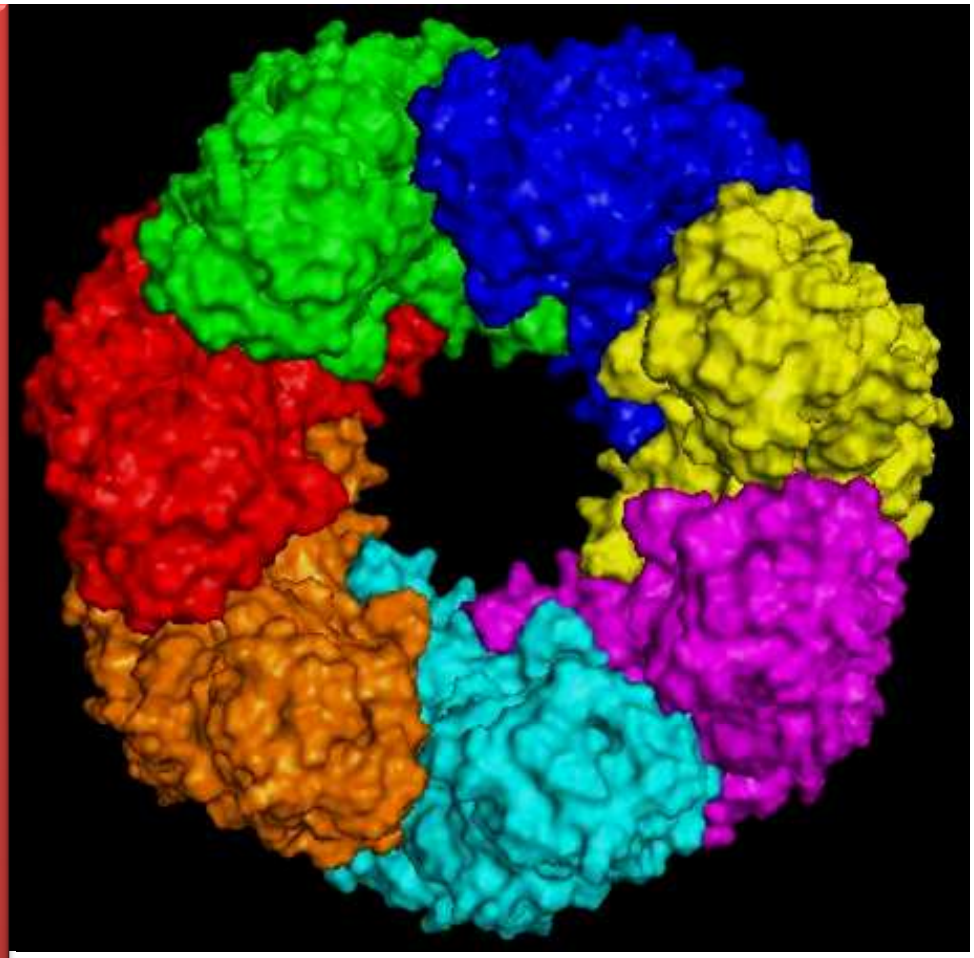
MOLECULAR CHAPERONES

Chaperonins



Oriol Bel, Esther Llaudet, Laura Luque i Rebeca Reus

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UPF

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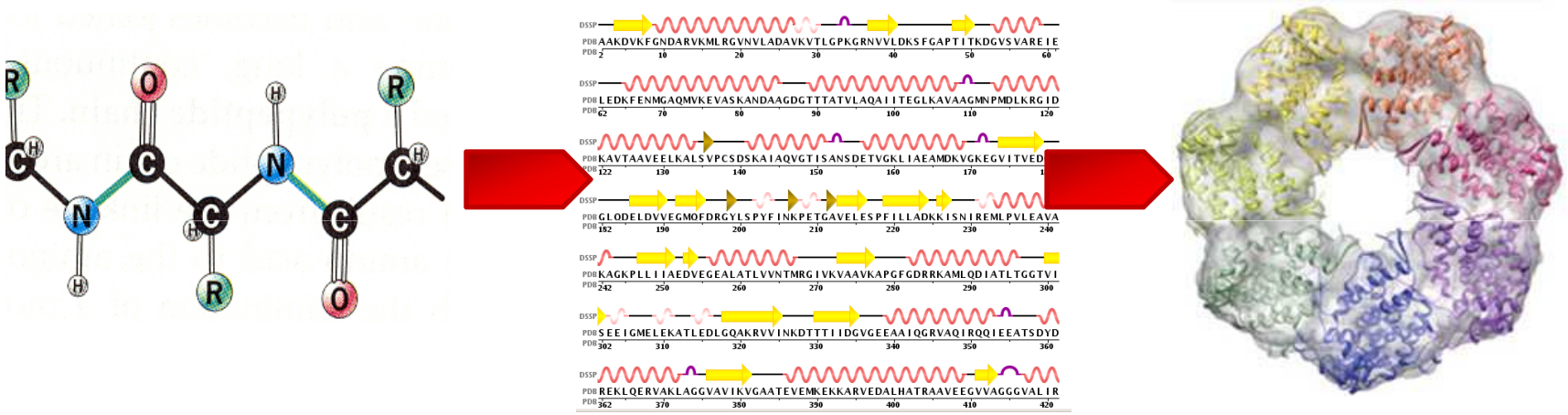
Introduction > Protein folding

How is tertiary structure determined in a protein?



PRIMARY STRUCTURE **SECONDARY STRUCTURE** **TERTIARY STRUCTURE**

Introduction > Molecular chaperones

Chaperone: protein that interacts, stabilizes or helps non-native proteins to acquire their native conformation.

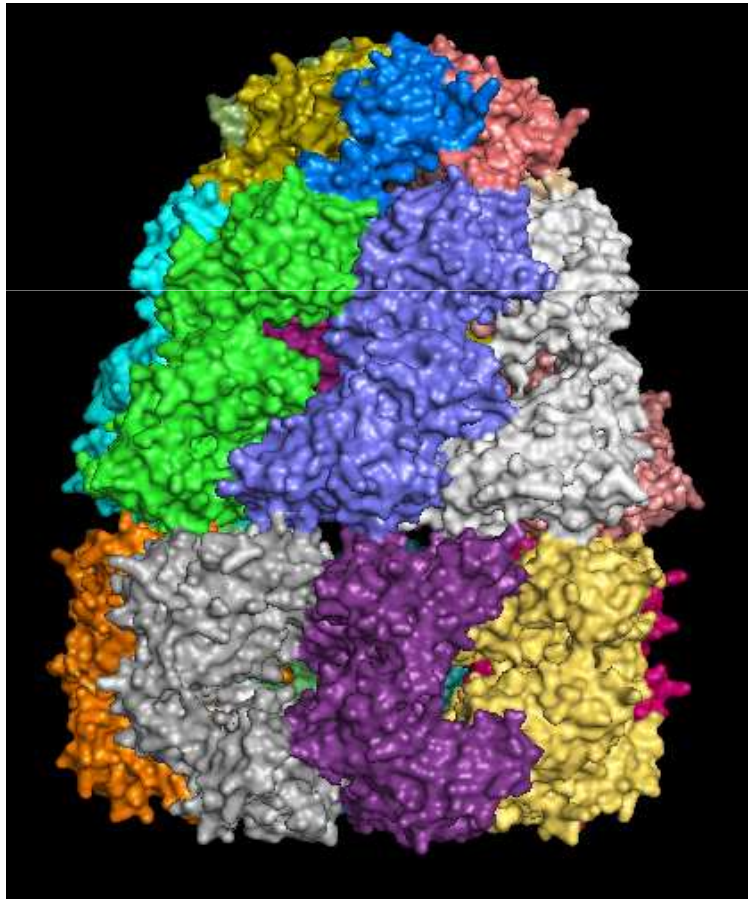


Fig1. GroEL/GroES chaperone complex (1AON)

Not present in the final functional structure.

Functions:

- *De novo* folding.
- Refolding of denatured species.
- Disruption of unspecific aggregations.

Introduction > Protein aggregation

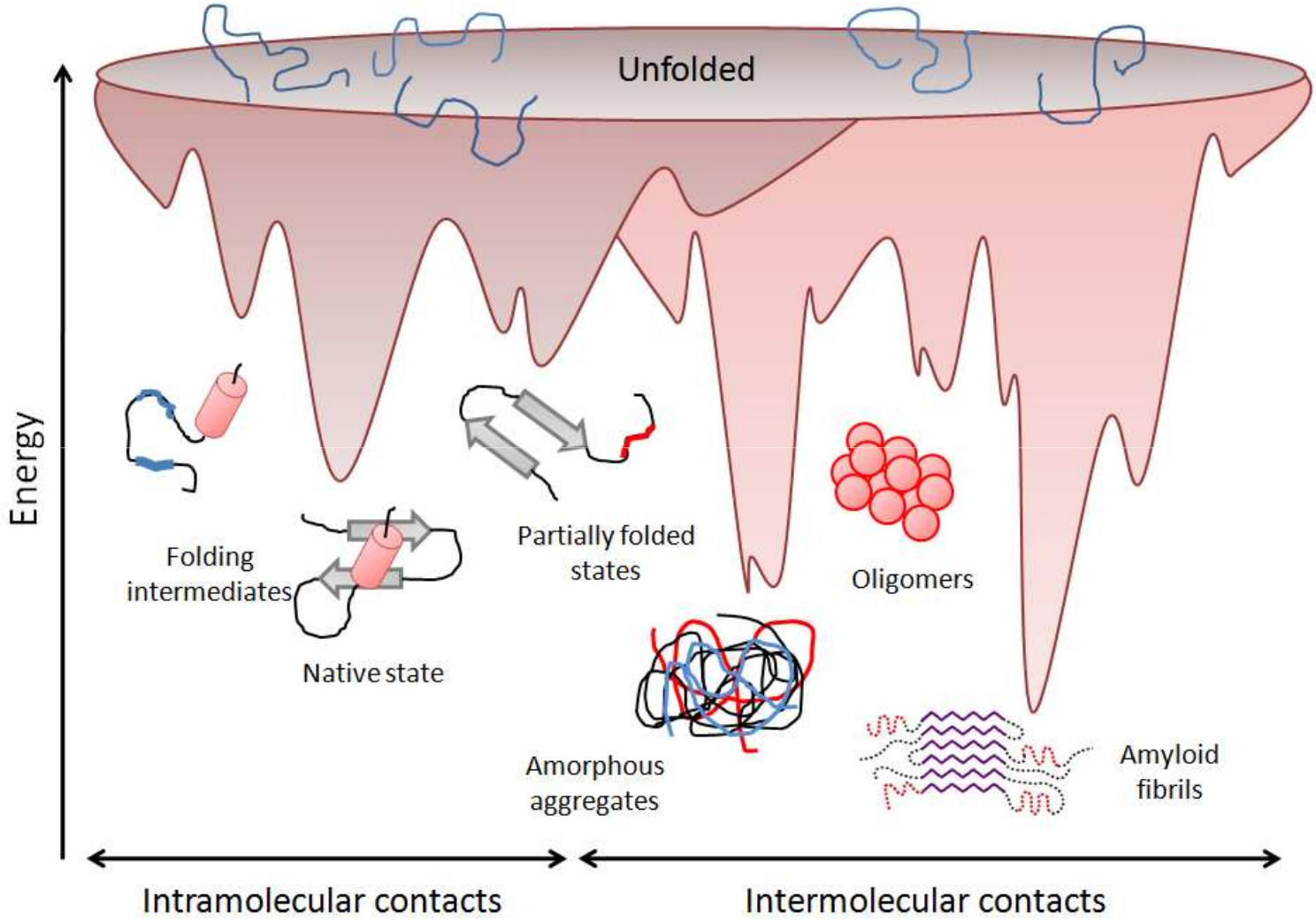


Fig2. Energy landscape scheme of protein folding and aggregation

Molecular chaperones > General features

- Recognition of exposed hydrophobic groups.
- ATP-regulated cycle.
- Unrelated, heterogeneous proteins.
- Network organization.

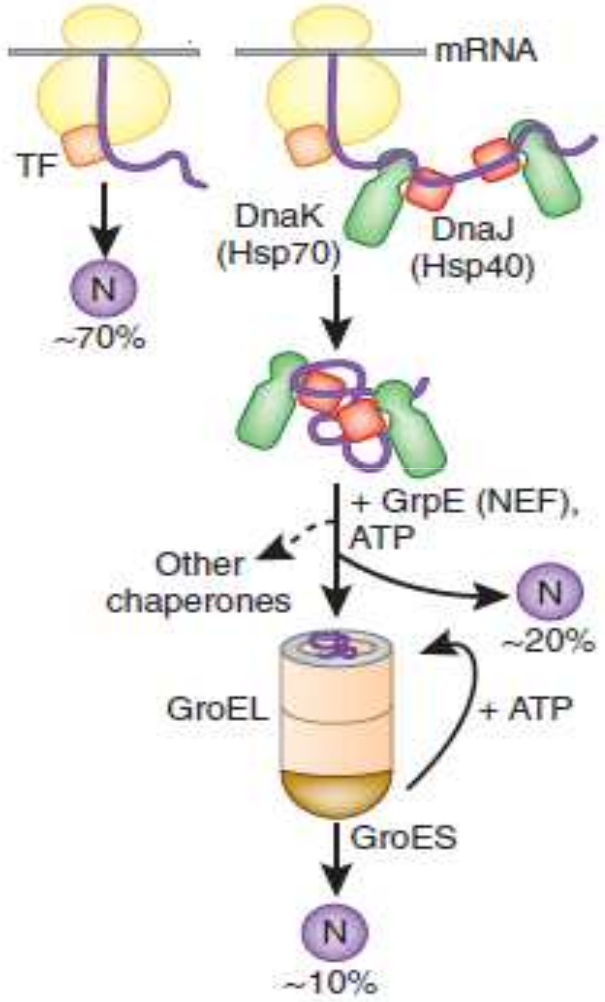


Fig3. Protein folding in the bacterial cytosol, extracted from:
Hartl FU, Hayer-Hartl M. Converging concepts of protein folding in vitro and in vivo. Nat Struct Mol Biol. 2009; 16(6): 574-81.

Chaperone groups > Trigger factor

- **Prokaryotic**
- **Ribosome-associated**
- **Not ATP binding**
- **Channel-shaped**

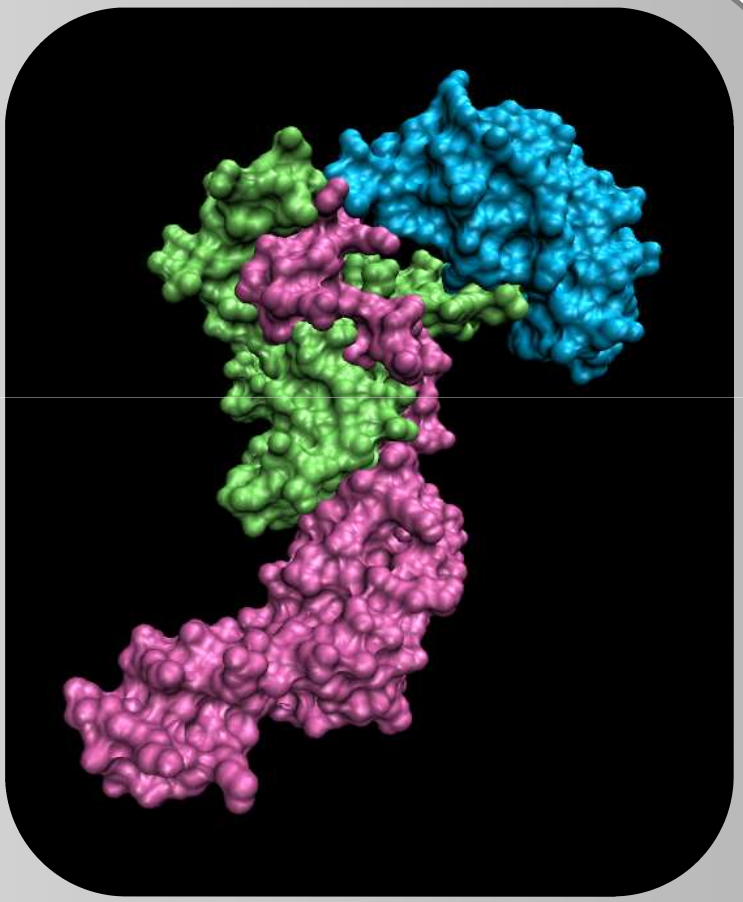


Fig4. Trigger factor of *V. Cholerae* (1T11)

Chaperone groups > Hsp70

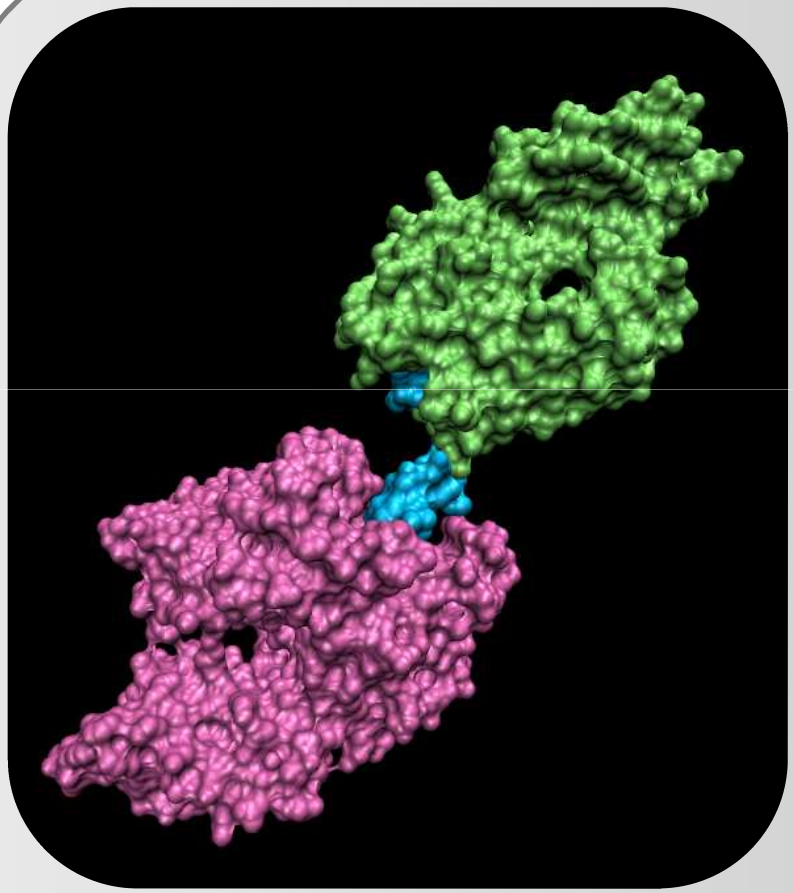


Fig5. DnaK of *E. Coli* (2KHO)

- **Prokaryotes and eukaryotes**
- **ATP-driven cycle**
- **Central organizer of the chaperone network**

Chaperone groups > Hsp90

- **Eukaryotes and bacteria**
- **ATP-driven cycle**
- **Homodimer with 3 domains per subunit**

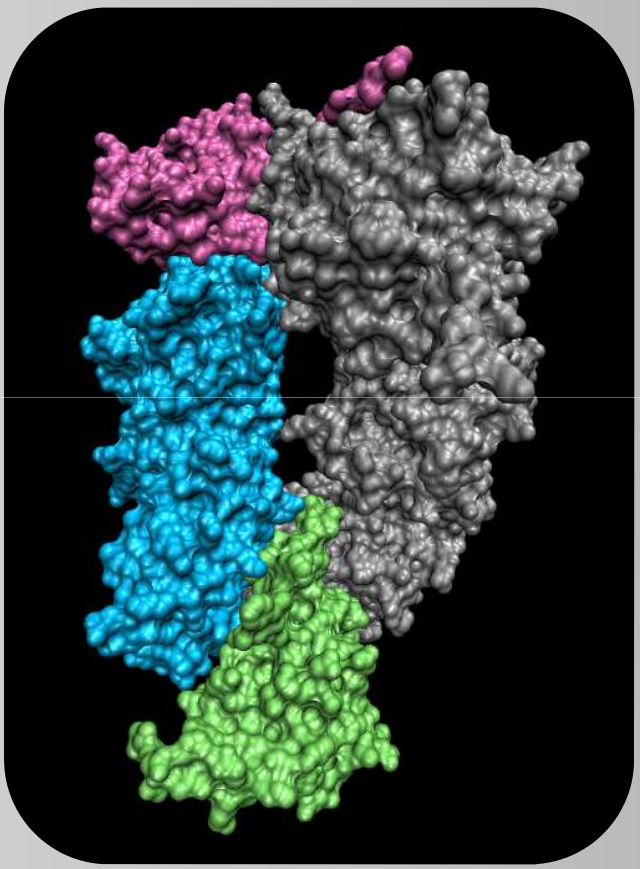


Fig6. Hsp90 of S. *cerevisiae* (2CG9)

Chaperone groups > Chaperonins

- Large, cage-like cylindrical complexes
- Eukaryotes and prokaryotes
- ATP-driven cycle
- 3 domains
- Organization in rings

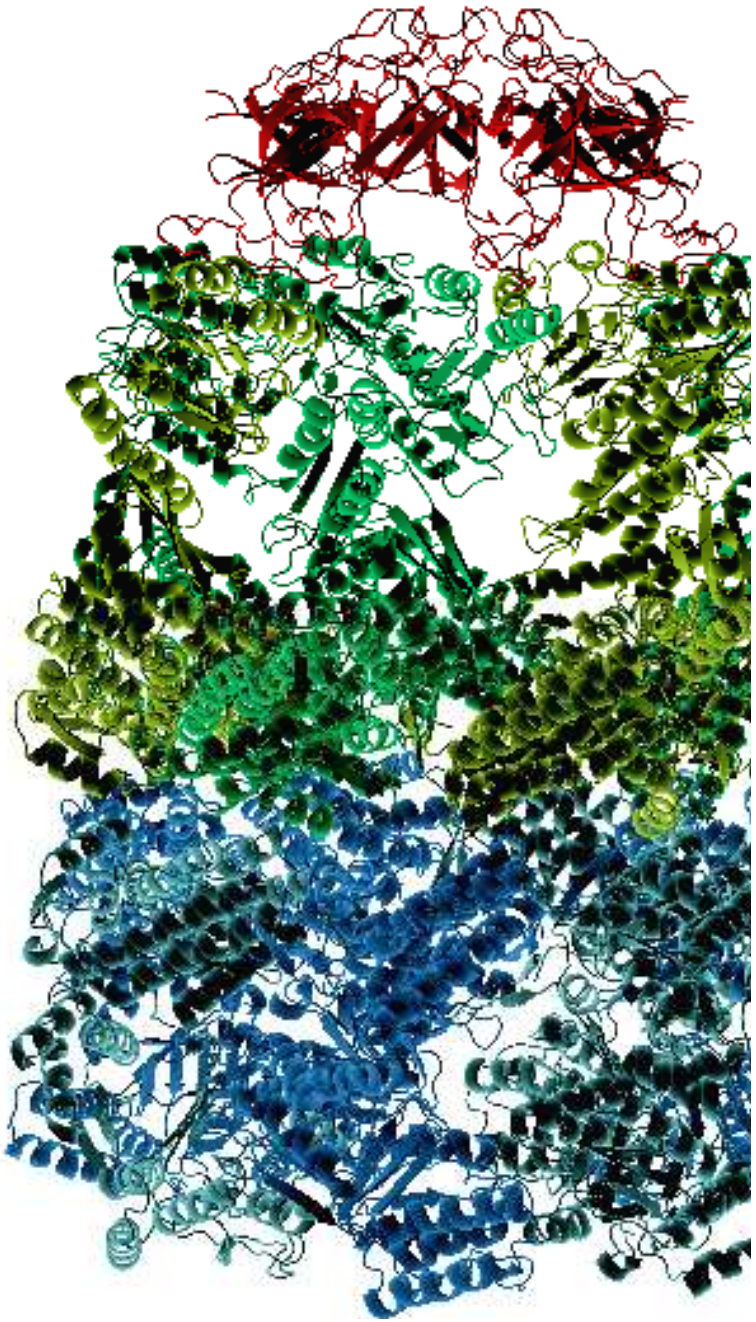


Fig7. GroEL/GroES complex of *E. coli* (1AON)

Chaperone groups > Chaperonins

GroEL apical domain-like superfamily

SCOP classification

Root: SCOP hierarchy in SUPERFAMILY [SCOP 0] (11)
Class: Alpha and beta proteins (a/b) [SCOP 51349] (147)
Fold: The "swivelling" beta/beta/alpha domain [SCOP 52008] (10)
Superfamily: **GroEL apical domain-like** [SCOP 52029] (2)
Families: GroEL-like chaperone, apical domain [SCOP 52030]
Group II chaperonin (CCT, TRIC), apical domain [SCOP 52034]

GroEL-intermediate domain like superfamily

SCOP classification

Root: SCOP hierarchy in SUPERFAMILY [SCOP 0] (11)
Class: Alpha and beta proteins (a+b) [SCOP 53931] (376)
Fold: GroEL-intermediate domain like [SCOP 54848]
Superfamily: **GroEL-intermediate domain like** [SCOP 54849] (2)
Families: GroEL-like chaperone, intermediate domain [SCOP 54850]
Group II chaperonin (CCT, TRIC), intermediate domain [SCOP 54853]

GroEL equatorial domain-like superfamily

SCOP classification

Root: SCOP hierarchy in SUPERFAMILY [SCOP 0] (11)
Class: All alpha proteins [SCOP 46456] (284)
Fold: GroEL equatorial domain-like [SCOP 48591]
Superfamily: **GroEL equatorial domain-like** [SCOP 48592] (2)
Families: GroEL chaperone, ATPase domain [SCOP 48593]
Group II chaperonin (CCT, TRIC), ATPase domain [SCOP 48596]

GroES-like superfamily

SCOP classification

Root: SCOP hierarchy in SUPERFAMILY [SCOP 0] (11)
Class: All beta proteins [SCOP 48724] (174)
Fold: GroES-like [SCOP 50128] (2)
Superfamily: **GroES-like** [SCOP 50129] (2)
Families: GroES [SCOP 50130] (2)

