

(a)

10 20 30 40 50 60 70
| | | | | | |
MKG N K I L Y I L G T G I F V G S S C L F S S L F V A A E E Q V Y S E S E V S T V L S K L E K E A I S E A A A E Q Y T V V D R K E D A W G
c t t c e e e e e e t c c e e e c c h h h h h h h h h h h h h h h h c c h h h h h h h h h h h h h h h h h h h e e e e e c c c t t t
M K H L K L E K Q T E G V T V D S D N V I I H L D K N G A V T S V T G N P V D Q V V K I Q S V D A I G E E G V K K I I A S D N P E N K D L V
c e e e e e c c c t t c c c c c e e e e e e c t t c c e e e e h c c c c c c c c h h h h h h h h h h h h h h h h c c c c c c c c c c c
F L A I D K R V N N E G Q L F Y K V R V T S S P T G D P V S L V Y K V N A T D G T I M E K Q D L T E H V G S E V T L K N S F Q V T F N V P V
c e e e e e e c t t c e t t c c e e e h h h h h h h h h c c c c e e c c c c c e e c c c c
E K S N T G I A L H G T D N T G V Y H A V V D G K N N Y S I I Q A P S L A T L N Q N A V D A Y T H G K F V K T Y Y E D H F Q R H S I D D R G
c c c c e e e e c c c c c c c c c c e e e e e e e c c c c c c c c c e e e e c c h h h h h h h h h h h h h h h h c c c c c c t t t
M P I L S V V D E Q H P D A Y D N A F W D G K A M R Y G E T S T P T G K T Y A S S L D V V G H E M T H G V T E H T A G L E Y L G Q S G A L N
c e e e e e e e c c c c c c h h e e t t c e e e e c c c c c e e c c c c h h h h h h h h h h h h h h h h h c c c e e e e c c c t t c h h
E S Y S D L M G Y I I S G A S N P E I G A D T Q S V D R K T G I R N L Q T P S K H G Q P E T M A Q Y D D R A R Y K G T P Y Y D Q G G V H Y N
h h h h h h h h h h h h c c c e e c c e e e e c c c c c c c c h h h h c c c c c c c c c c c c h h c c c c c c c c c c c c e e e c
S G I I N R I G Y T I I Q N L G I E K A Q T I F Y S S L V N Y L T P K A Q F S D A R D A M L A A A K V Q Y G D E A A S V V S A A F N S A G I
t t c c c h h e e e e e t t c c c c c h h h h h h h h h h e e c c c c c c h h h h h h h h h h h h h h c c c c c h h h h h h h h h t t c
G A K E D I Q V N Q P S E S V L V N E
C c c c e e e c c c c c e e e e h

Sequence length: 509

SOPMA:

Alpha helix	(Hh)	:	162	is	31.83%
Extended strand	(Ee)	:	110	is	21.61%
Beta turn	(Tt)	:	27	is	5.30%
Random coil	(Cc)	:	210	is	41.26%

(b)

10 20 30 40 50 60 70
| | | | | | |
MKG N K I L Y I L G T G I F V G S S C L F S S L F V A A E E Q V Y S E S E V S T V L S K L E K E A I S E A A A E Q Y T V V D R K E D A W G
c c c c e e e e e e e e c c c c e e c c c c c c c c h h h h h h h h h h c c c c c h
M K H L K L E K Q T E G V T V D S D N V I I H L D K N G A V T S V T G N P V D Q V V K I Q S V D A I G E E G V K K I I A S D N P E N K D L V
h h h h h h c c c c c e h h h h h h h c e e e e e e e e e e c c c h h h
F L A I D K R V N N E G Q L F Y K V R V T S S P T G D P V S L V Y K V N A T D G T I M E K Q D L T E H V G S E V T L K N S F Q V T F N V P V
h h h h h h h c c c c c e c c c c c h h h h h h c c c c c c e e e e e e e e e e e e e c c
E K S N T G I A L H G T D N T G V Y H A V V D G K N N Y S I I Q A P S L A T L N Q N A V D A Y T H G K F V K T Y Y E D H F Q R H S I D D R G
c c c e e e e e e e c c c c e e e e e e e e e e e e e e e e c c c h h h h h h c h h h h h h c c c e e e e e e e e e e e e e e c c c c c c
M P I L S V V D E Q H P D A Y D N A F W D G K A M R Y G E T S T P T G K T Y A S S L D V V G H E M T H G V T E H T A G L E Y L G Q S G A L N
c e e e e e e c c c c e c c h h h h h h h c c c c c c c c c c c c c c c c
E S Y S D L M G Y I I S G A S N P E I G A D T Q S V D R K T G I R N L Q T P S K H G Q P E T M A Q Y D D R A R Y K G T P Y Y D Q G G V H Y N
h h h h h h h e e e e e c c c c c c c c c c c c c c h h h h c e e e e e e e e e e e e c c c c c c h h h h h h h h h c c c c e e e e c c c c c c c c
S G I I N R I G Y T I I Q N L G I E K A Q T I F Y S S L V N Y L T P K A Q F S D A R D A M L A A A K V Q Y G D E A A S V V S A A F N S A G I
c c c e e e c c h h h h h h c c h h h h h h h h h h h h h h c c c c c h c c h h h h h h h h h h h h h h c c c
G A K E D I Q V N Q P S E S V L V N E
C c c c h h h h c c c c c e e e e c

