Y L E D I A I L T G G

GroEL 301 310 320 330 340 350 360 370 380 390 400
 α T V I S E E I G M E L E K A T L E D L G Q A K R V V I N K D T T T I I D G V G E E A A I Q G R V A Q I R Q Q I E E A T S D Y D R E K L Q E R V A K L A G G V A V I K V G A A T E V E M K E K K A R V E D
 β1 E F I A K D L G M K V E G A V V E Q L G V A R K V T V A N N T T L I A D A A S K D E I E M R I A Q L K K E L A E T D S V Y D T E K L S E R I A K L S G G V A V I K V G A A T E A E L E D R K L R I E D
 β2 T V V R D E M G V S L E Q A T D A V L G T A A K I T I K E R T T V V G D G S T A A D V A A R V K Q I R N L Q M Q T D Q D Y E R E K L Q E R I A R L S G G V A I I Q V G A Q T E T E L K E K K L R V E D

GroEL 401 410 420 430 440 450 460 470 480 490 500
 α A L H A T R A A V E E G V V V A G G G V A L I R V A S K L A D L R G - - Q N E D Q N V G I K V A L R A M E A P L R Q I V L N C G E E P S V V A N T V K G - - G D G N Y G Y N A A T E E Y G N M I D M G I L
 β1 A L N A T F A A V E E G I V P G G G A L L H L S E L V P A F K E T L T D A E E K L G A D I V M K S L R A P C R L I A D N A G V E G E V I V Q R L L G - - K P F E V G Y N A M I D K V E N L L D A G V I
 β2 A L N A T K A A V E E G I V I G G G C T L L R L S Q K V D S I K E T L S N E E Q K M G A D I I K R A L S Y P I K L I A N N A G T N G S V V M Q R V M D N I D Q P Y Y G Y N A T D T F E D L M E A G I I

GroEL 501 510 520 530
 α D P T K V T R S A L Q Y A A S V A G L M I T T E C M V T D L P K
 β1 D P A K V T R N G L L N S V S I A G I M L T T Q A V M V E - -
 β2 D P S K V V R C S M E N A V S V A K T F L L A D V V V T E L K E

Fig. S1 Sequence alignment of Cpn60 α , β 1 and β 2 and their homolog GroEL and residue number

aa				β 1 β 1				β 2 β 2			
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