Chaperone groups > Chaperonins

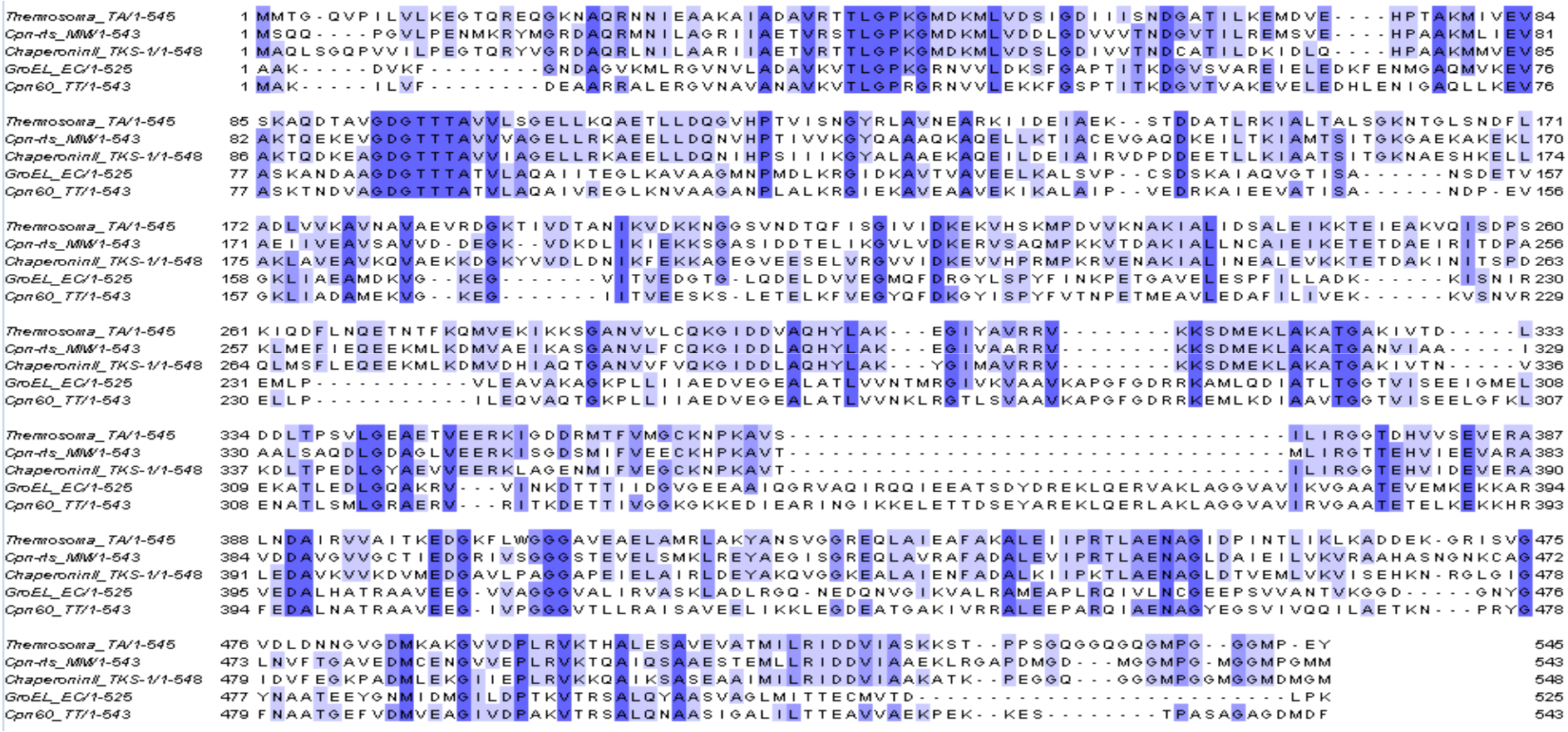


Fig8. Sequence alignment between members of both group I and II of chaperonins

Chaperone groups > Chaperonins

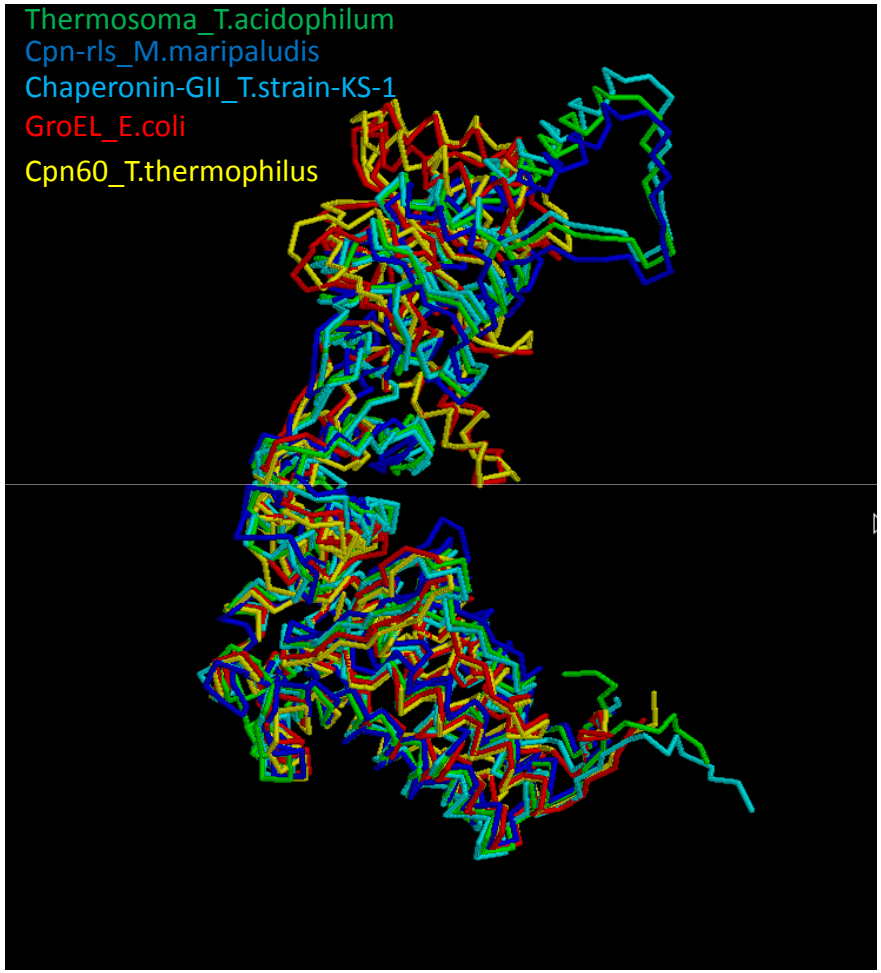


Fig9. Chaperonin whole-subunit structural alignment

RMSD 2.58
Sc 6.88

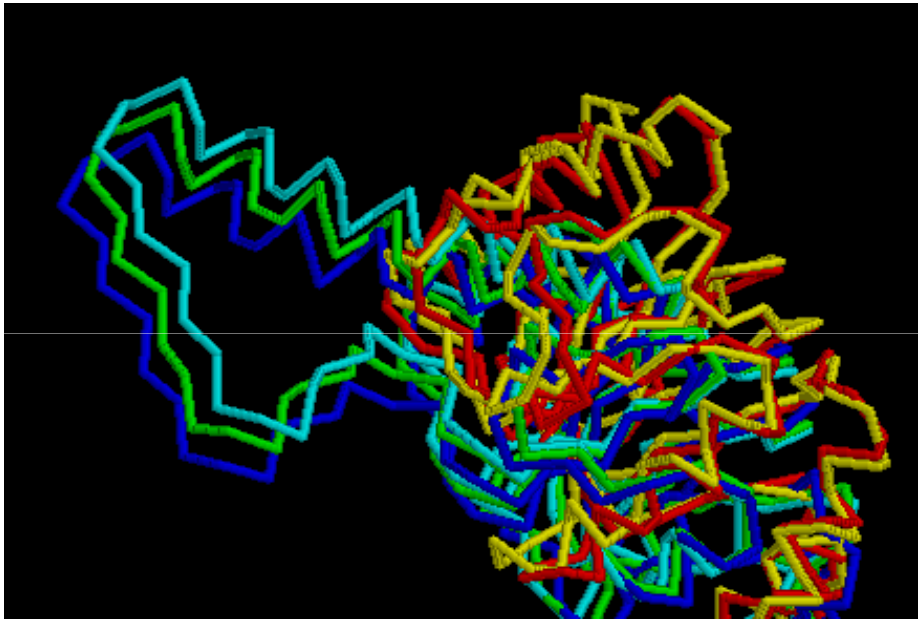


Fig10. Chaperonin apical domain structural alignment

GROUP I CHAPERONINS

Chaperonins group I > Main characteristics

- Eubateria, mitochondria and chloroplasts
- Cochaperonin-dependent
- GroEL-GroES from *E. coli*

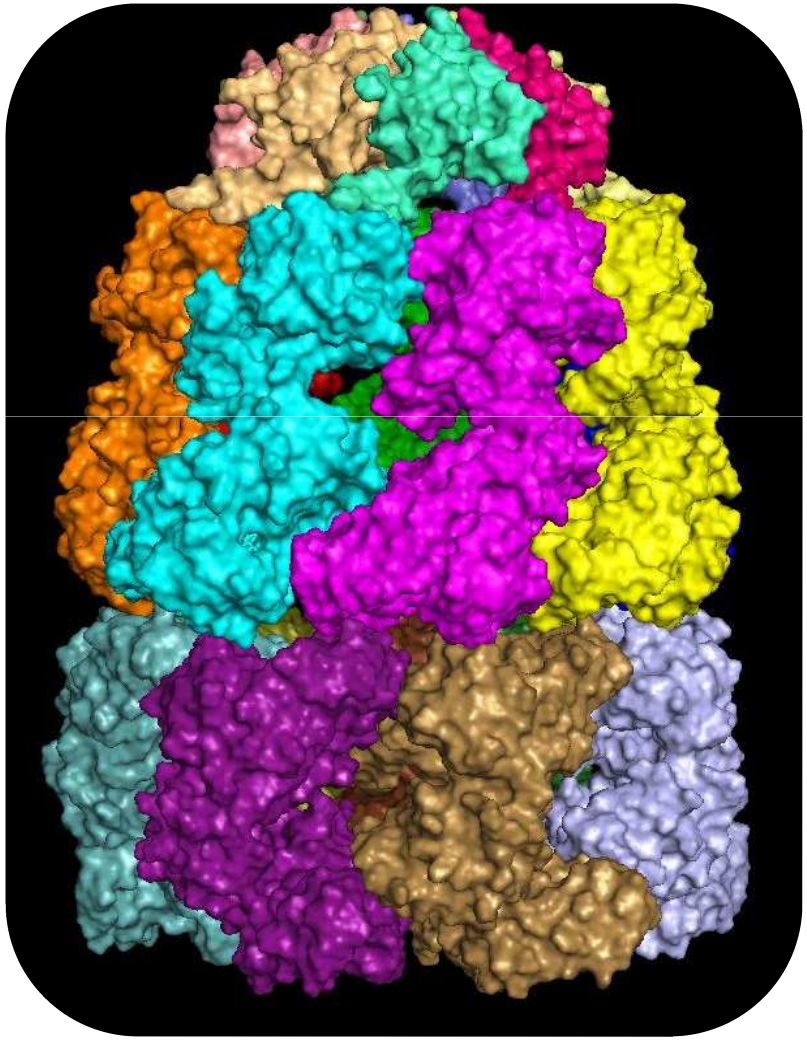


Fig11. GroEL complex with the cochaperonin GroES of *E. coli* (1AON)

Chaperonins group I > Sequence conservation

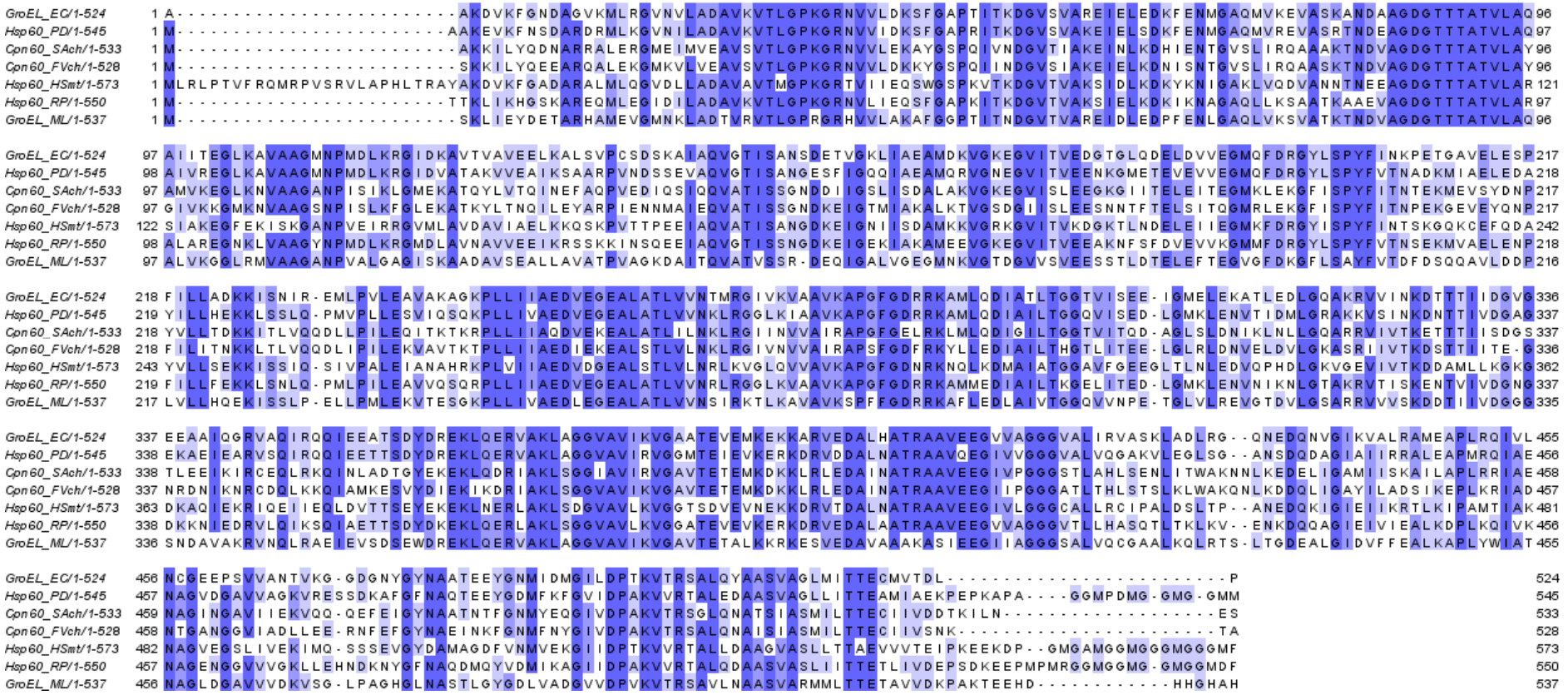


Fig12. Sequence alignment between members of the group I chaperonins

GroEL/GroES > General structure

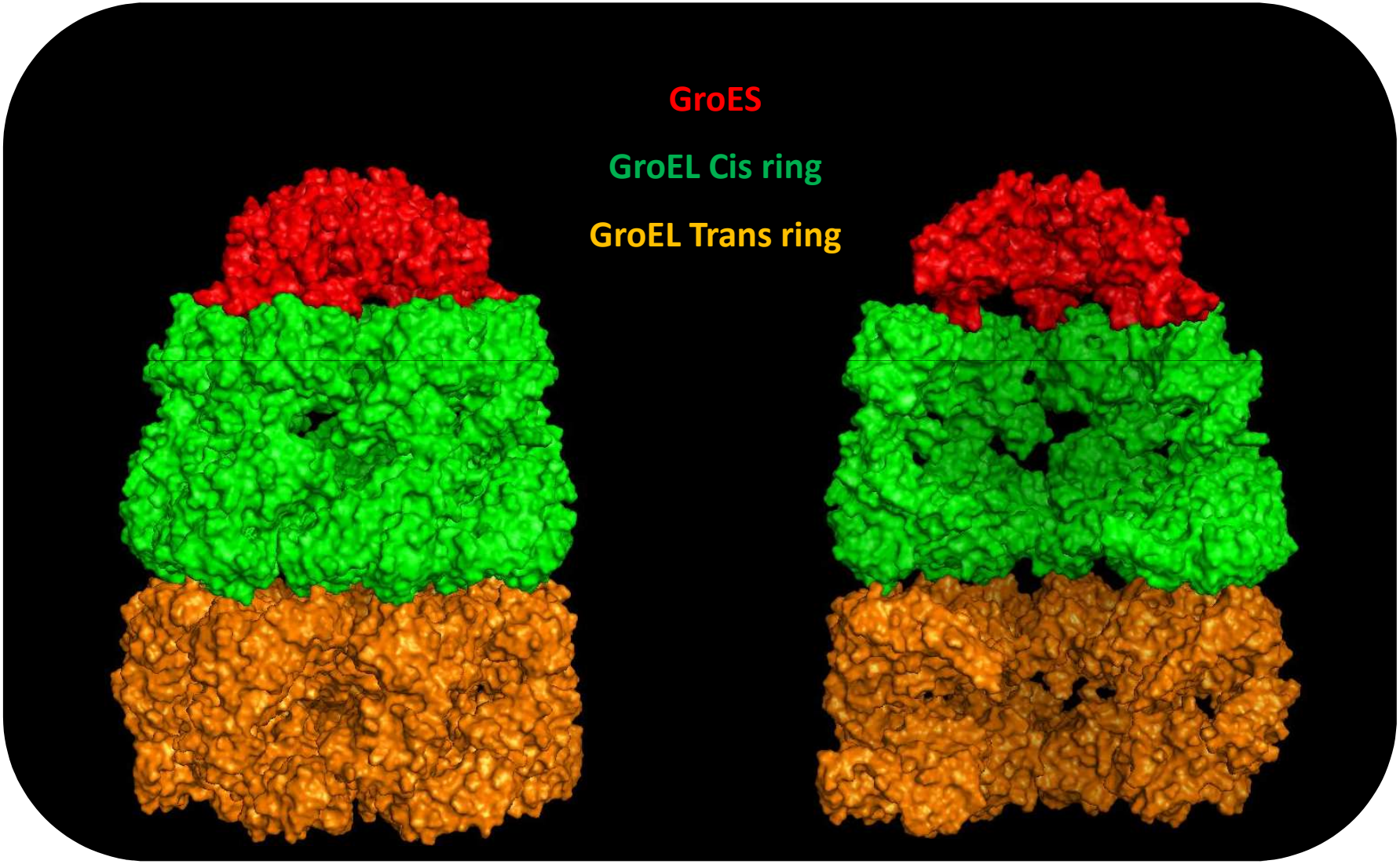


Fig13. GroEL/GroES surface (1AON)

Fig14. GroEL/GroES internal cavity (1AON)

GroEL/GroES > General structure

GroES → 7 subunits

GroEL Cis ring → 7 subunit

GroEL Trans ring → 7 subunit

119,553 atoms

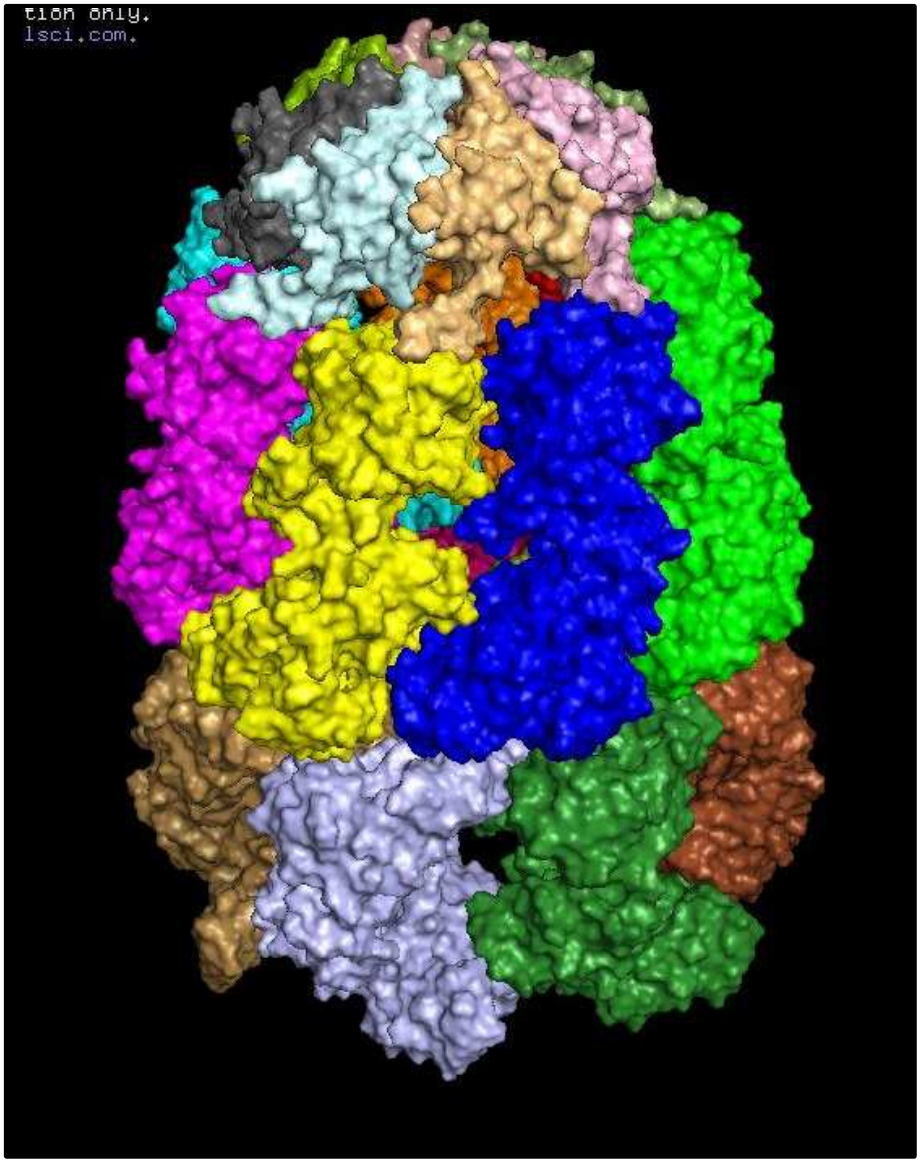


Fig15. GroEL/GroES subunit reconstruction (1AON)

GroEL/GroES> General structure GroEL

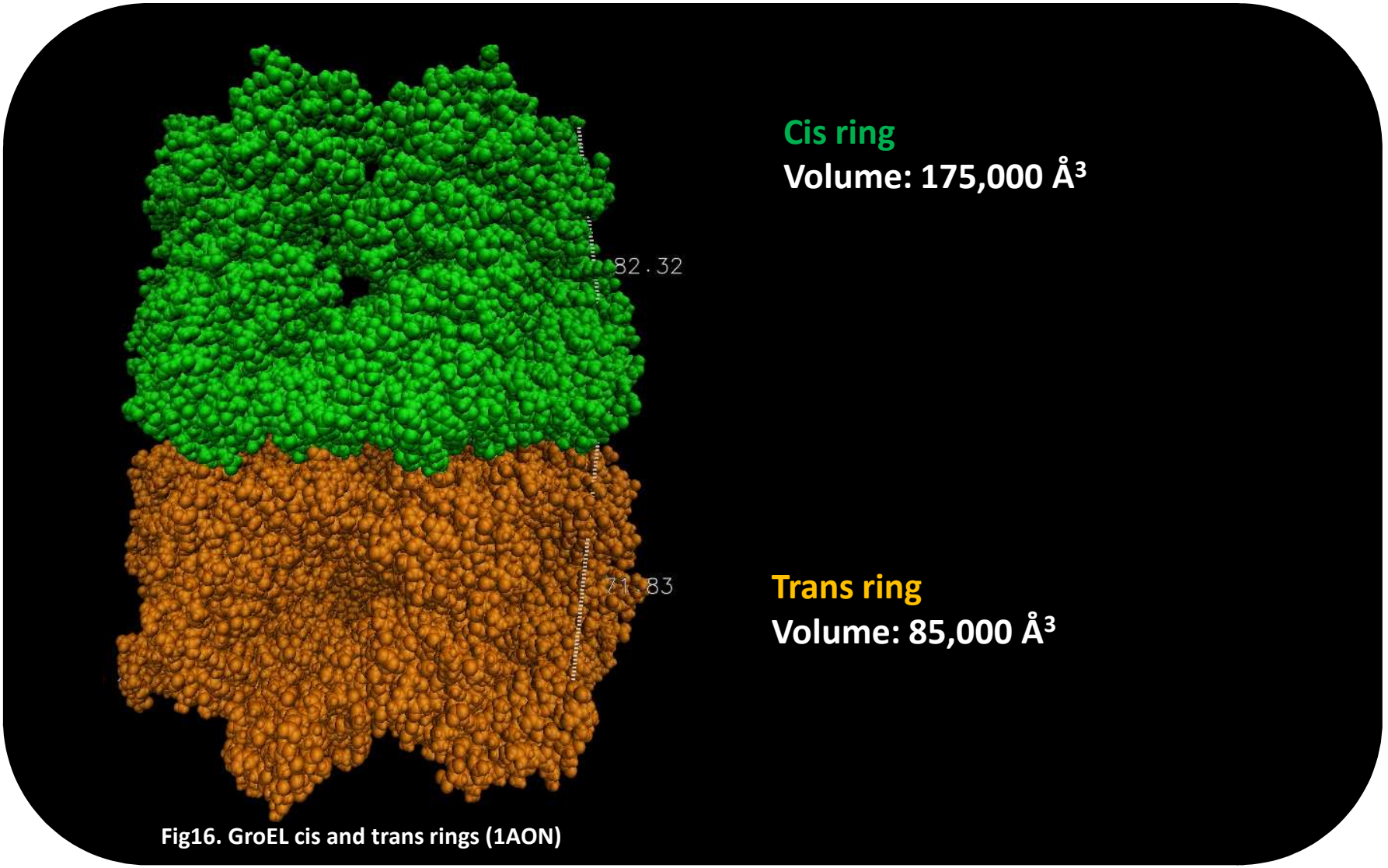


Fig16. GroEL cis and trans rings (1AON)