Sequence length: 509

GOR4:

Alpha helix	(Hh)	:	158	is	31.04%
Extended strand	(Ee)	:	119	is	23.38%
Random coil	(Cc)	:	232	is	45.58%

Figure S1 Secondary structure prediction by (a) SOPMA and (b) GOR4 programme.

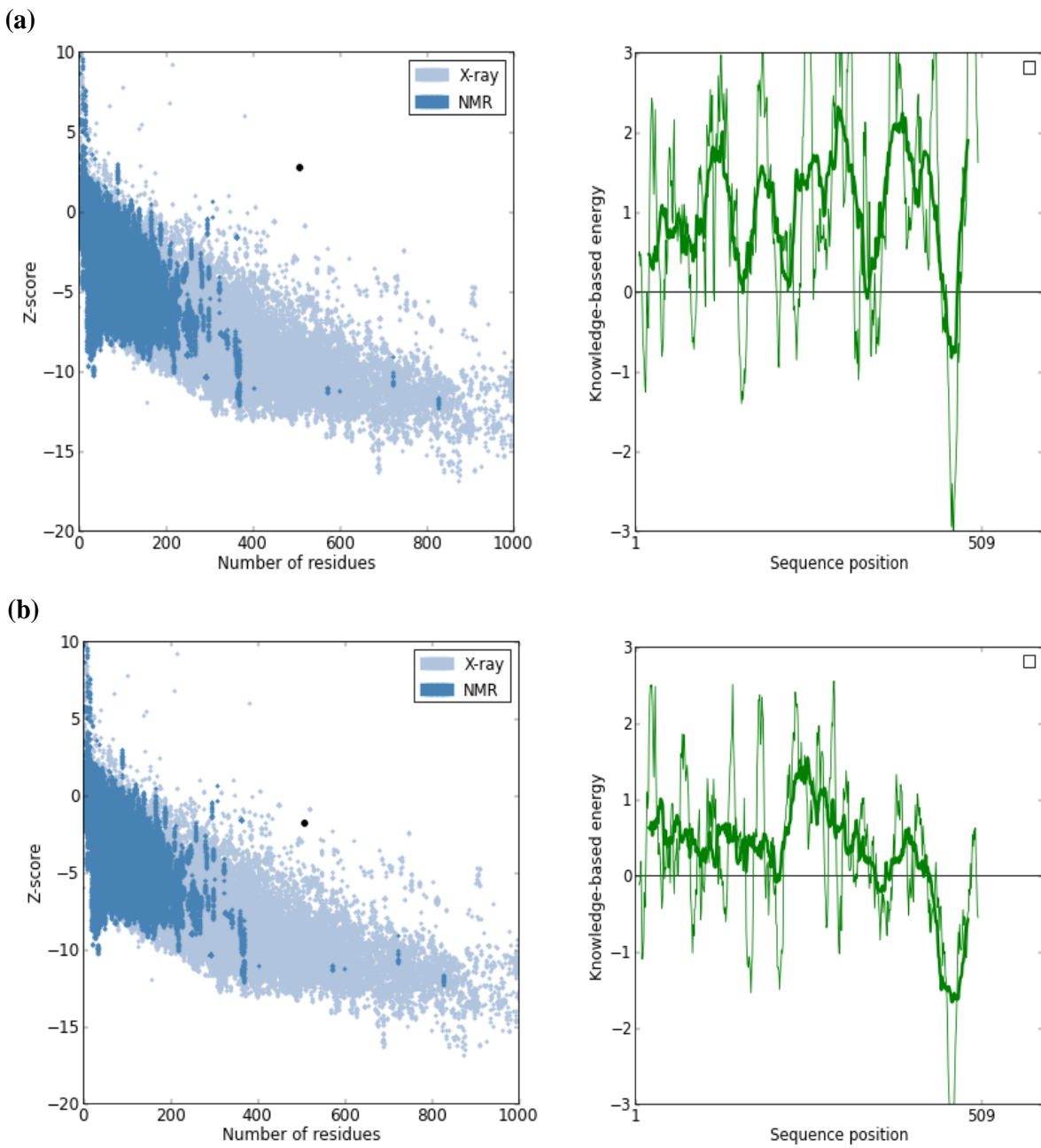


Figure S2 ProSA-web Z-scores of models (a) MUSTER and (b) MODELLER indicated by black dot and residue energies averaged over a sliding window.