GroEL/GroES> General structure GroEL

The cis ring has the internal cavity **polar** to promote producting folding

The trans ring has the internal cavity **hydrophobic**

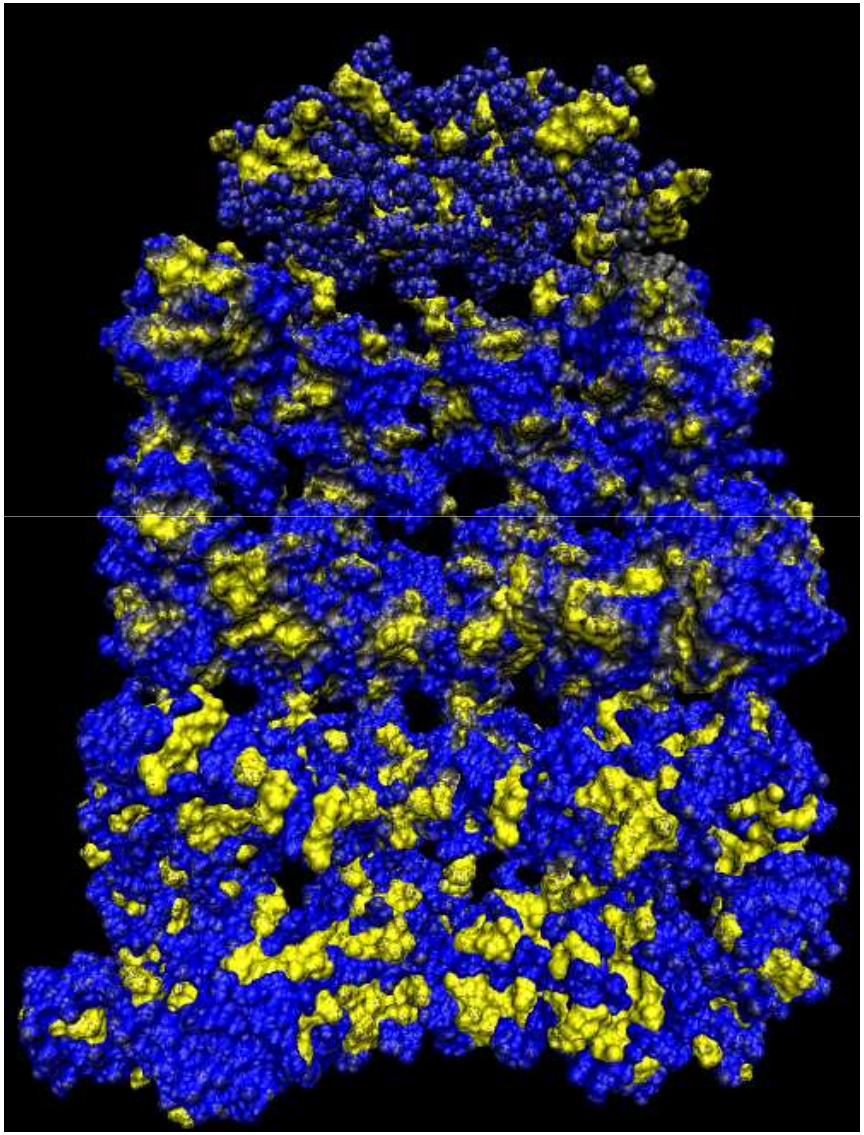


Fig17. GroEL/GroES internal cavity (1AON)

GroEL/GroES> General structure GroEL

Subunits of 548 aa

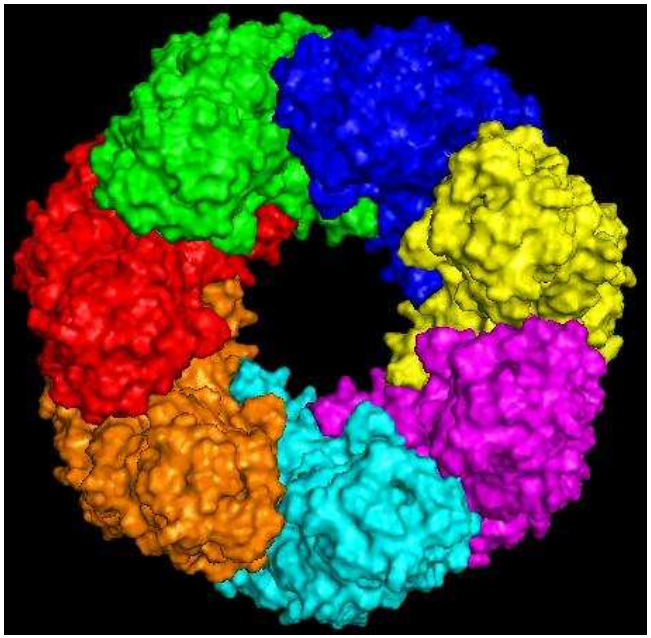


Fig18. GroEL cis ring subunits (1AON)

Domains: apical
intermediate
equatorial

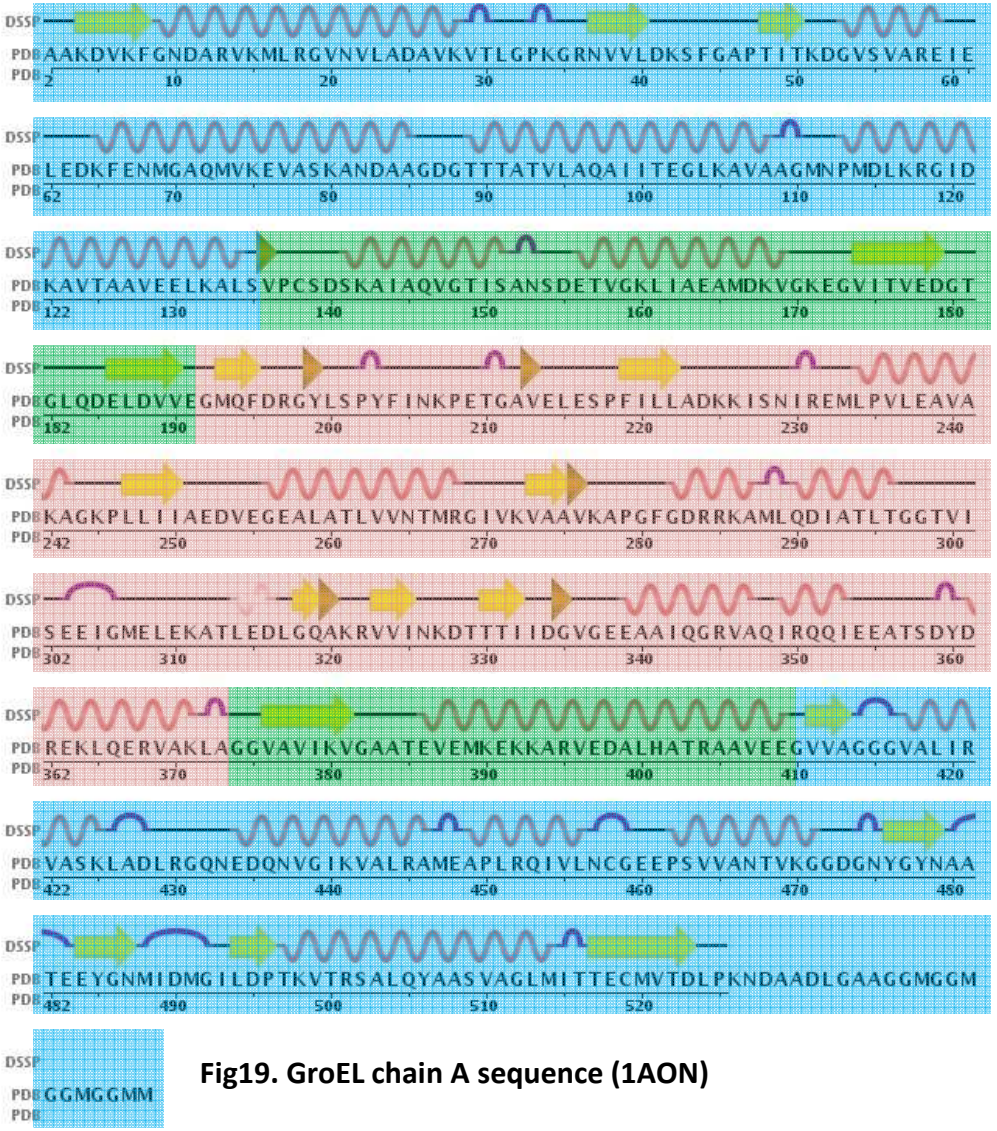


Fig19. GroEL chain A sequence (1AON)

GroEL/GroES> Subunit structure

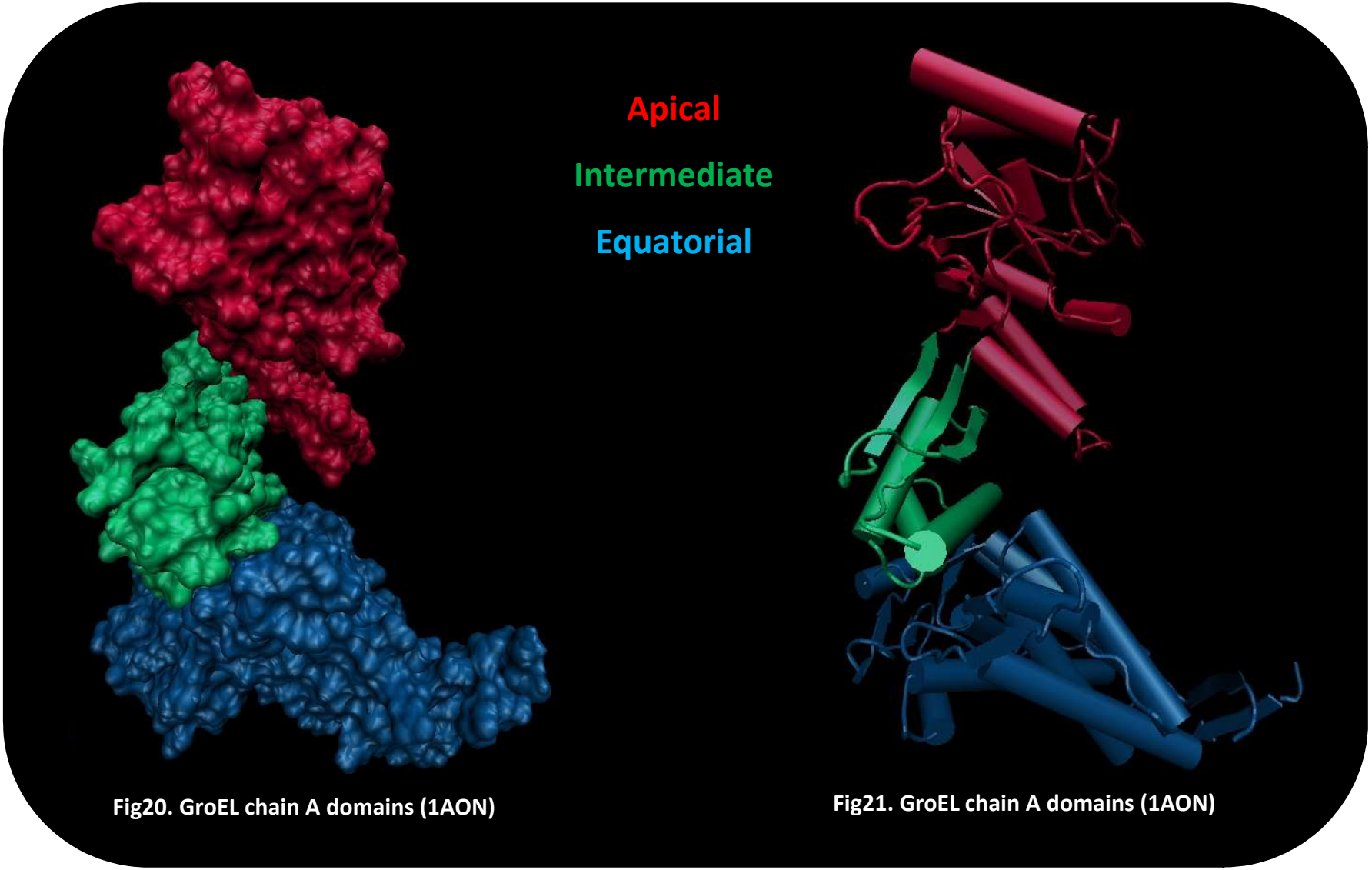


Fig20. GroEL chain A domains (1AON)

Fig21. GroEL chain A domains (1AON)

GroEL/GroES> Inter-ring interactions

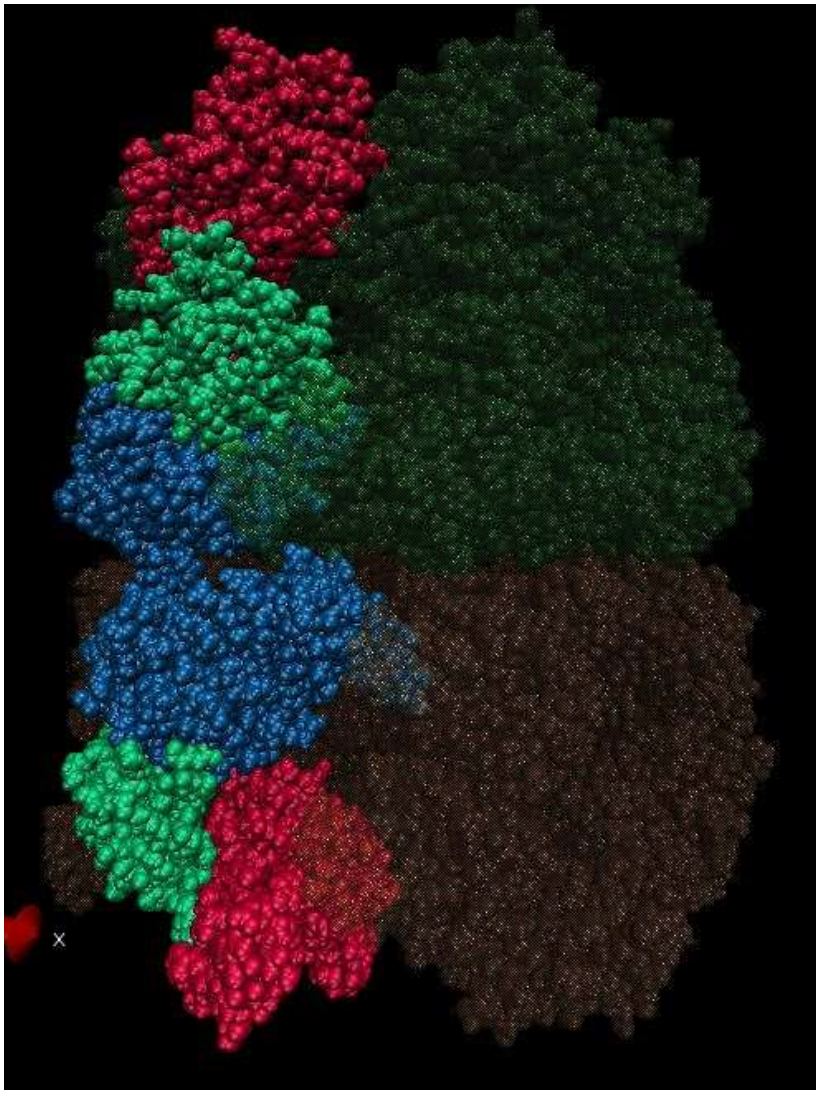


Fig22. GroEL chain A and H (1AON)

LEFT SITE: interaction between adjacent subunits

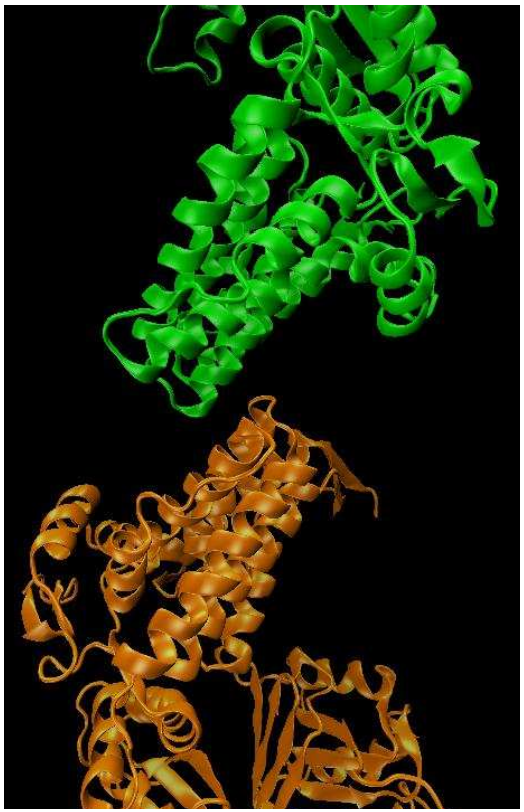


Fig23. GroEL equatorial domains chain A and H (1AON)

GroEL/GroES> Inter-ring interactions

LEFT SITE

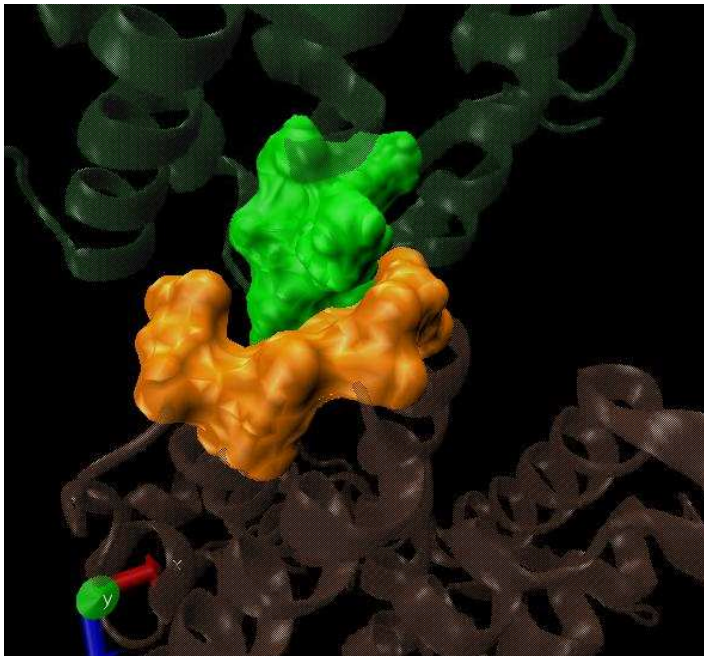


Fig24. Inter-ring interaction residues, surface (1AON)

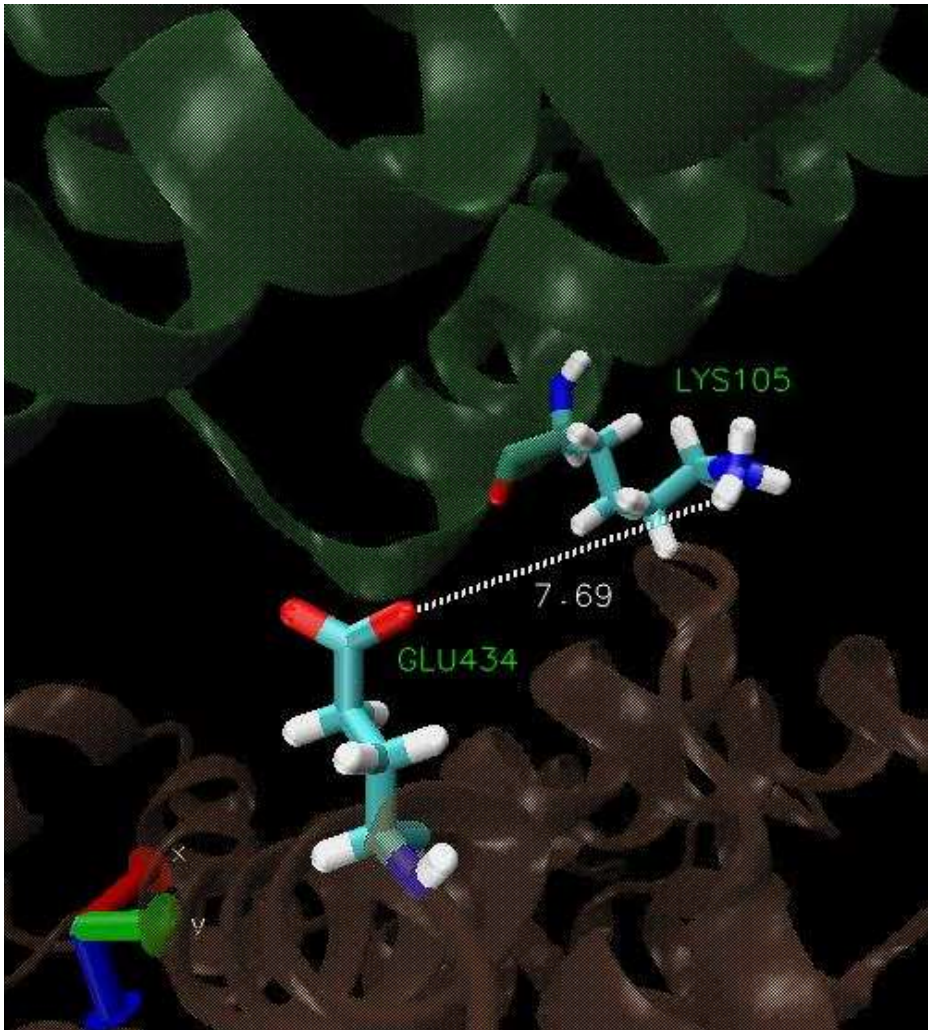


Fig25. Inter-ring interaction residues, salt bridge (1AON)

GroEL/GroES> Inter-ring interactions

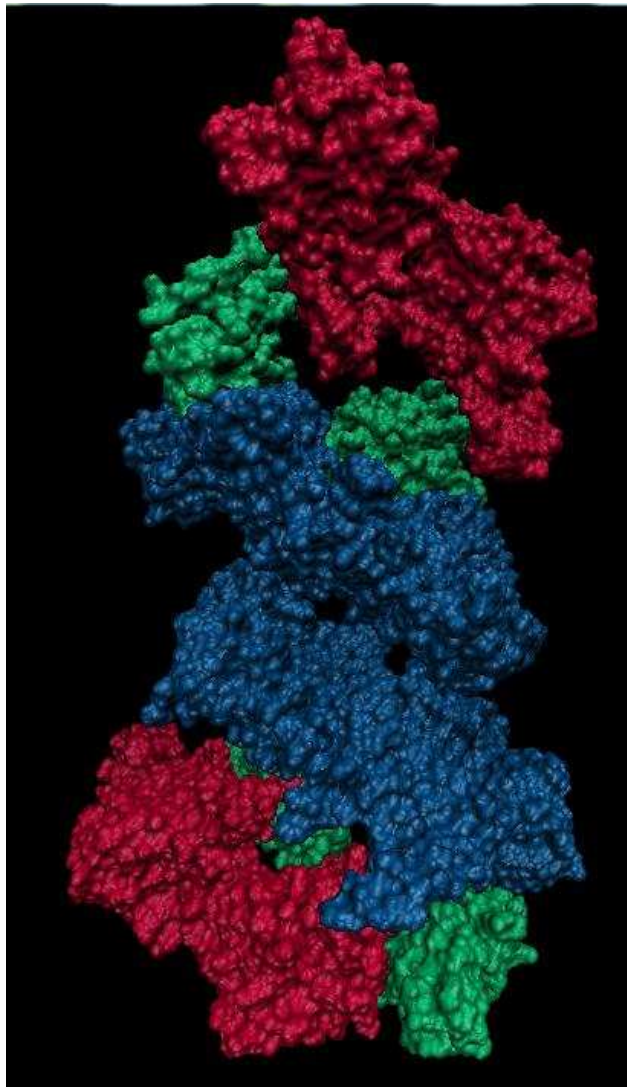


Fig26. GroEL chains A-B (cis) and H-I (trans) (1AON)

RIGHT SITE: interaction between one cis subunit and the left subunit from the trans ring

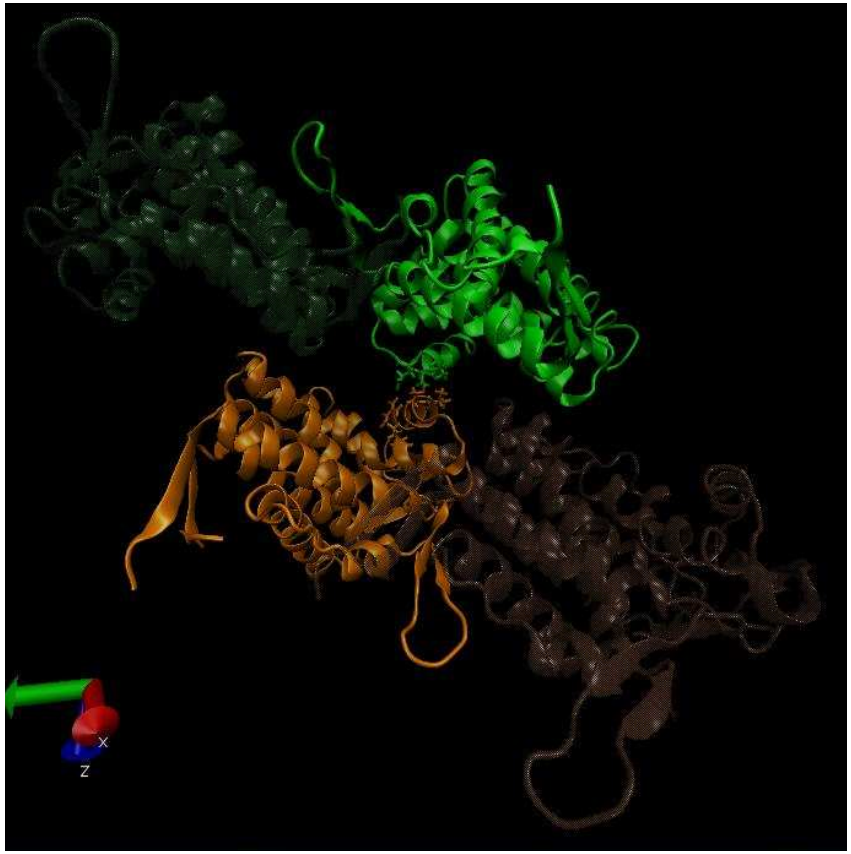


Fig27. GroEL chains B and H, equatorial domains (1AON)

GroEL/GroES> Inter-ring interactions

RIGHT SITE

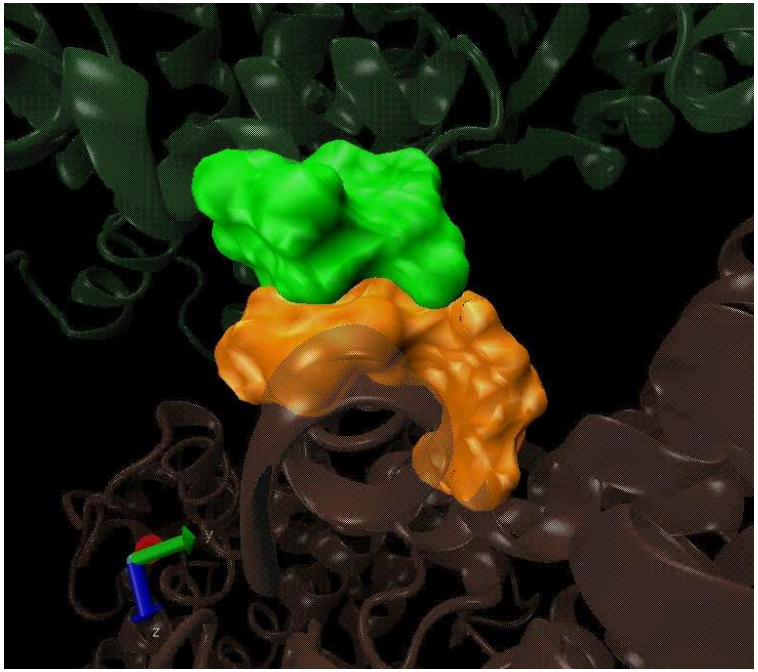


Fig28. Inter-ring interaction residues, surface (1AON)

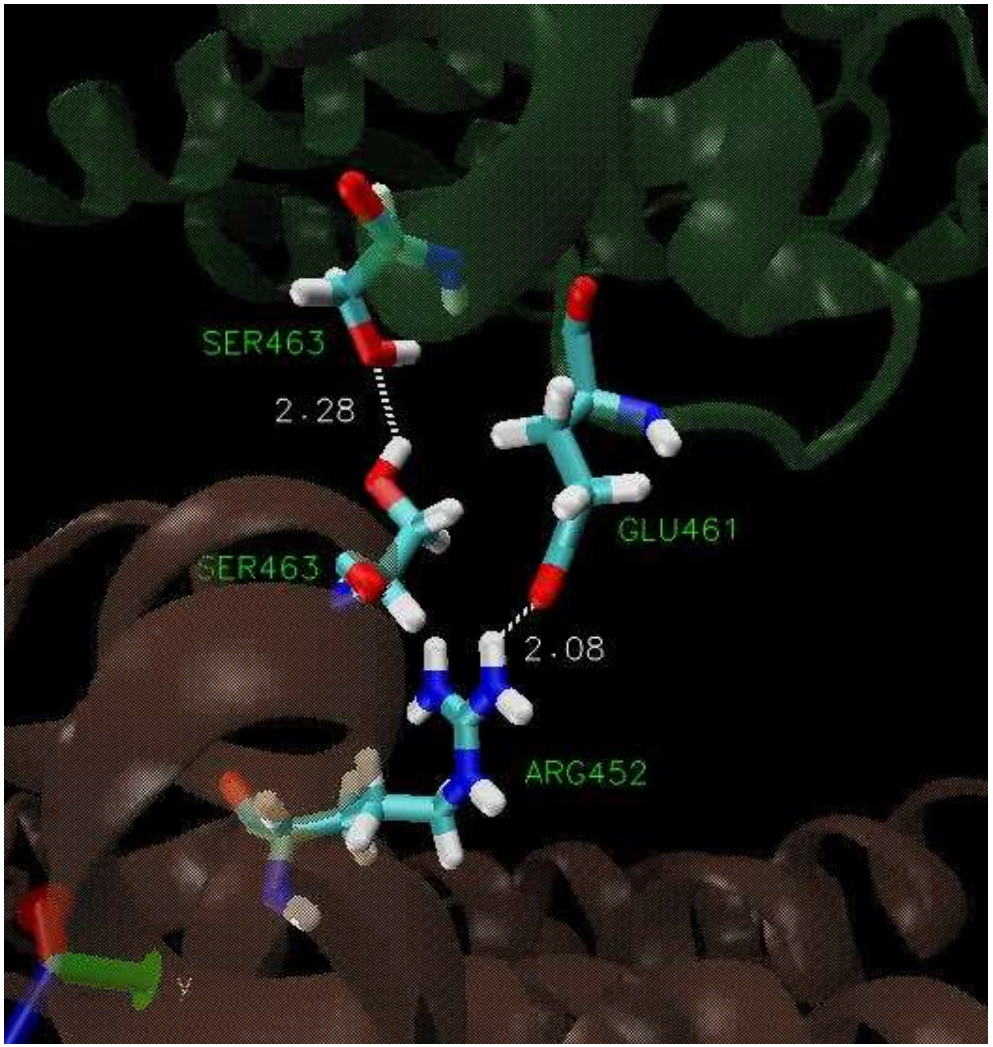


Fig29. Inter-ring interaction residues, salt bridge and Hbond (1AON)

GroEL/GroES> Intra-ring interactions

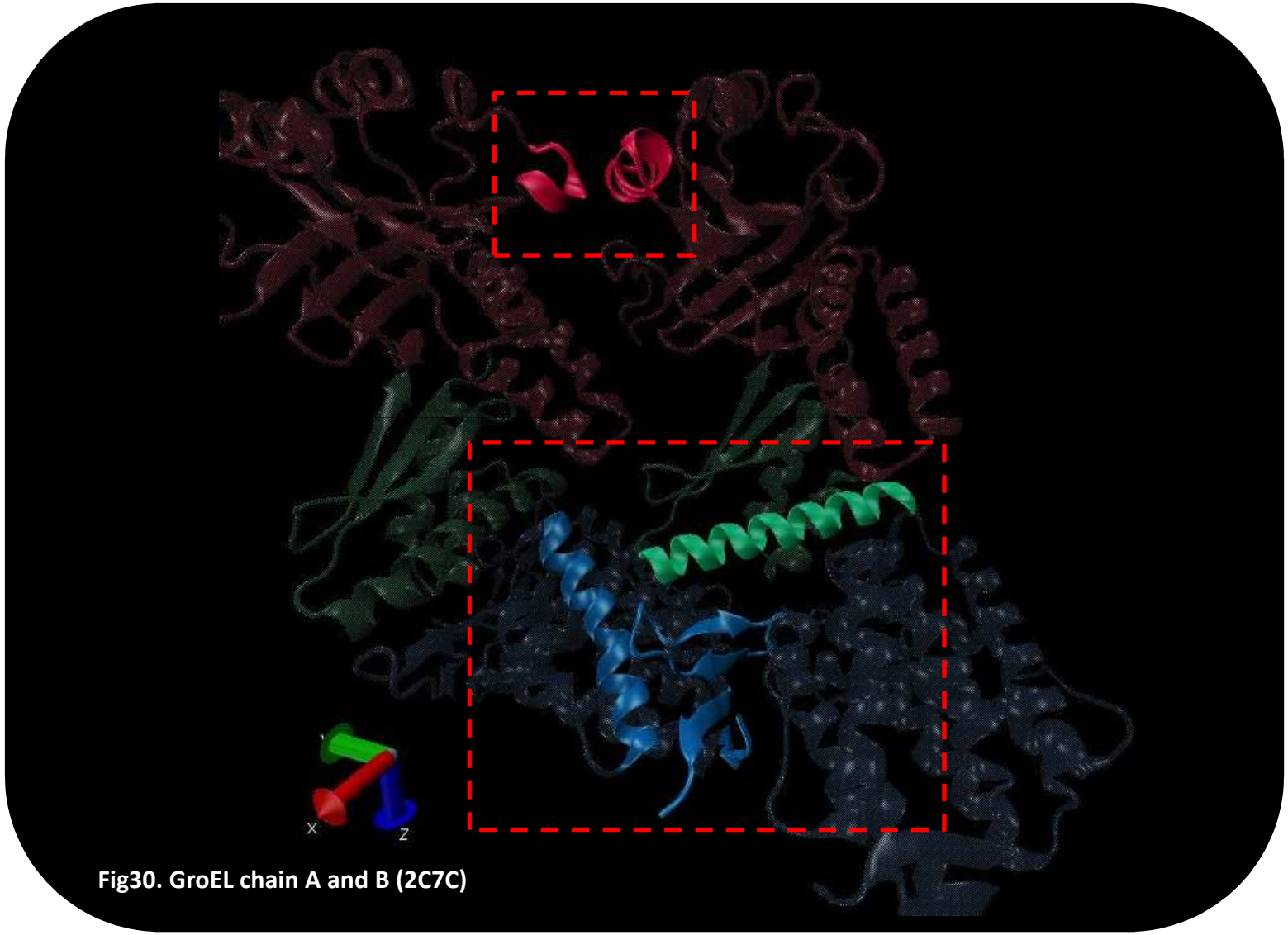


Fig30. GroEL chain A and B (2C7C)

GroEL/GroES> Intra-ring interactions

Hydrophobic interactions between apical domains

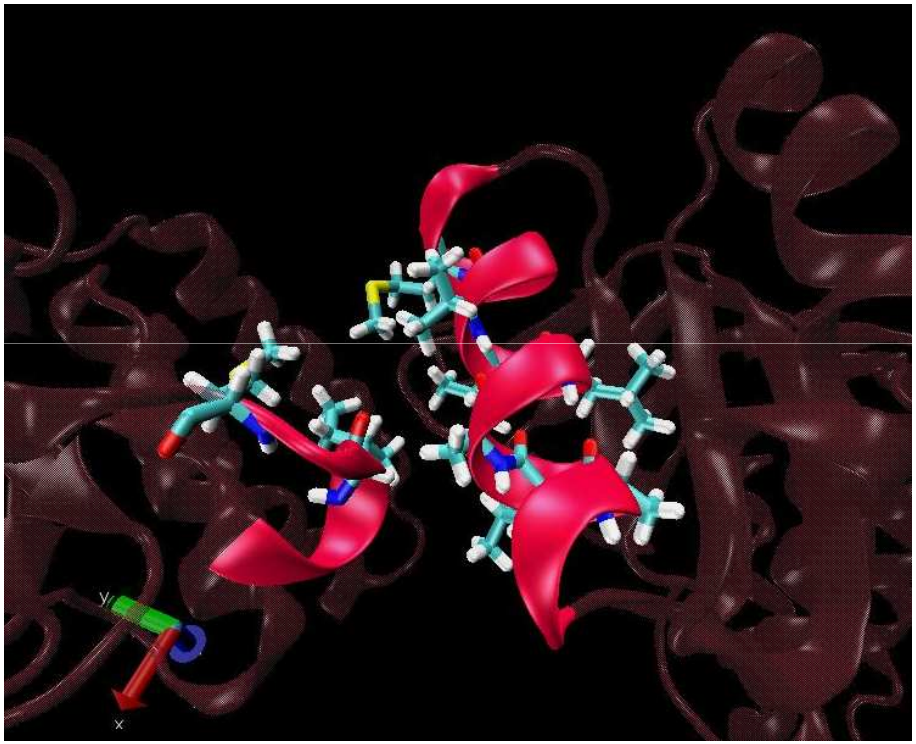


Fig31. GroEL chain A and B, hydrophobic apical interactions (2C7C)

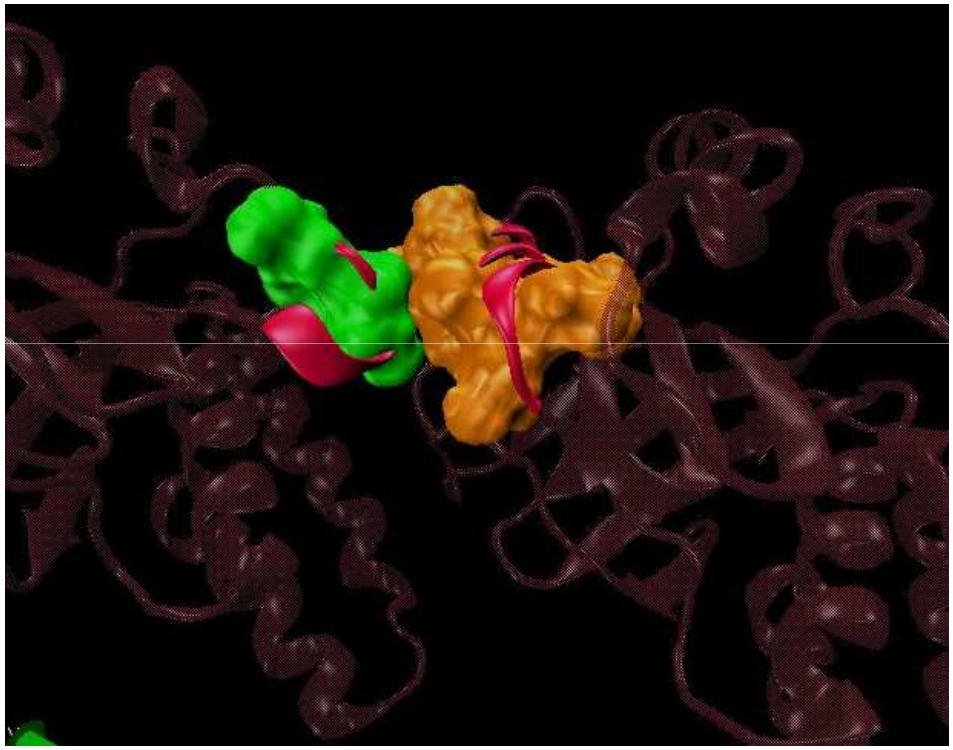


Fig32. GroEL chain A and B, surface hydrophobic apical interactions (2C7C)

GroEL/GroES> Intra-ring interactions

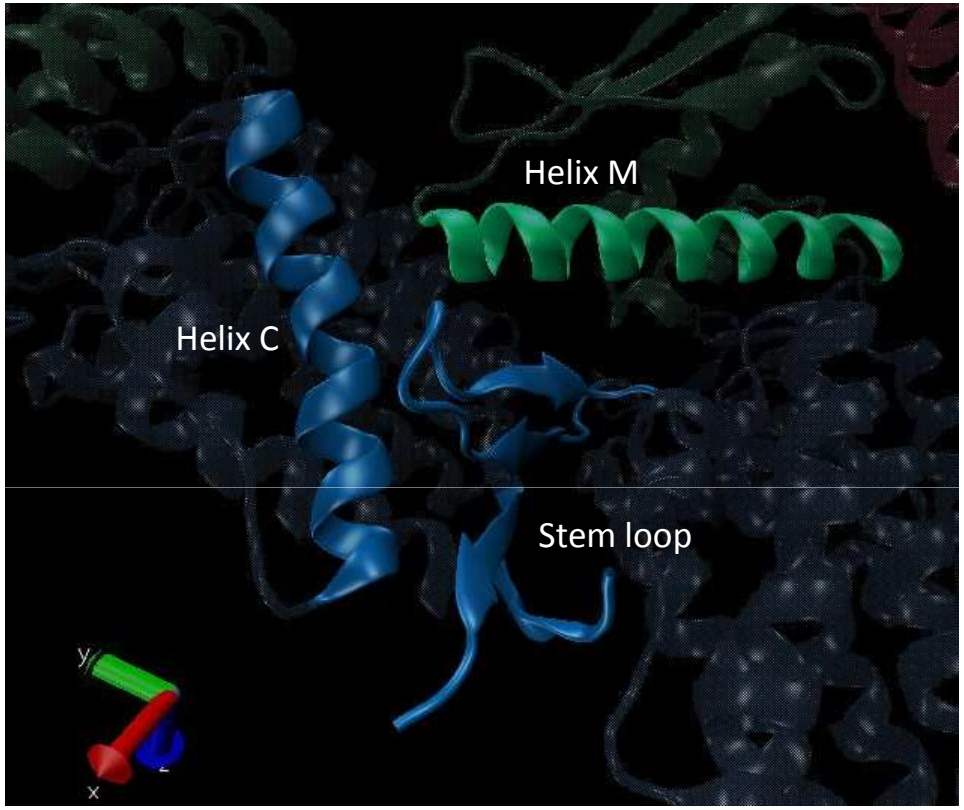


Fig33. GroEL chain A and B, intermediate and equatorial interactions (2C7C)

B-sheet inner contacts and hydrogen bonds between intermediate and equatorial domains

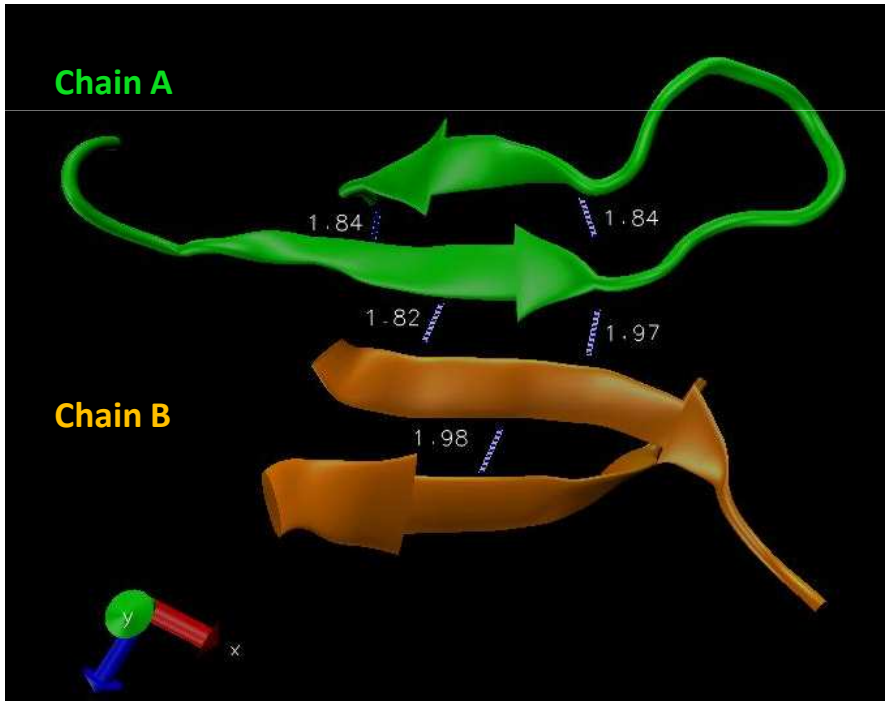


Fig34. β-sheet inner contacts (2C7C)

GroEL/GroES> Intra-ring interactions

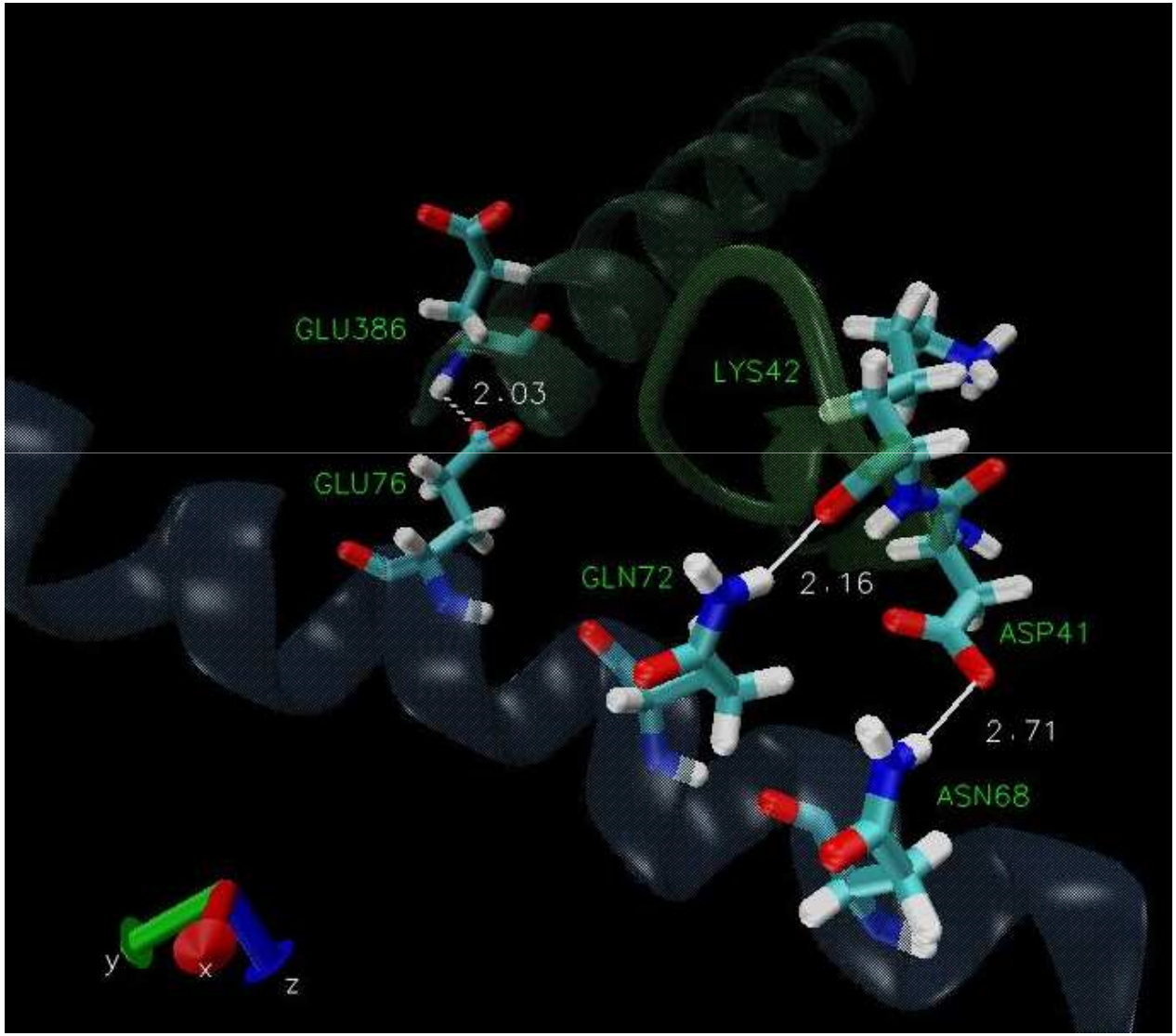


Fig35. Intra-ring interactions, Hbonds (2C7C)

GroEL/GroES> General structure GroES

Subunits of 97 aa

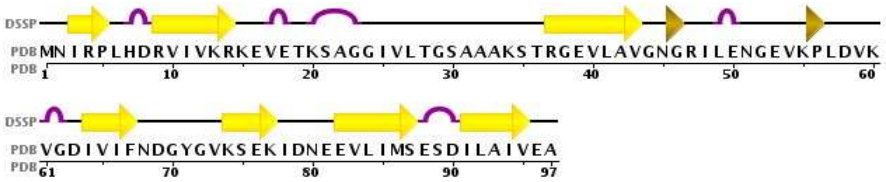


Fig36. GroES chain O sequence (1AON)

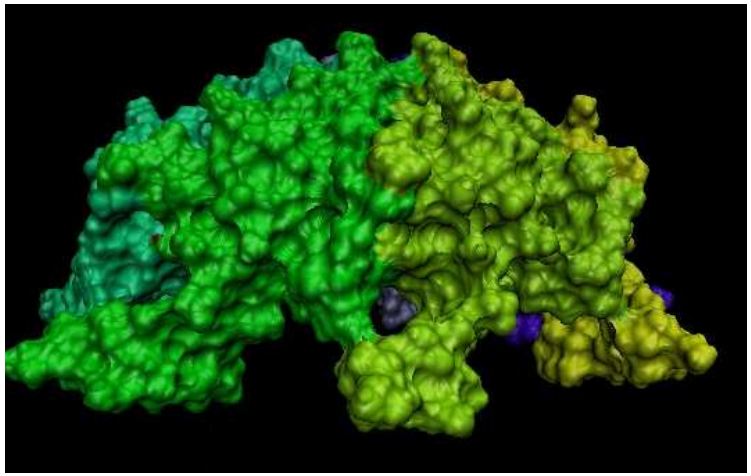


Fig37. GroES subunits, lateral view (1AON)

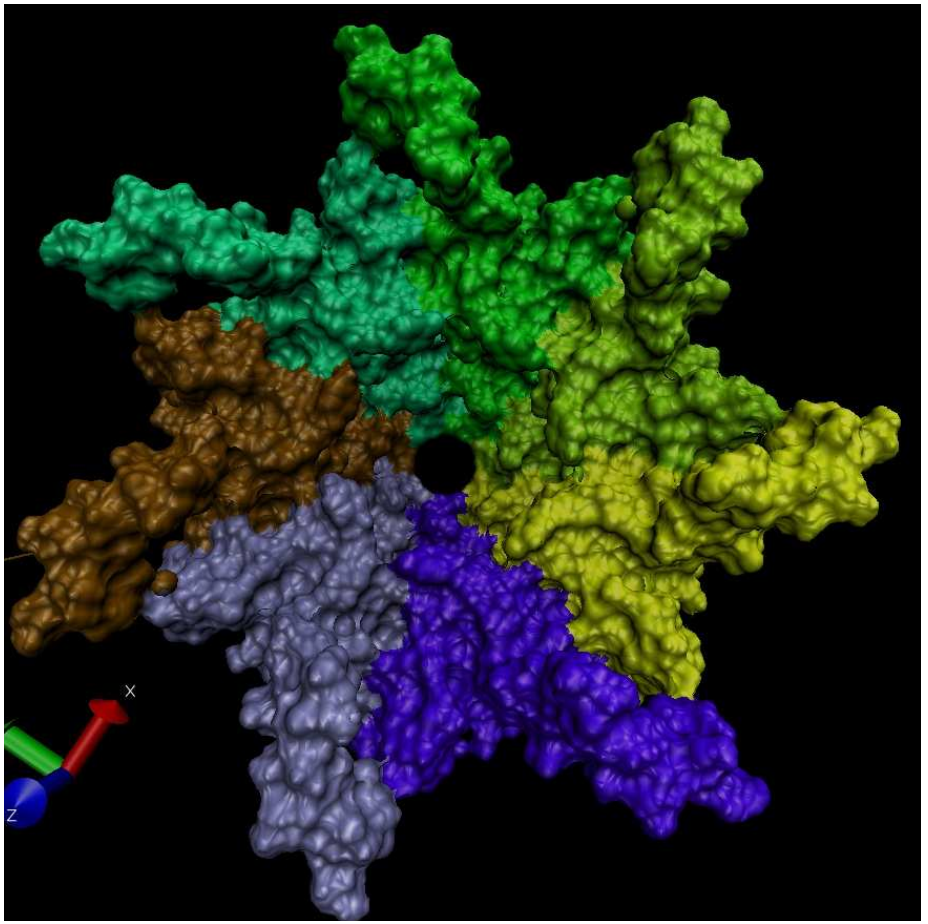


Fig38. GroES subunits, internal view(1AON)