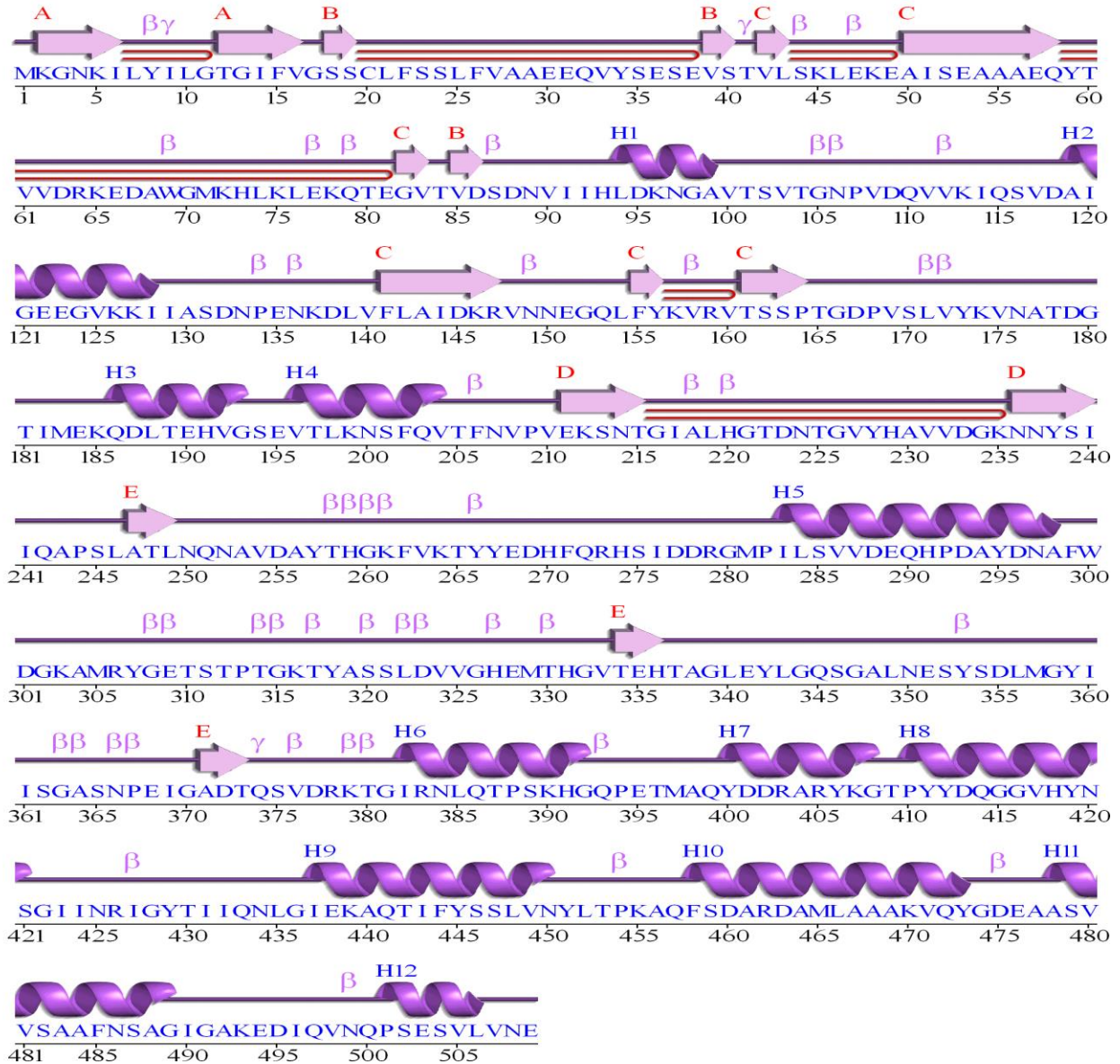


Figure S3 Structural details of predicted model of gelatinase from *Enterococcus faecalis* obtained by PDBsum. Helices are labeled with letter H followed by number (blue), strands with A, B (red), β and γ represents beta and gamma turn respectively.