GroEL/GroES> General structure GroES

One domain; β-barrel in the core and 2 β-hairpins loops

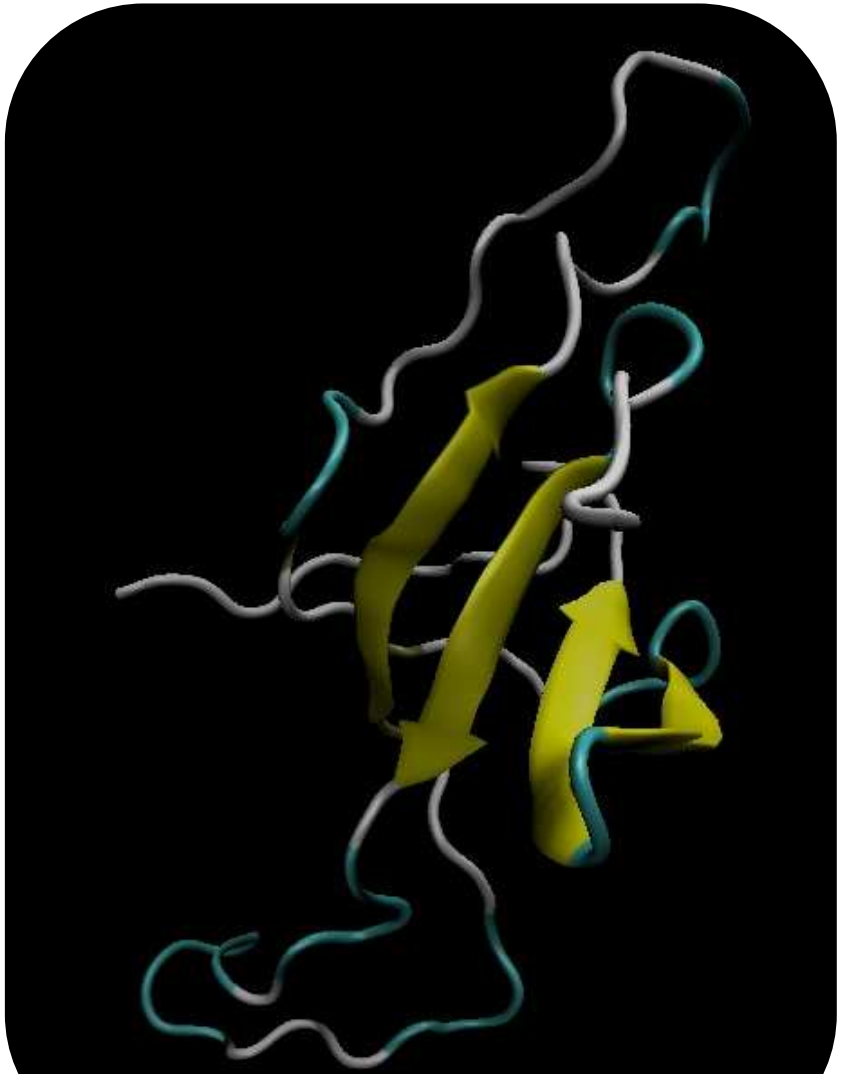


Fig39. GroES chain O (1AON)

GroEL/GroES> General structure GroES

One domain; β-barrel in the core and 2 β-hairpins loops

GroES structure free and bound to GroEL is very similar. Only changes de mobile loop residues (16-32)

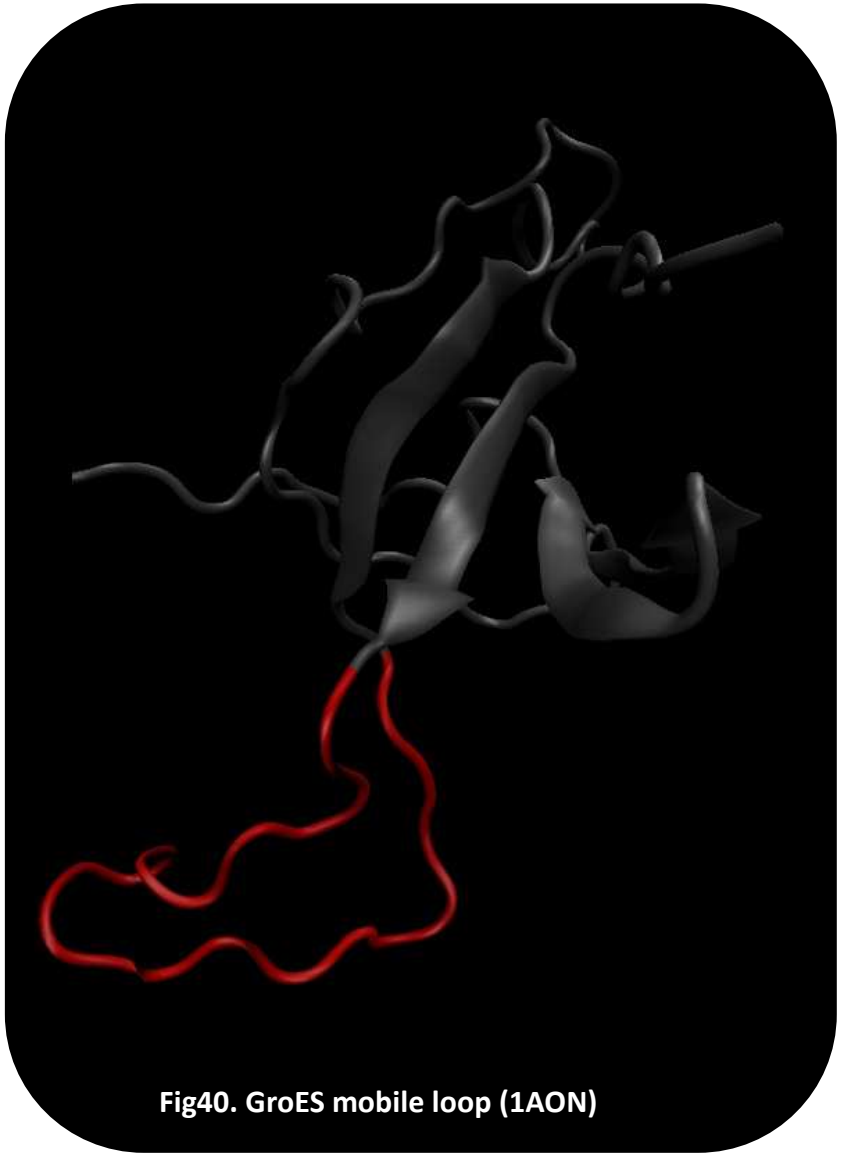


Fig40. GroES mobile loop (1AON)

GroEL/GroES> GroEL – polypeptide interaction

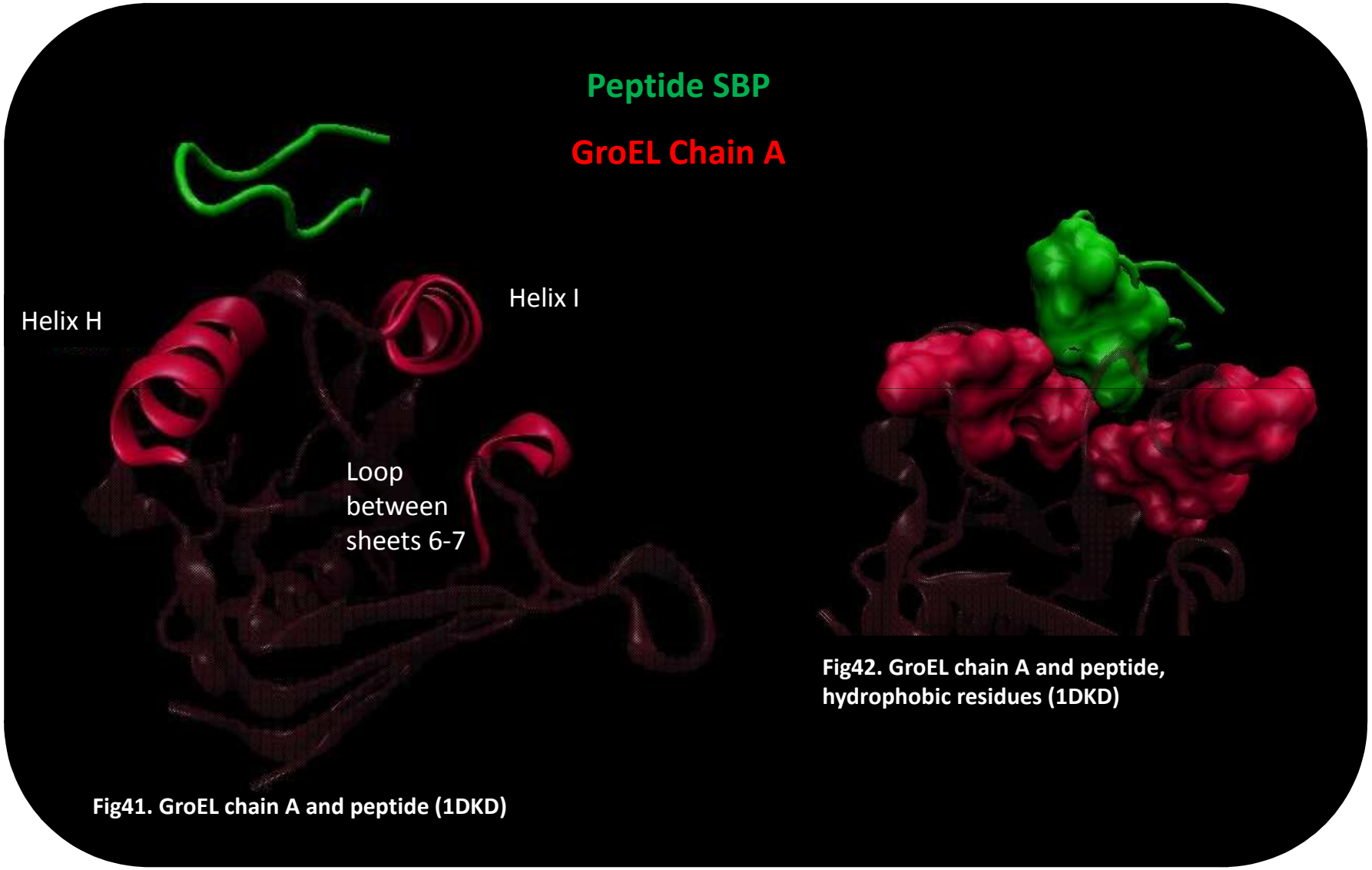


Fig41. GroEL chain A and peptide (1DKD)

Fig42. GroEL chain A and peptide, hydrophobic residues (1DKD)

GroEL/GroES> GroEL – polypeptide interaction

Hydrophobic interactions

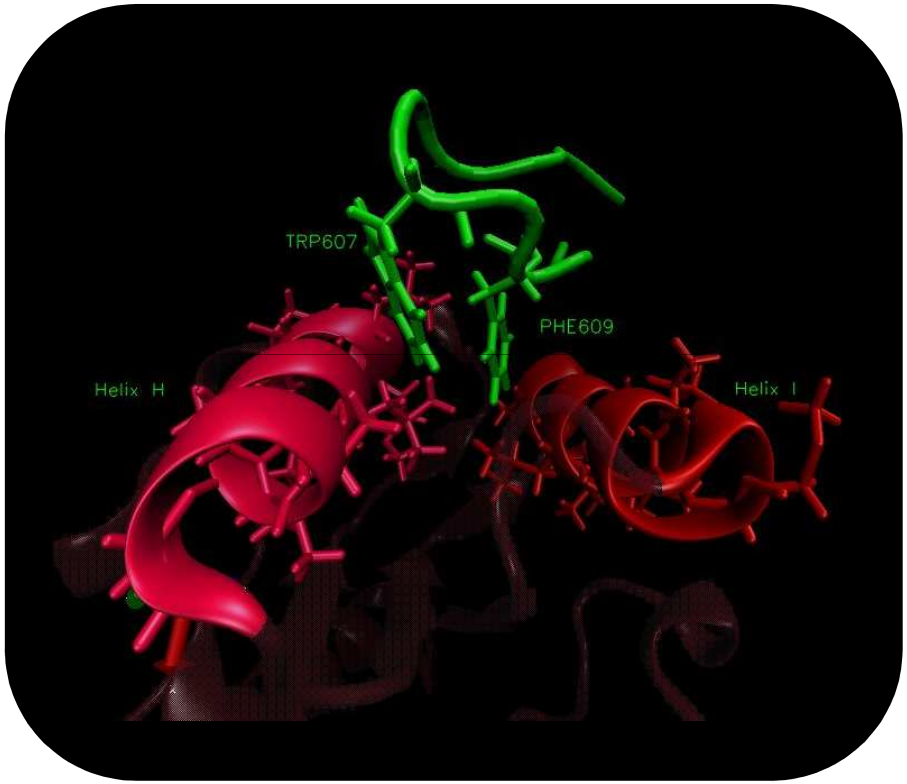


Fig43. GroEL - polypeptide interface, hydrophobic pocket (1DKD)

Hydrogen bonds

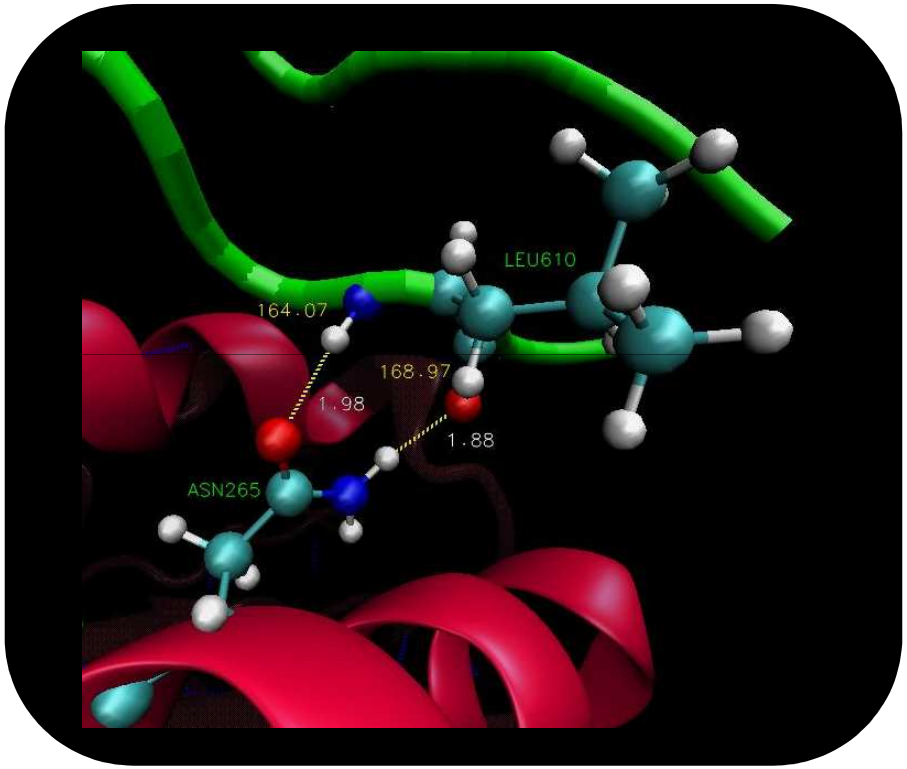


Fig44. GroEL – polypeptide interface, H bonds (1DKD)

GroEL/GroES> GroEL – polypeptide interaction

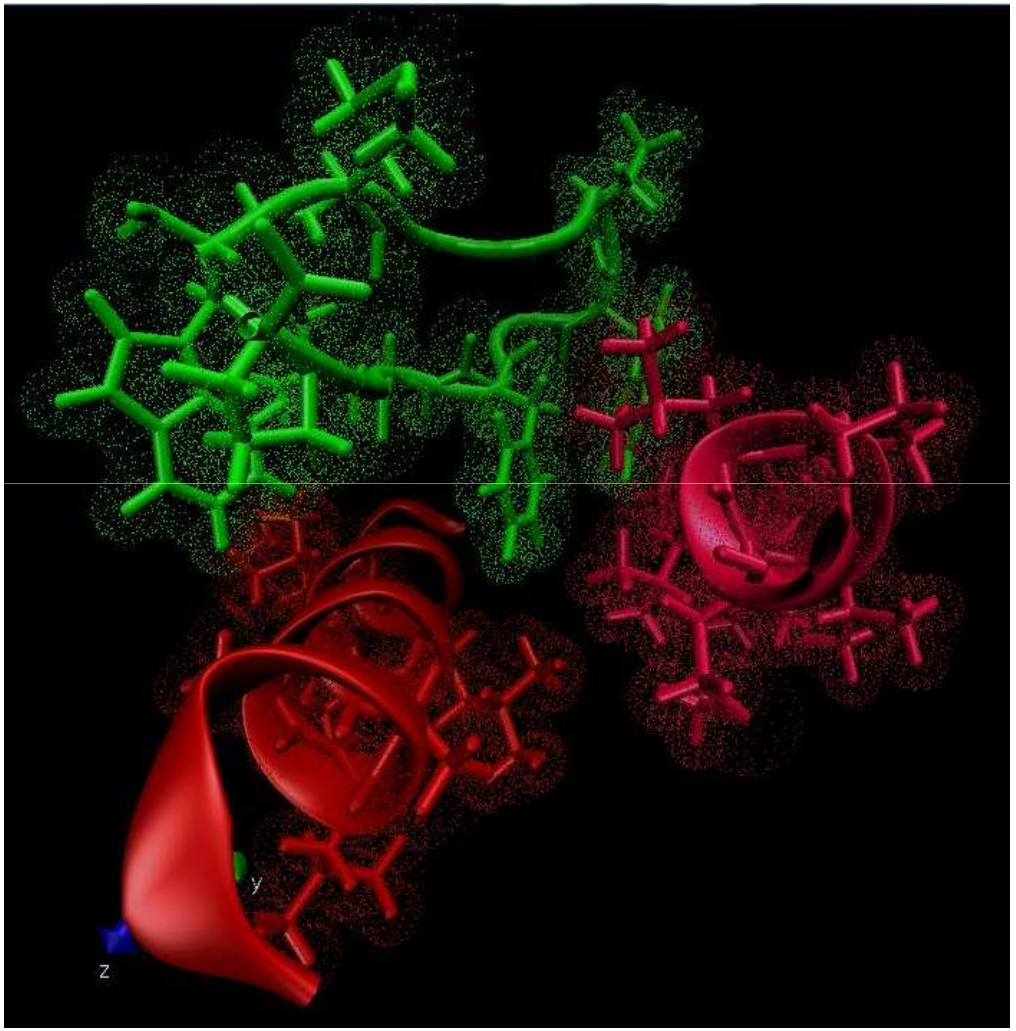


Fig45. GroEL – polypeptide interface, hydrophobic residues (1DKD)

GroEL/GroES> GroEL – GroES interaction

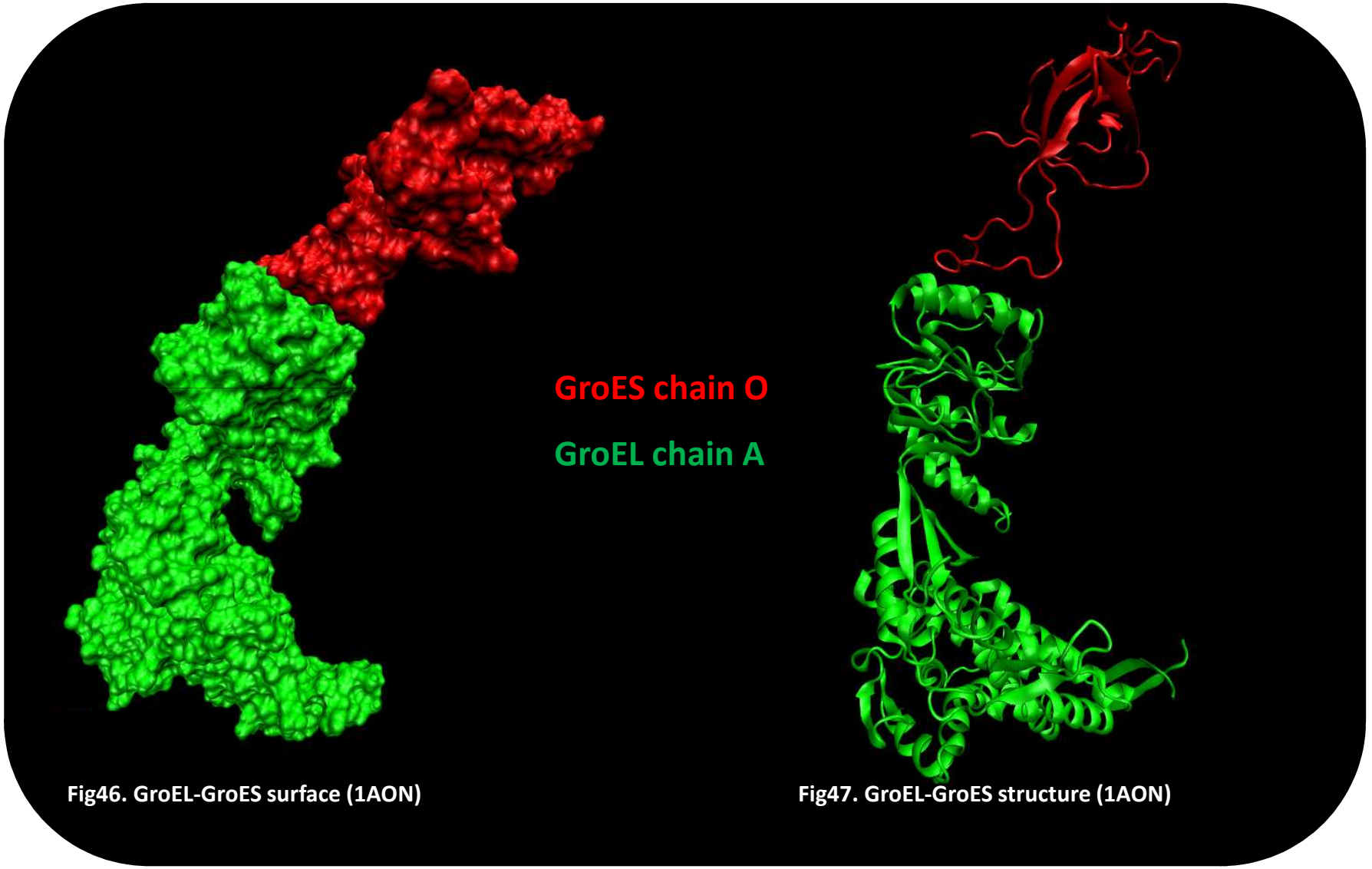


Fig46. GroEL-GroES surface (1AON)

Fig47. GroEL-GroES structure (1AON)

GroEL/GroES> GroEL – GroES interaction

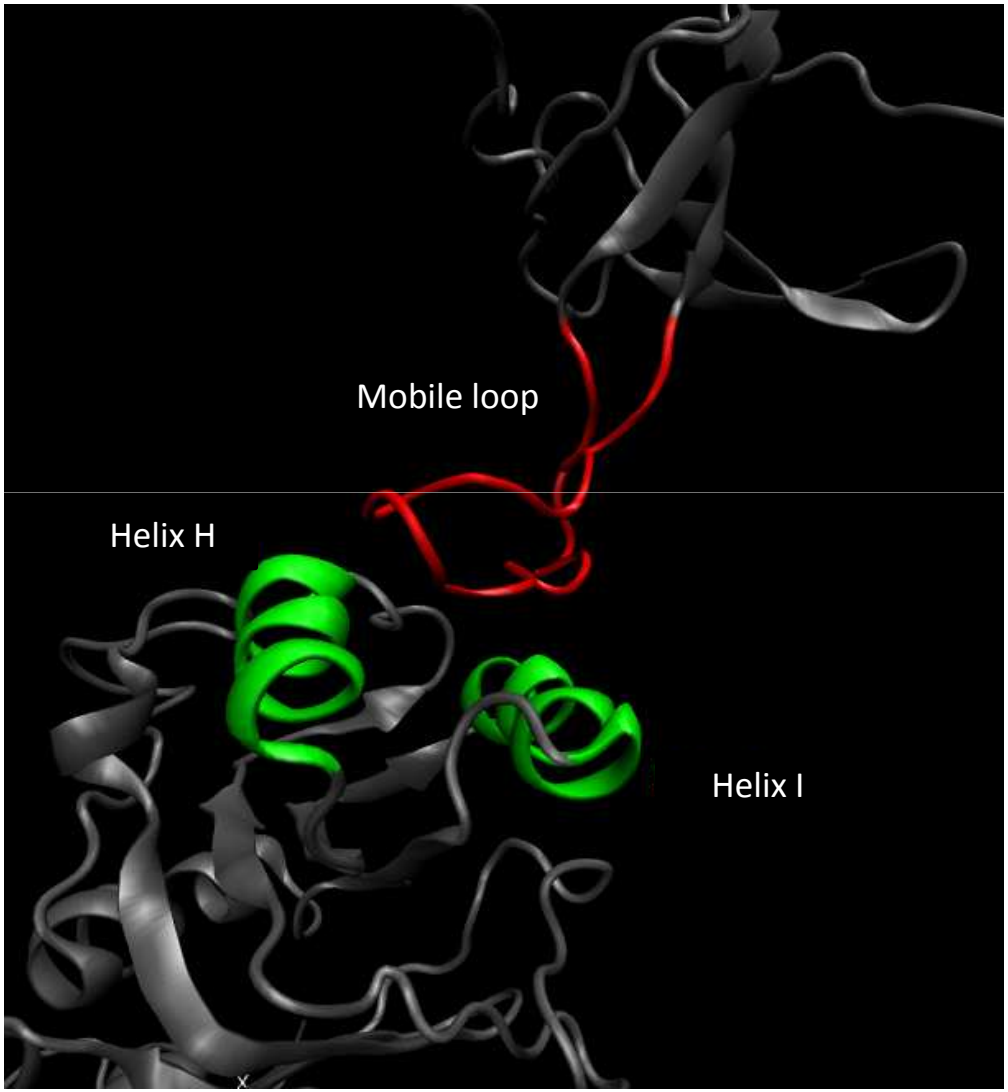


Fig48. GroEL-GroES chain A and O, interface zoom (1AON)

GroEL/GroES> GroEL – GroES interaction

Hydrophobic interactions

GroEL	Leu 234	Leu 237	Val 264
GroES	Val26	Ile25	Leu 27

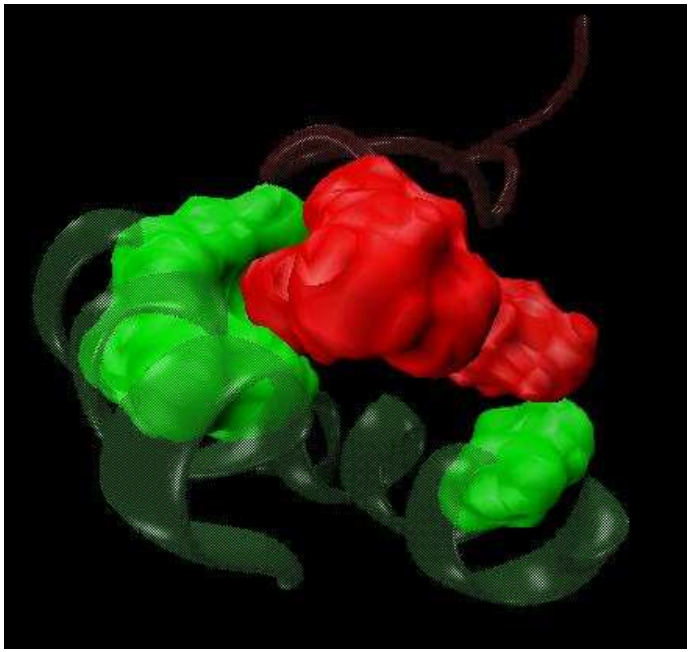


Fig49. GroEL-GroES interface, hydrophobic residues surface (1AON)

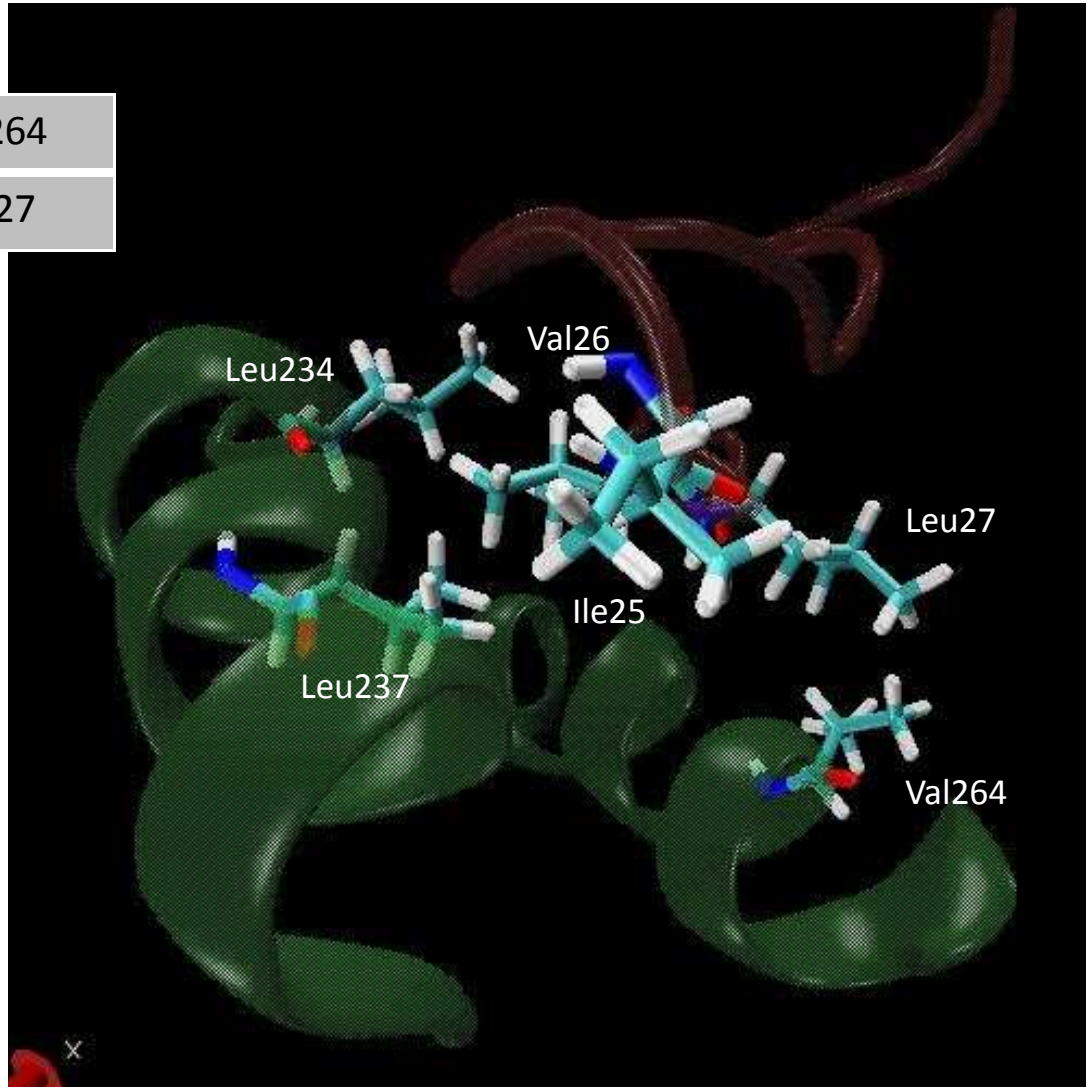


Fig50. GroEL-GroES interface, hydrophobic residues (1AON)

GroEL/GroES> GroEL – nucleotide interaction

Cis ring

Trans ring

Fig51. GroEL rings and ADP bound to the cis ring (1AON)

GroEL/GroES> GroEL – nucleotide interaction

NUCLEOTIDE BINDING SITE:

equatorial domain, but

intermediate domain acts as a lid

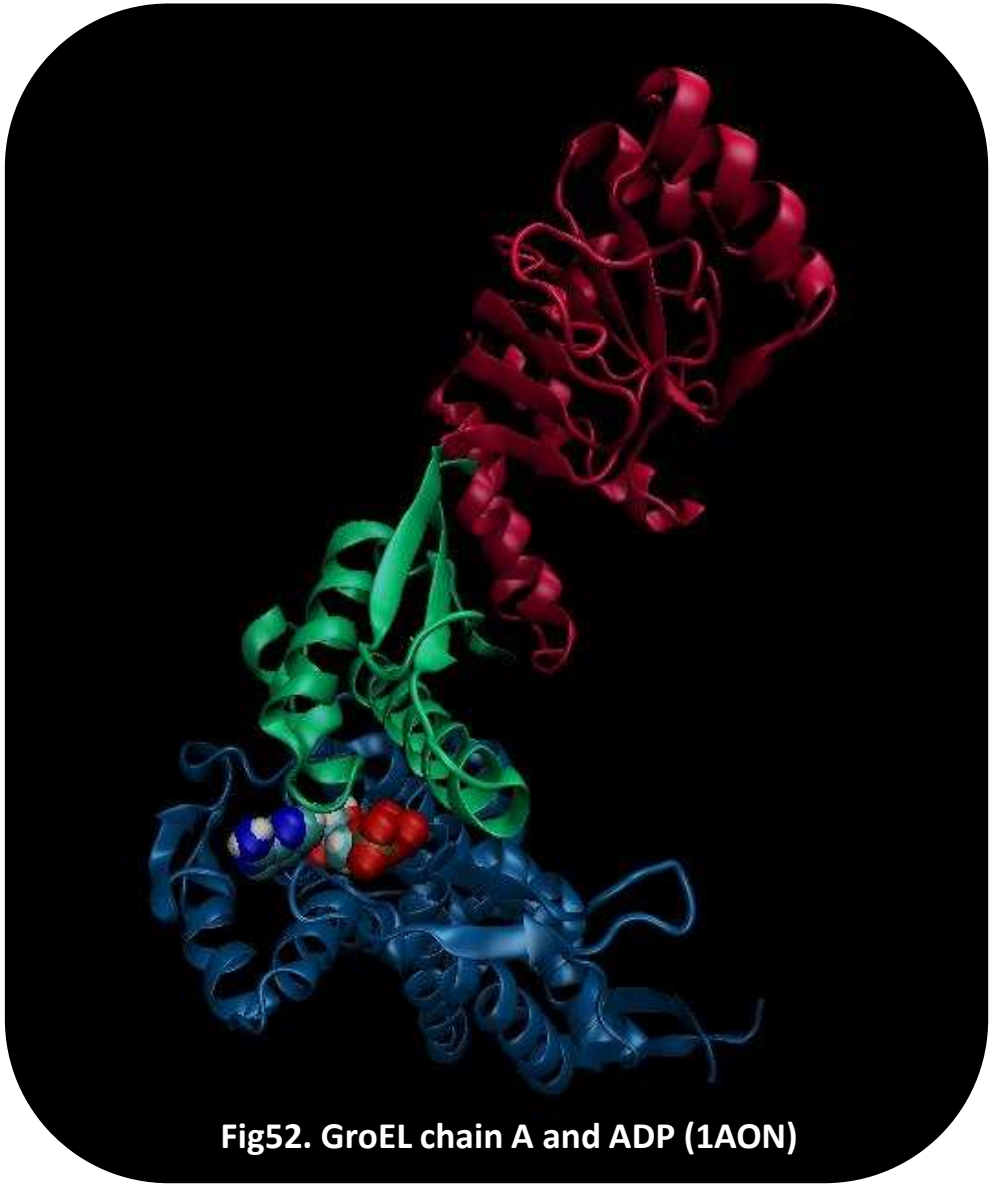


Fig52. GroEL chain A and ADP (1AON)

GroEL/GroES> GroEL – nucleotide interaction

NUCLEOTIDE BINDING SITE:

equatorial domain, but

intermediate domain acts as a lid

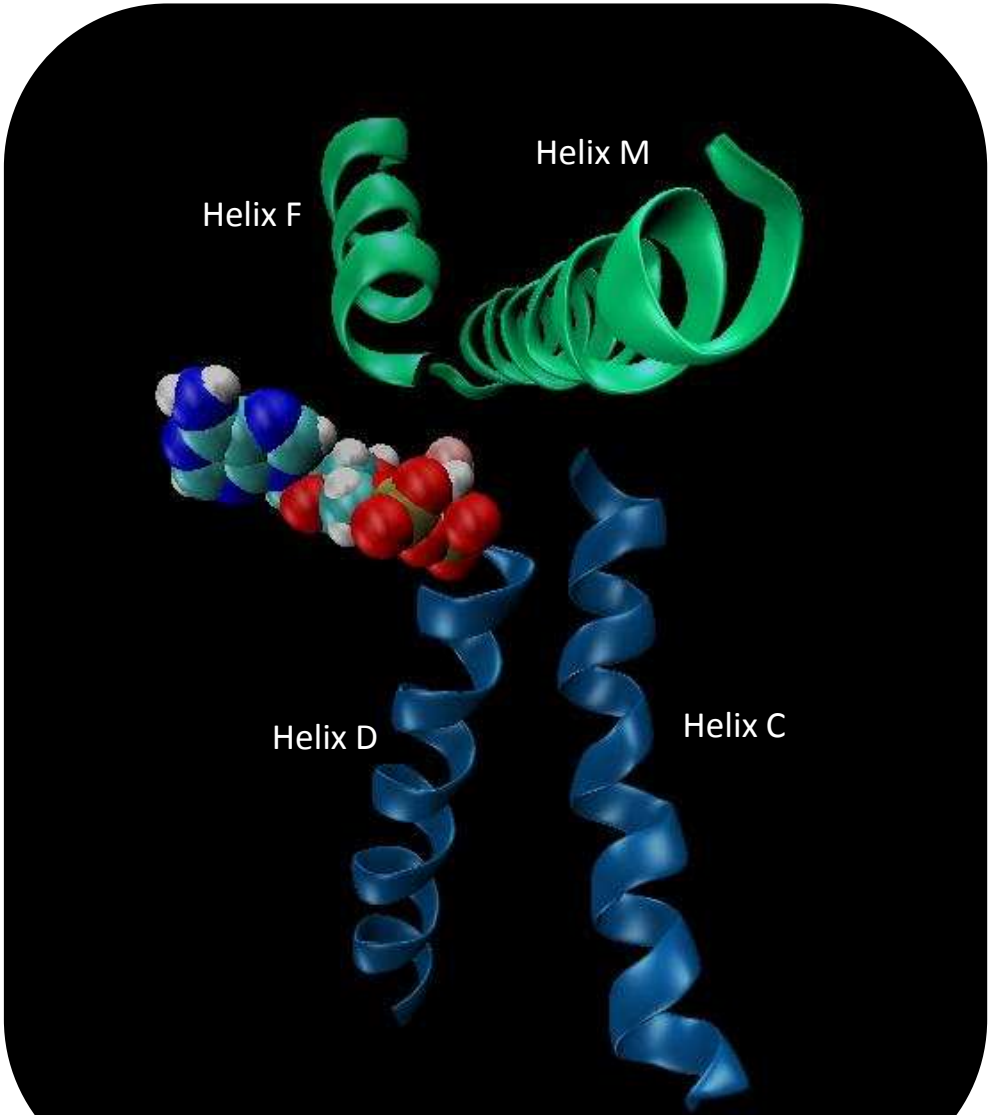


Fig53. Helixes of the nucleotide binding site (1AON)

GroEL/GroES> GroEL – nucleotide interaction

Phosphate binding loop (DGTTT) conserved in all chaperonin

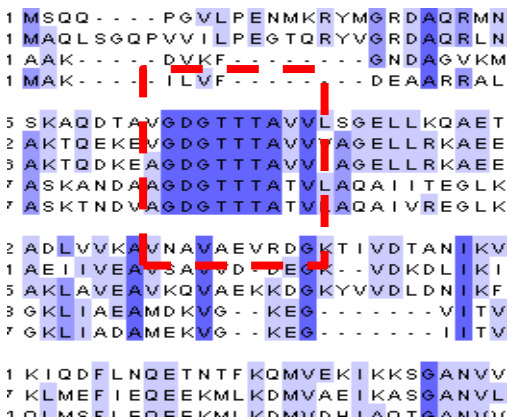


Fig54. Sequence alignment between members of both group I and II of chaperonins, conserved region.

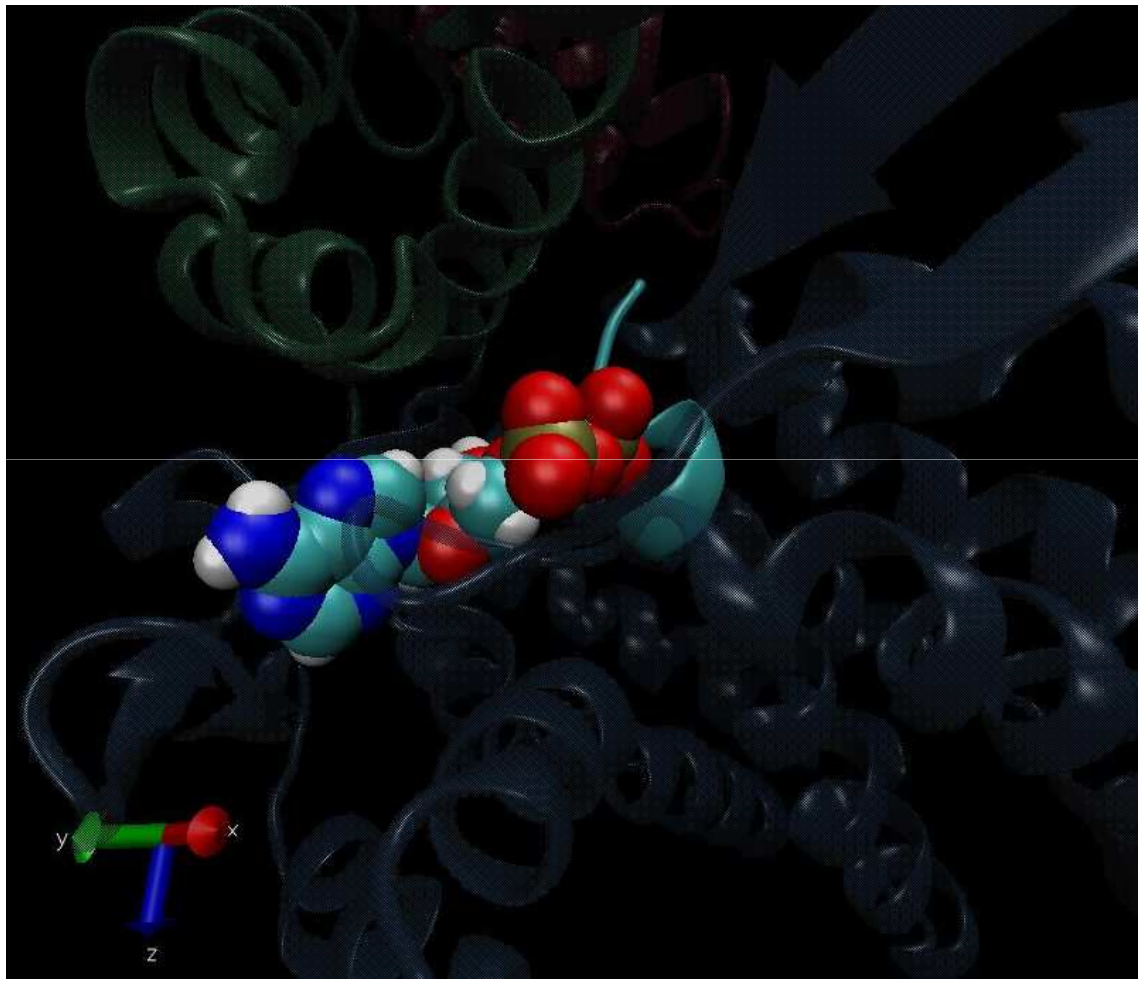


Fig55. Zoom nucleotide binding site (1AON)

GroEL/GroES> GroEL – nucleotide interaction

PHOSPHATE BINDING LOOP

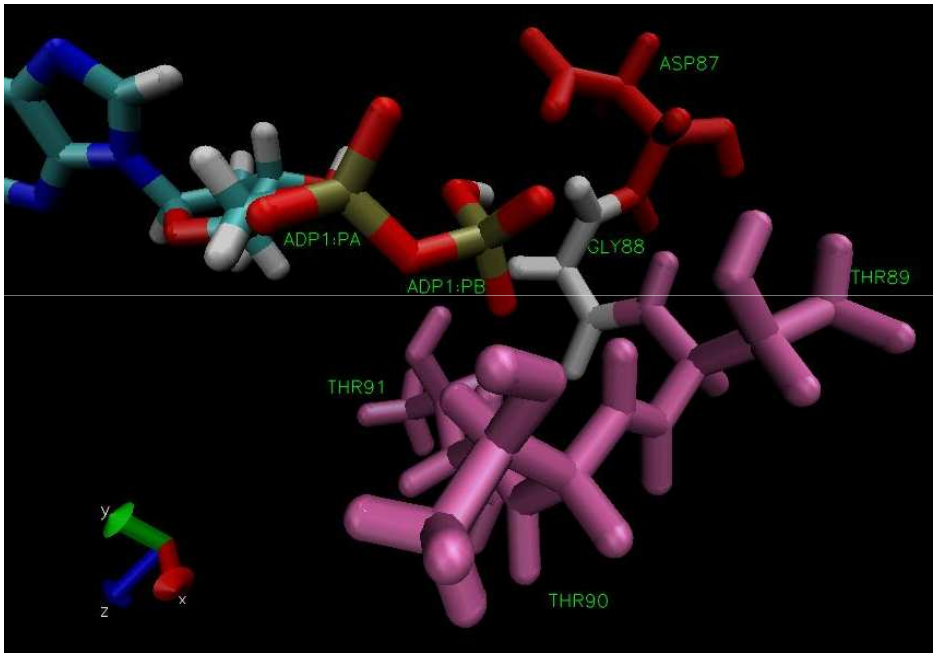


Fig56. Phosphate binding loop and ADP (1AON)

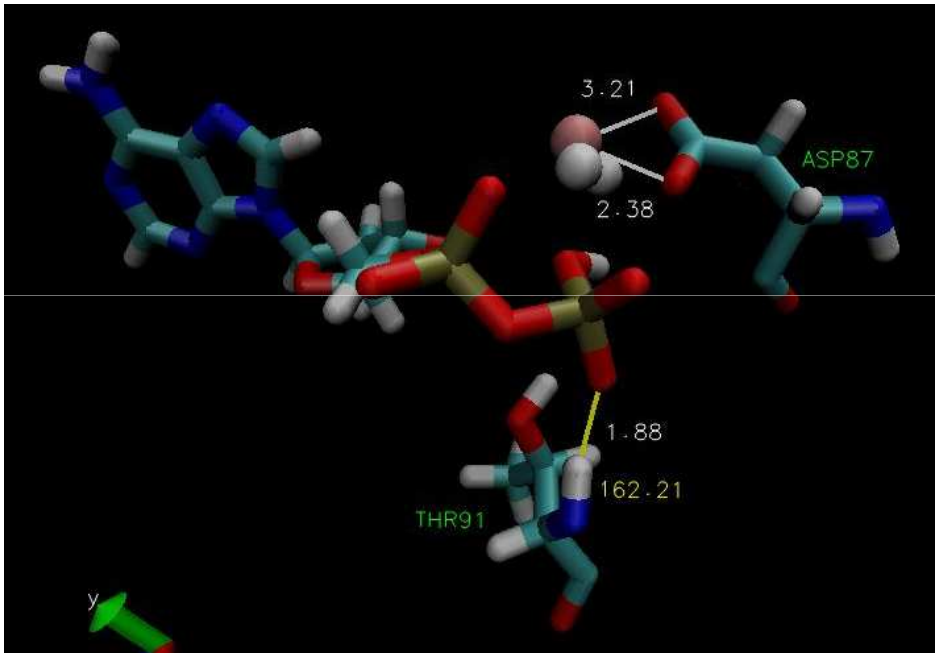


Fig57. Phosphate binding loop and ADP interactions (1AON)

GroEL/GroES> GroEL – nucleotide interaction

Hydrogen bonds

Magnesium coordinations

van der Waals contacts

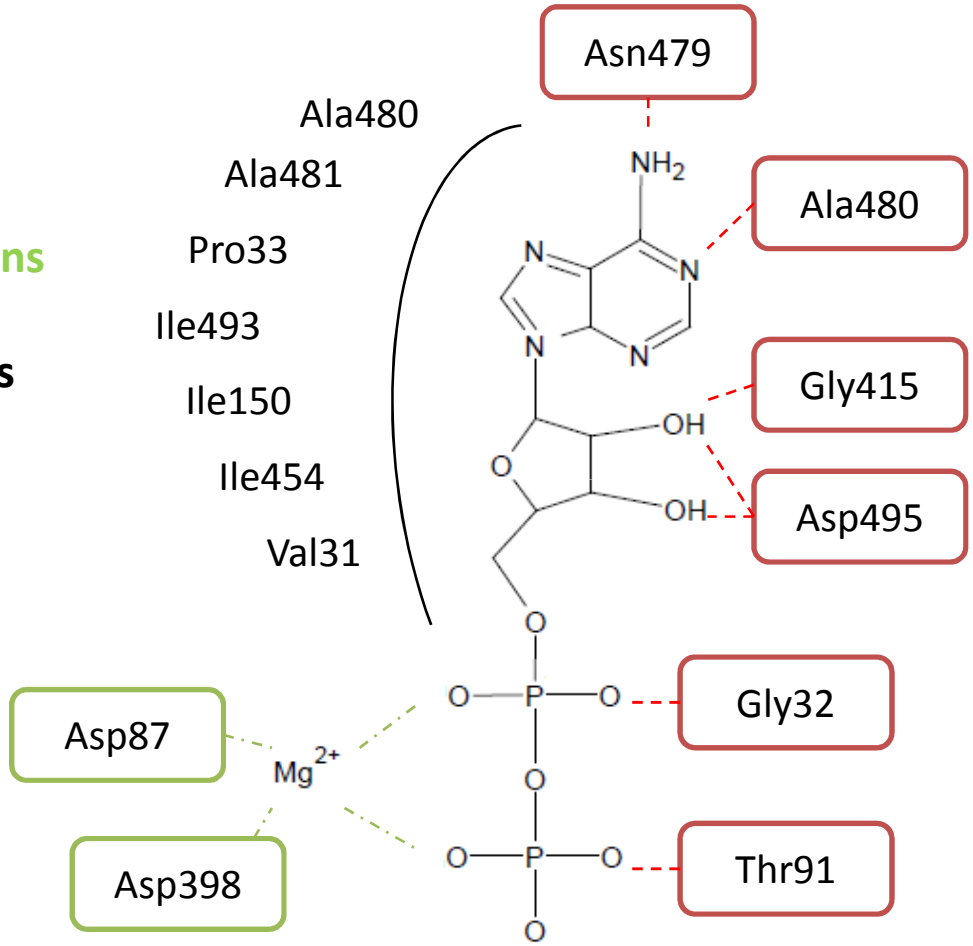


Fig58. Interactions between ADP, Mg^{2+} and GroEL residues (ChemSketch)

GroEL/GroES> GroEL – nucleotide interaction

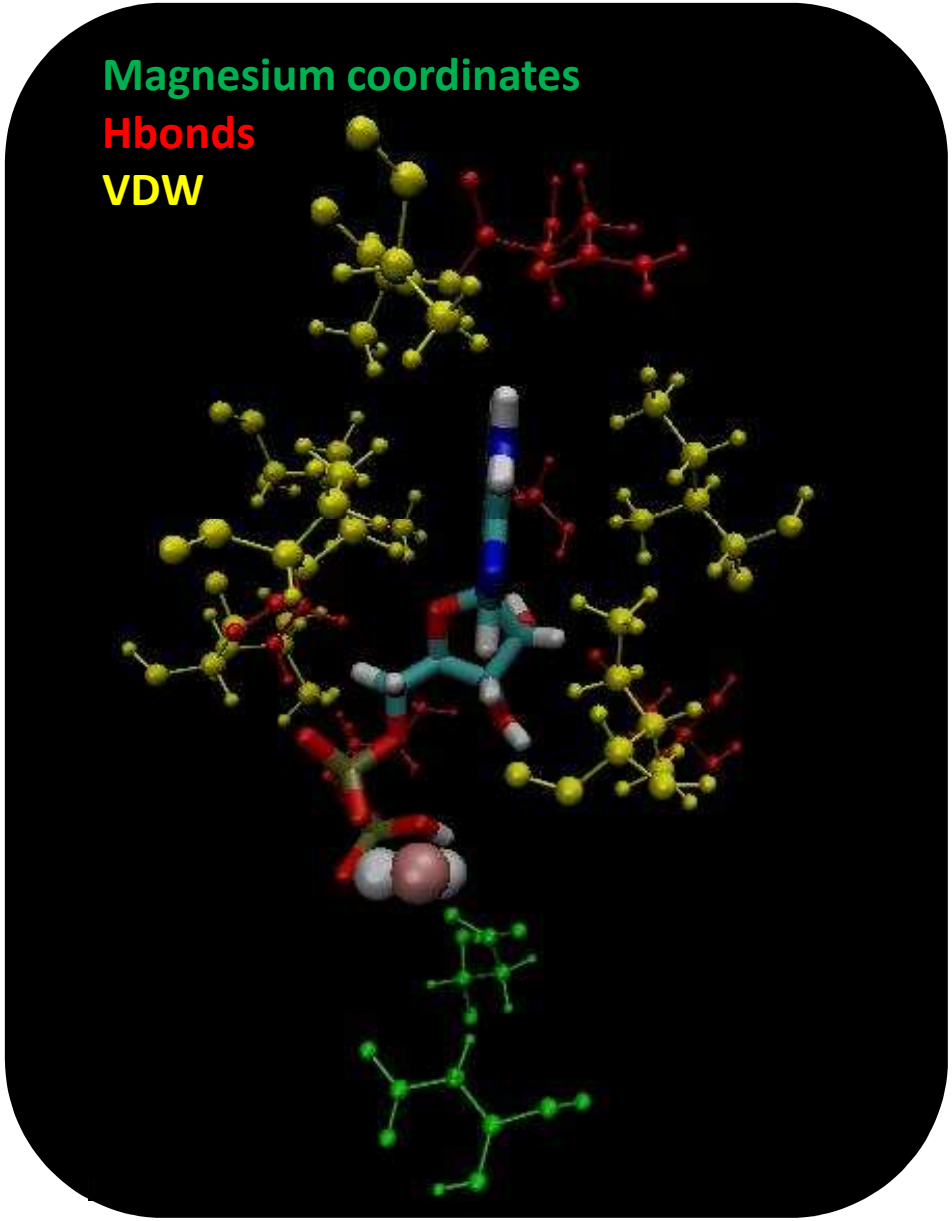


Fig59. Interactions between ADP, Mg^{2+} and GroEL residues (1AON)

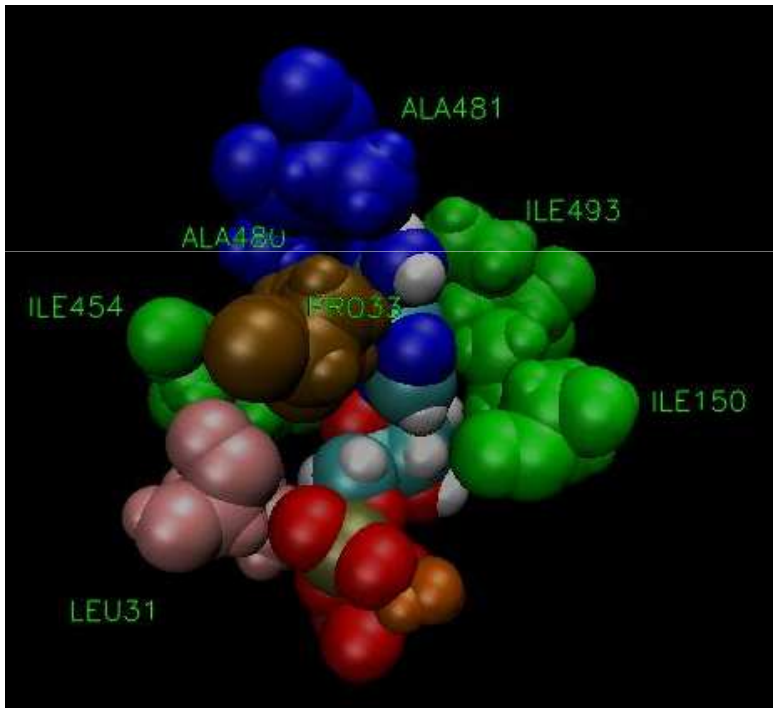


Fig60. Van der Waals interactions between GroEL and ADP (1AON)

GroEL/GroES> GroEL – nucleotide interaction

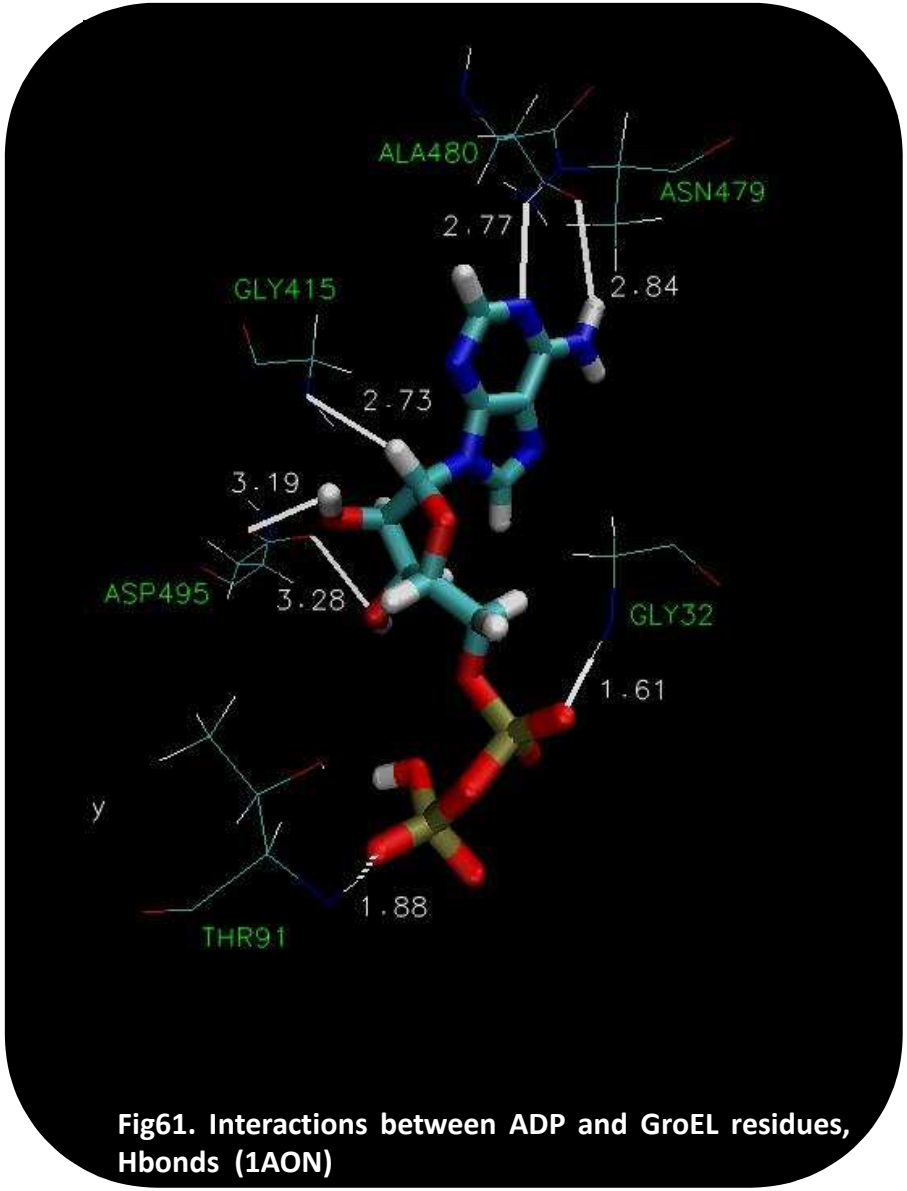


Fig61. Interactions between ADP and GroEL residues, Hbonds (1AON)

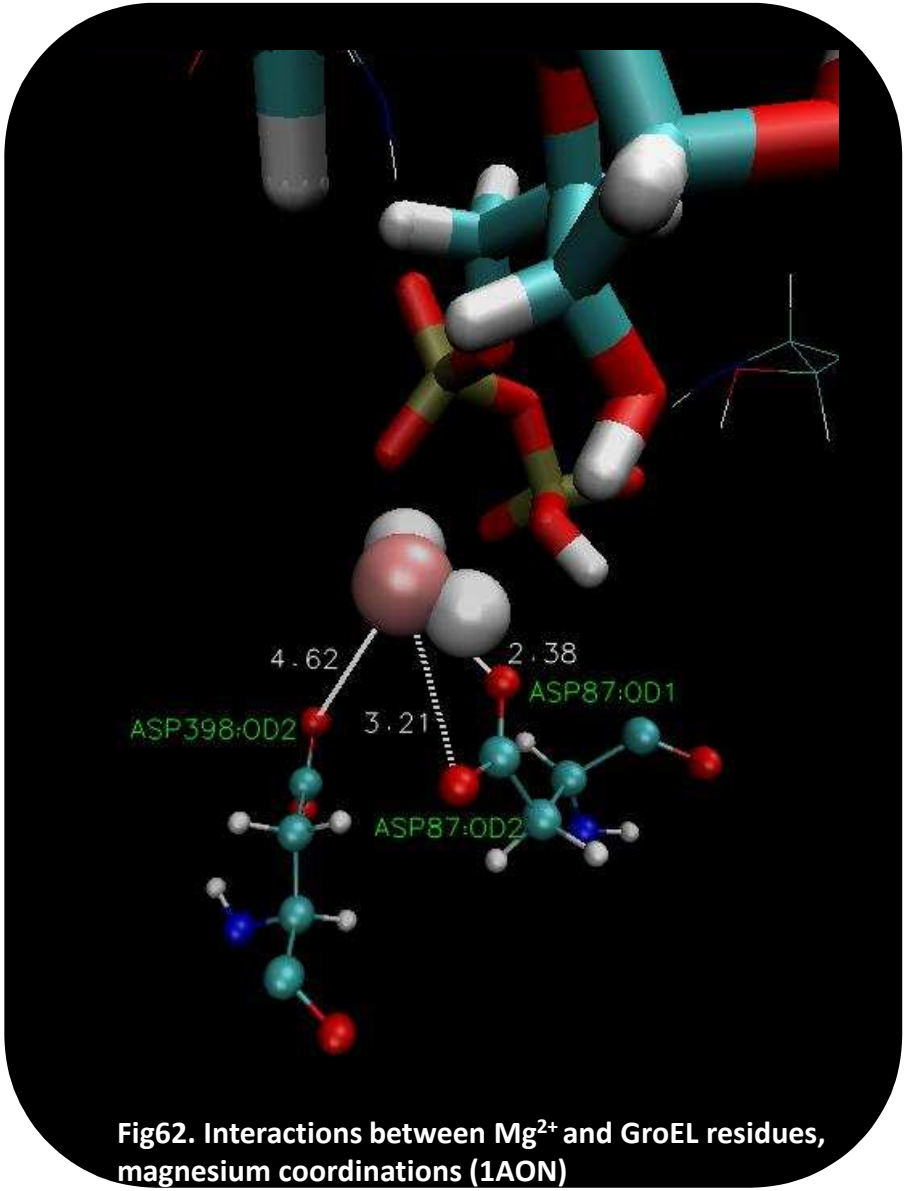


Fig62. Interactions between Mg^{2+} and GroEL residues, magnesium coordinations (1AON)

GroEL/GroES> GroEL – nucleotide interaction

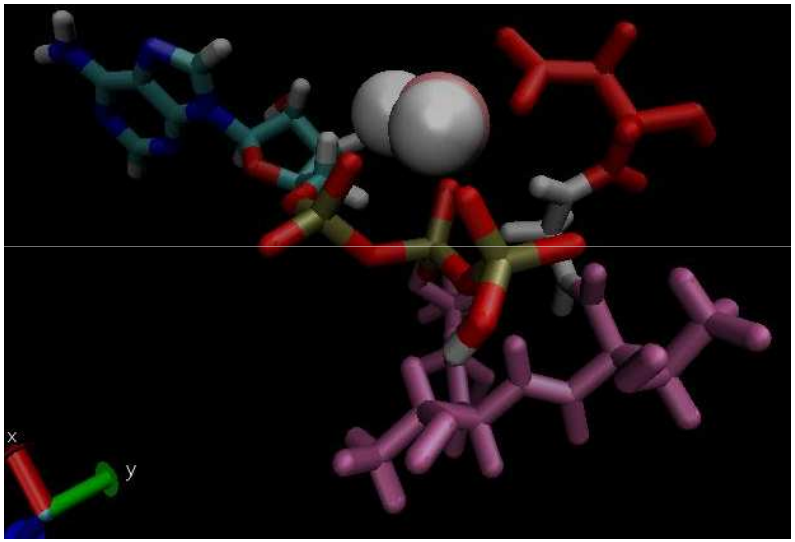


Fig63. Interactions between ATP and GroEL residues (1SX3)

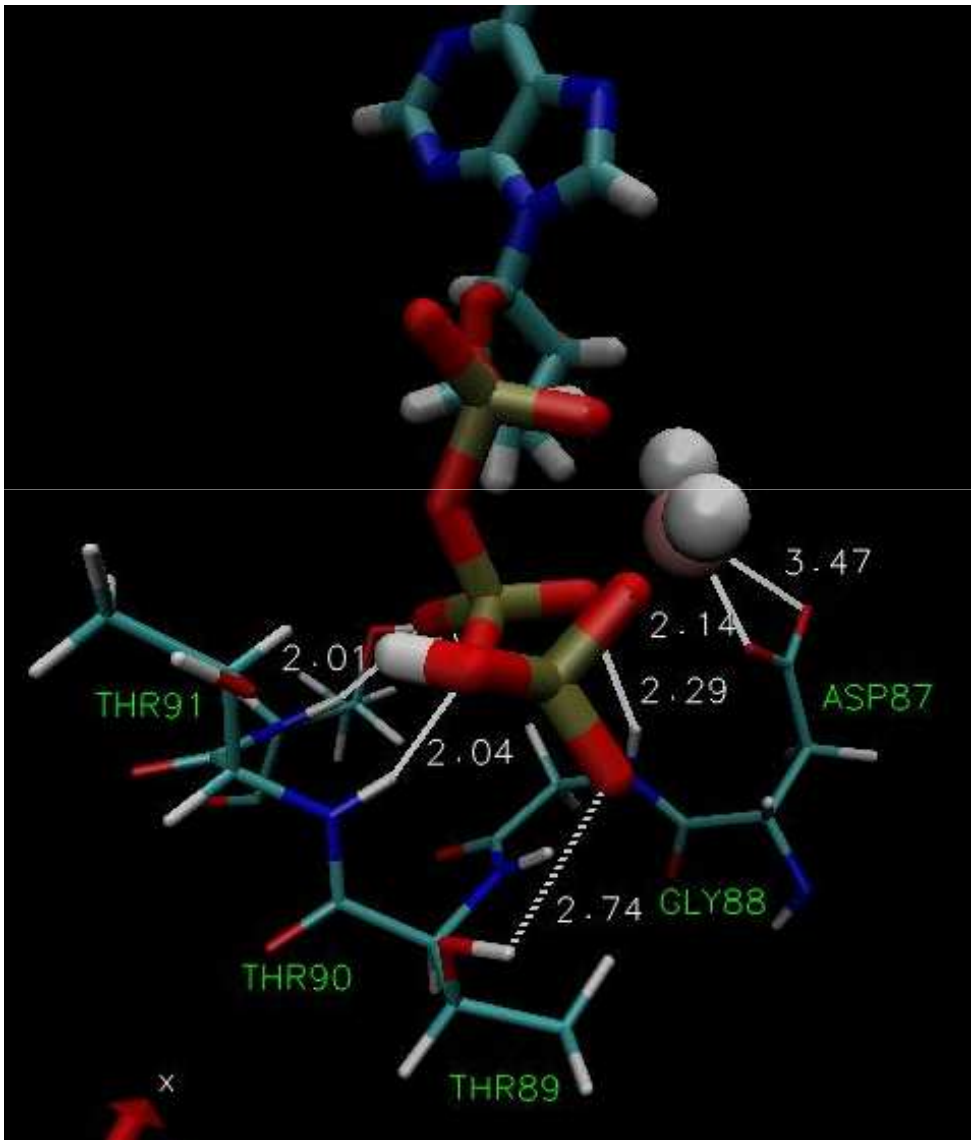


Fig64. Interactions between ATP and GroEL residues (1SX3).

GroEL/GroES> GroEL – nucleotide interaction

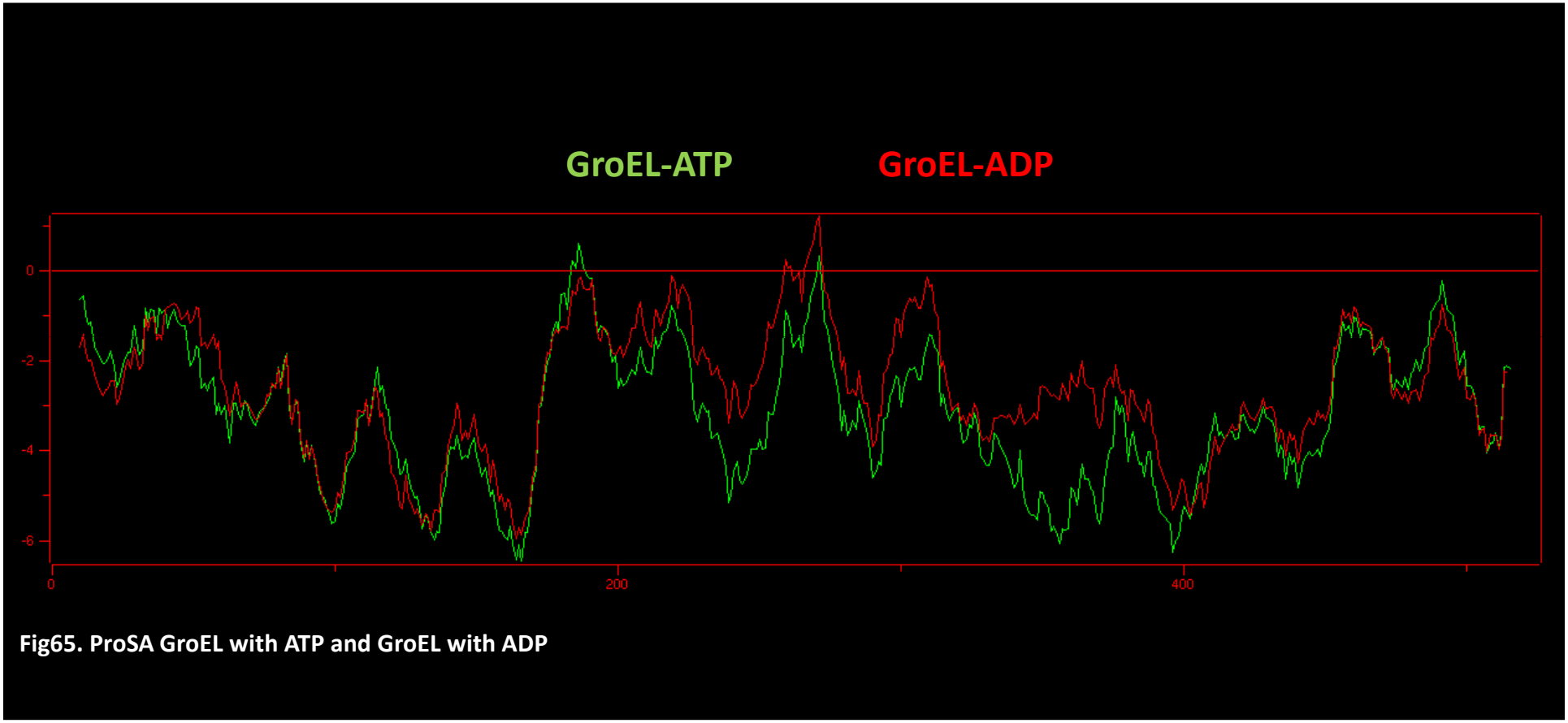


Fig65. ProSA GroEL with ATP and GroEL with ADP

GroEL/GroES> Folding cycle overview

This reaction cycle can be divided into four phases:

I. Polypeptide Binding

II. Nucleotide and GroES Binding

III. Polypeptide Release and Folding

IV. Protein Folding and Release of Ligands

GroEL/GroES> Folding cycle overview

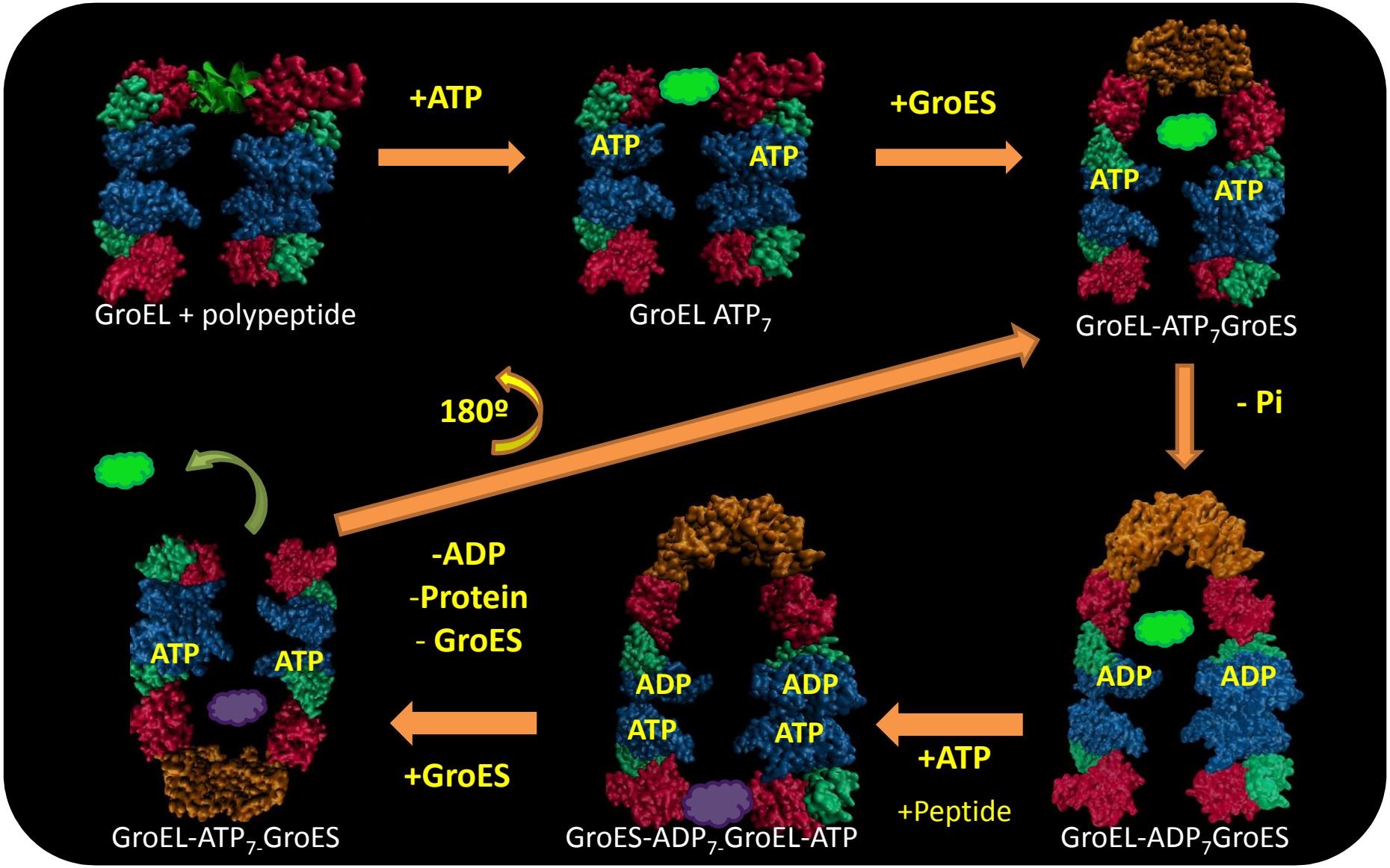


Fig55. GroEL-GroES cycle overview (1MNF, 1SX3, 1SVT, 1SX4, 1GRU)

GroEL/GroES> **Folding cycle >** Phase I

Polypeptide Binding

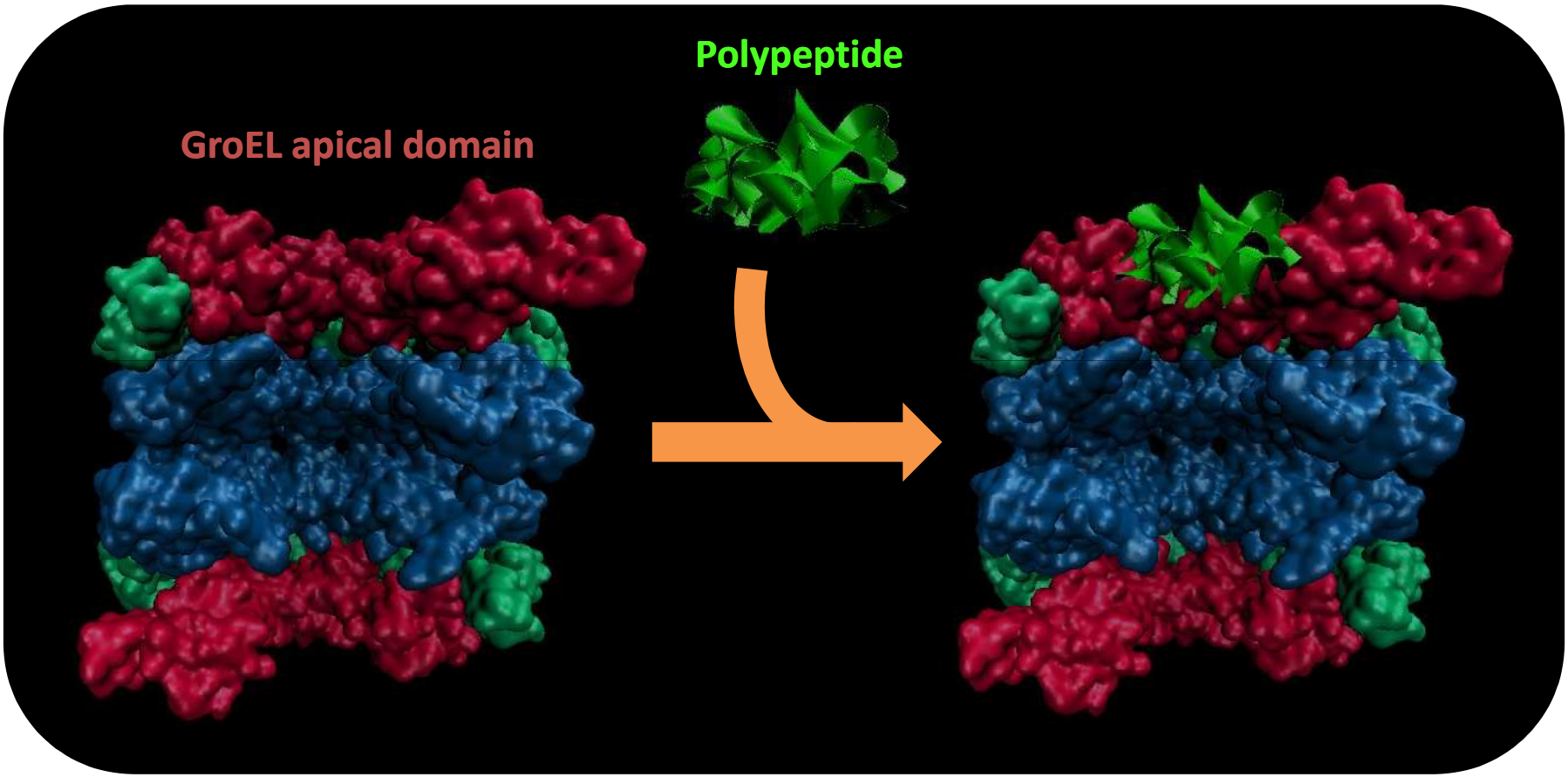


Fig67. Polypeptide binding (1MNF)

GroEL/GroES> **Folding cycle >** Phase II

Nucleotide and GroES Binding

Fig68. GroEL (1SS8), chain A

+ ATP

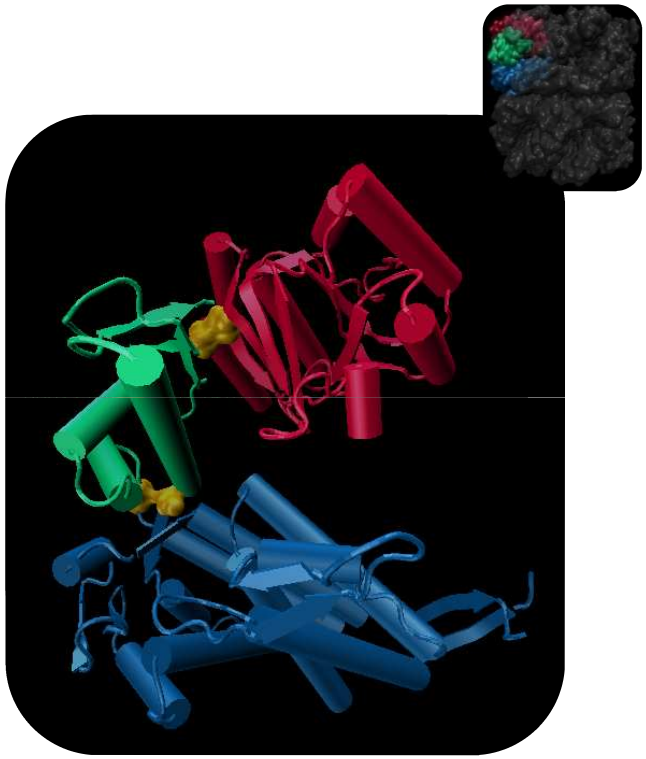


Fig69. GroEL ATP_7 (1SX3), chain A

GroEL/GroES> **Folding cycle >** Phase II

Nucleotide and GroES Binding

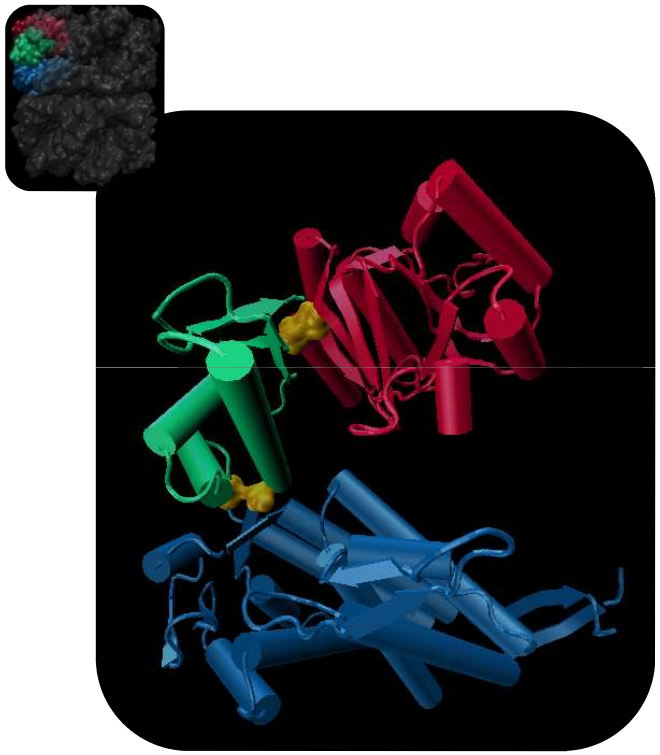


Fig70. GroEL ATP_7 (1SX3), chain A

+ GroES

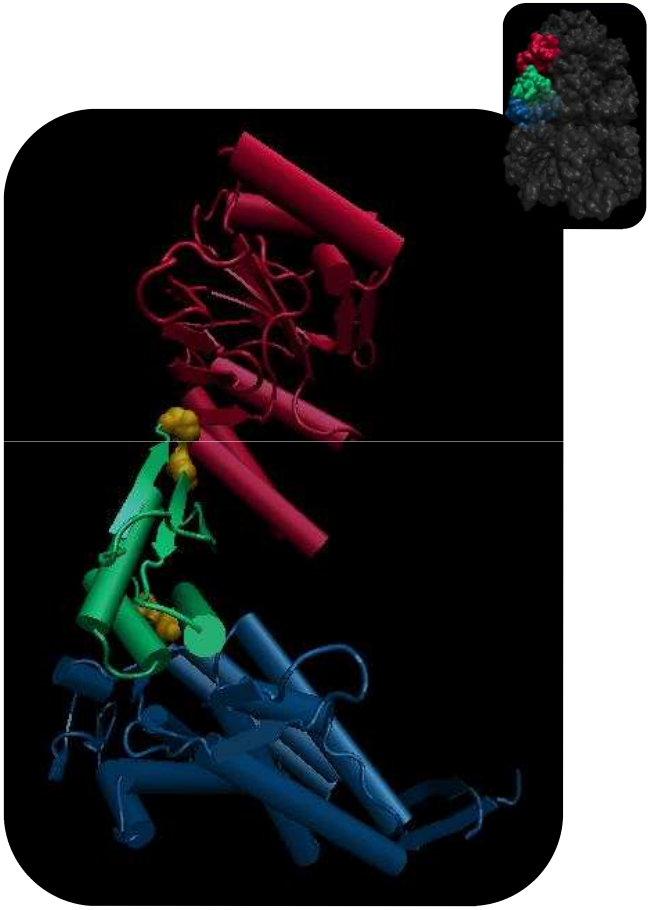
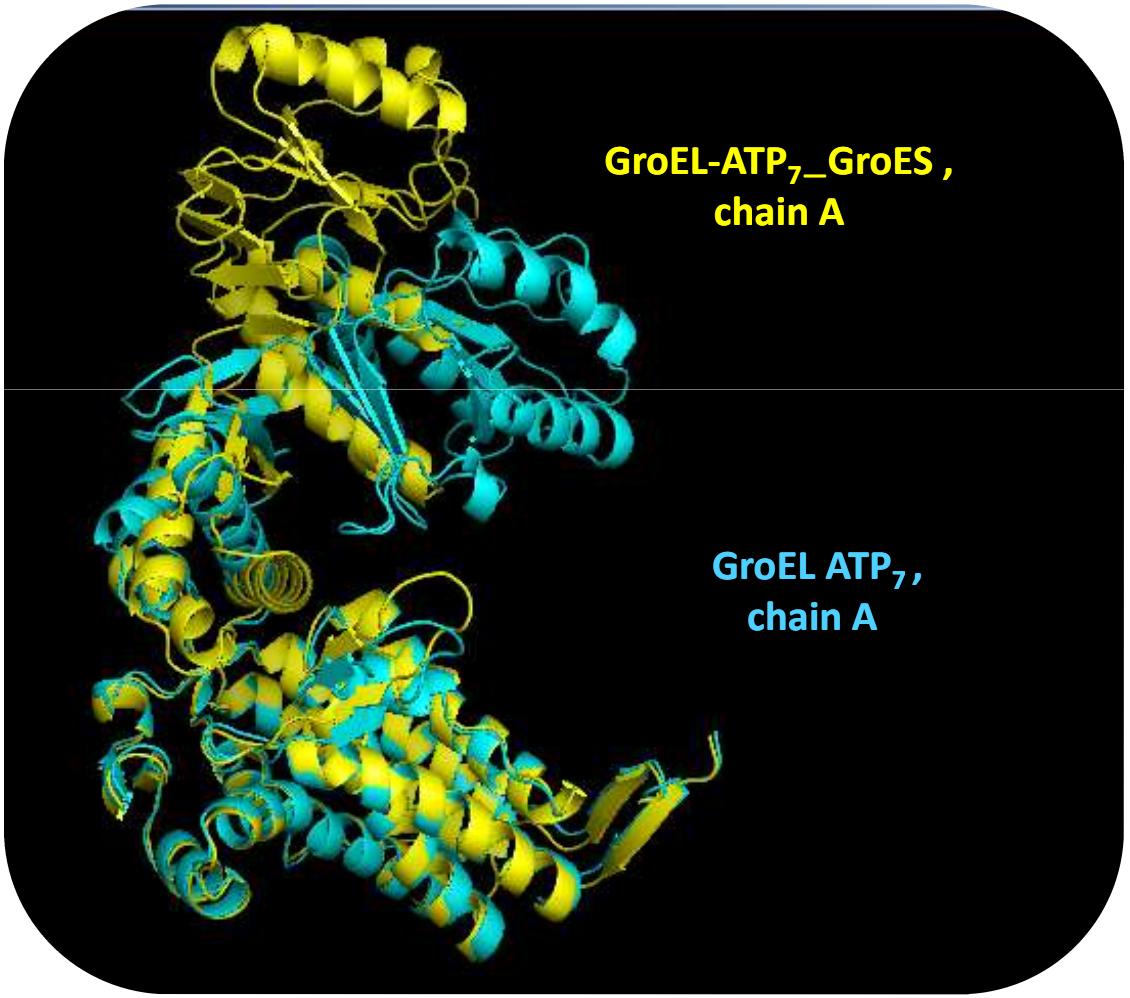


Fig71. GroEL-ATP_7-GroES (1SVT), chain A

GroEL/GroES> Folding cycle > Phase II

Nucleotide and GroES Binding



RMSD 1.12
Sc 3.91

Fig72. STAMP GroEL ATP_7 (1SX3), chain A vs GroEL-ATP_7-GroES (1SVT), chain A

GroEL/GroES> **Folding cycle >** Phase II

Nucleotide and GroES Binding

GroEL ATP_7, GroEL-ATP_7-GroES

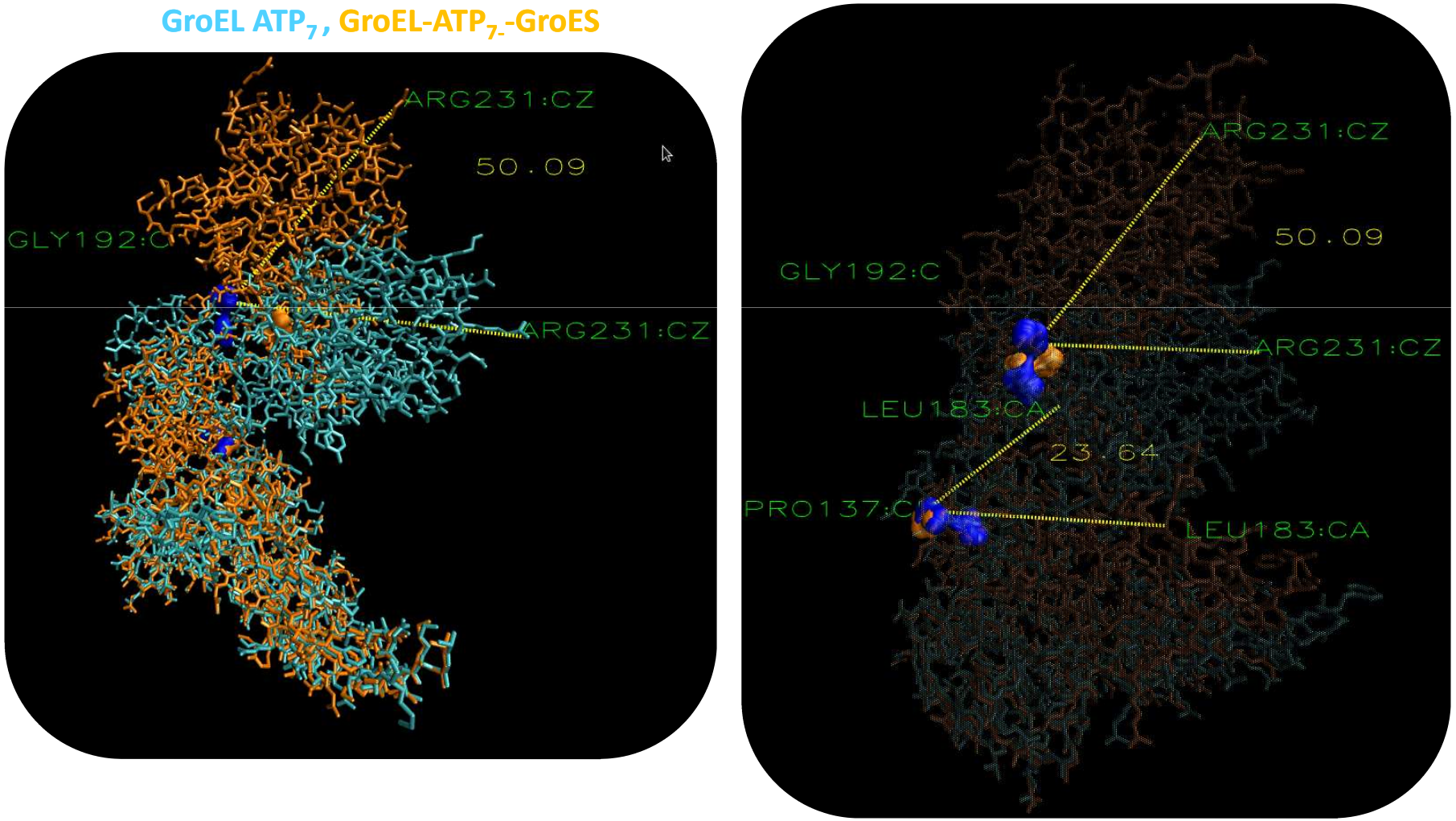


Fig73. STAMP GroEL ATP_7 (1SX3), GroEL-ATP_7-GroES (1SVT).

GroEL/GroES> **Folding cycle >** Phase II

Nucleotide and GroES Binding

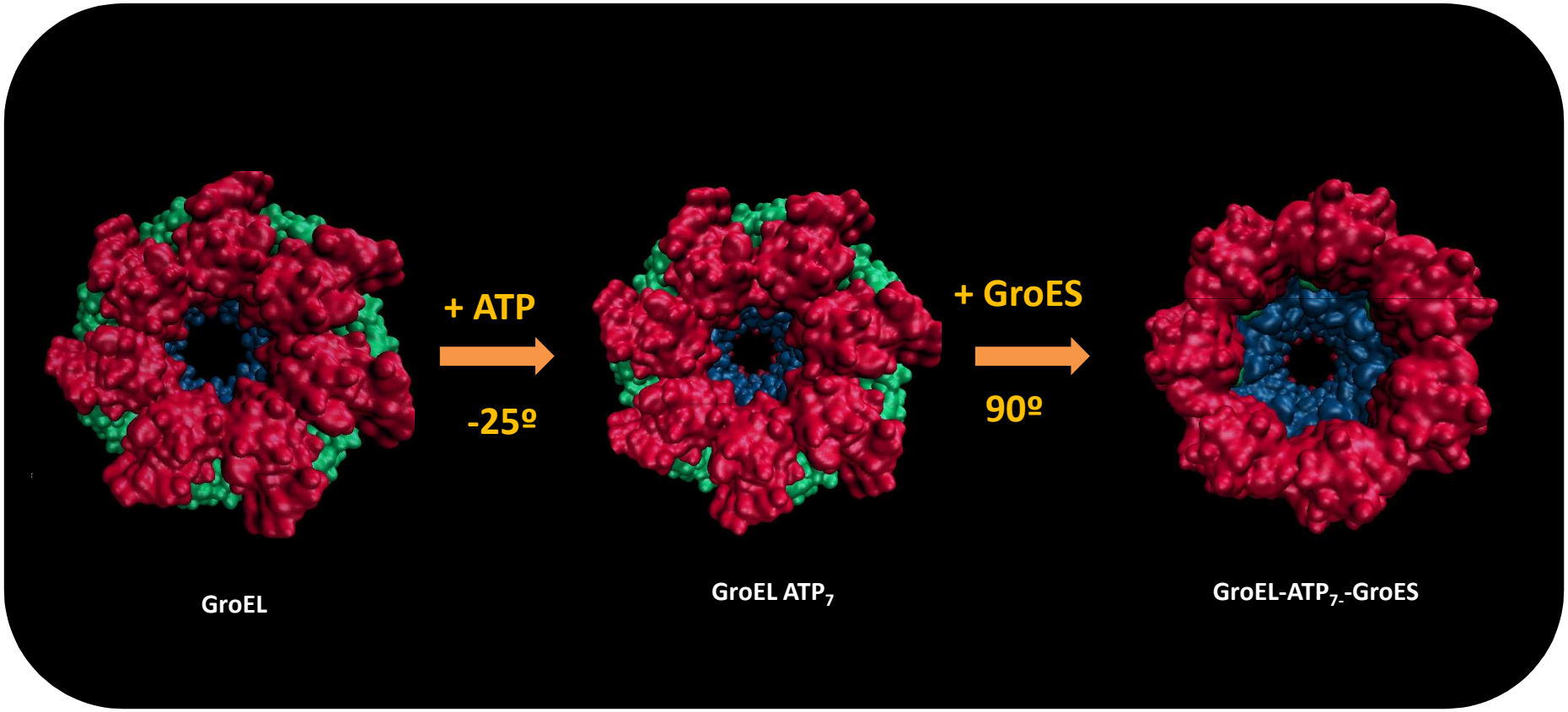
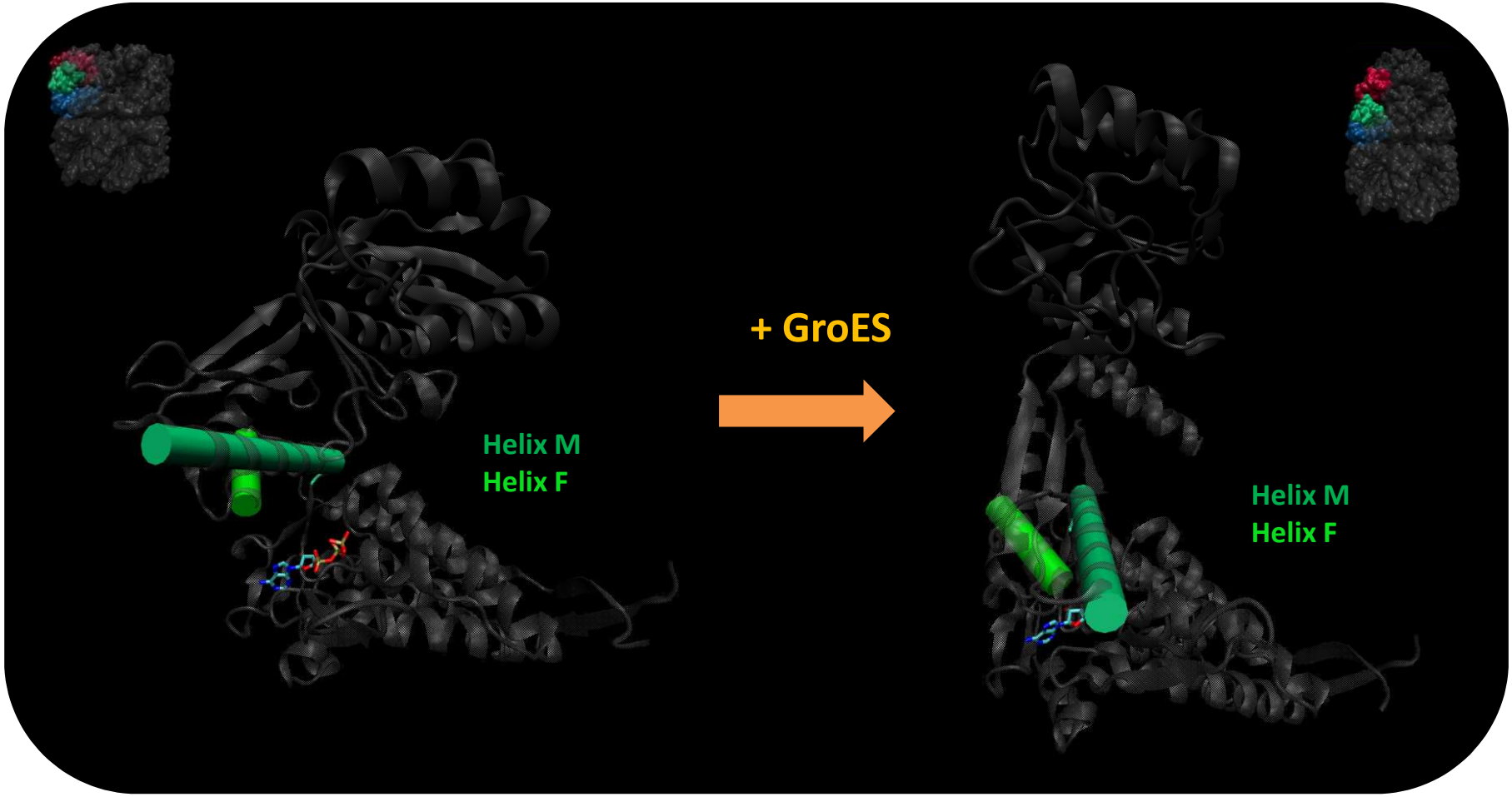


Fig 74. Twist of th apical domains (1SS8, 1SX3, 1SVT)

GroEL/GroES> **Folding cycle >** Phase II

Nucleotide and GroES Binding



GroEL ATP_7 (1SX3), chain A

GroEL-ATP_7-GroES (1SVT), chain A

Fig75. Closing the nucleotide binding site

GroEL/GroES> **Folding cycle >** Phase II

Nucleotide and GroES Binding

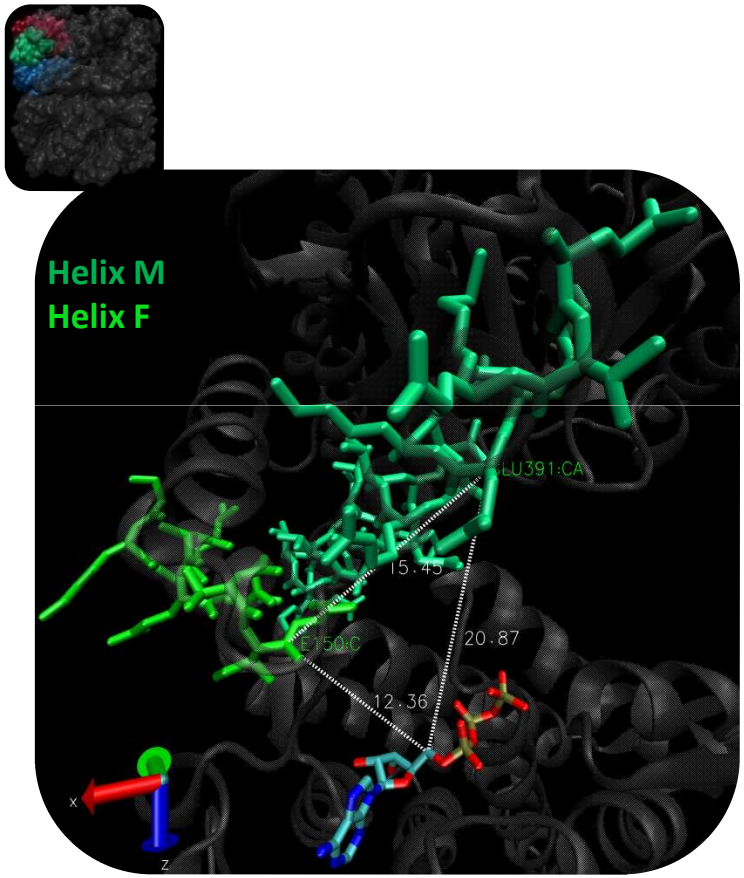


Fig76. GroEL (1SX3)

+ GroES

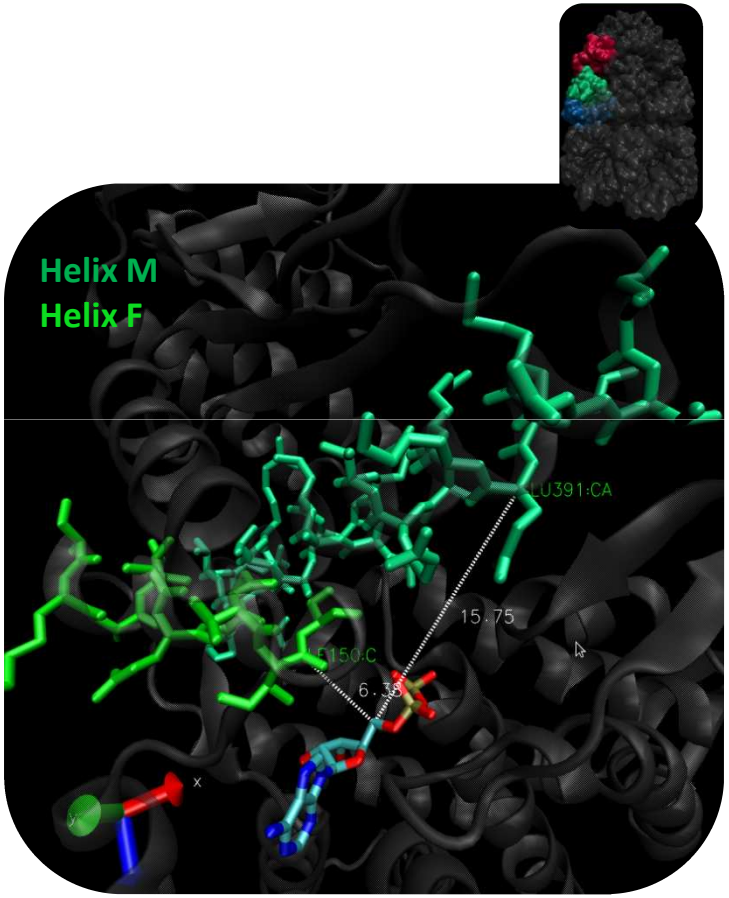


Fig77. GroEL-GroES (1SVT)

GroEL/GroES> Folding cycle > Phase II

Nucleotide and GroES Binding

GroEL ATP_7 , GroEL-ATP_7-GroES

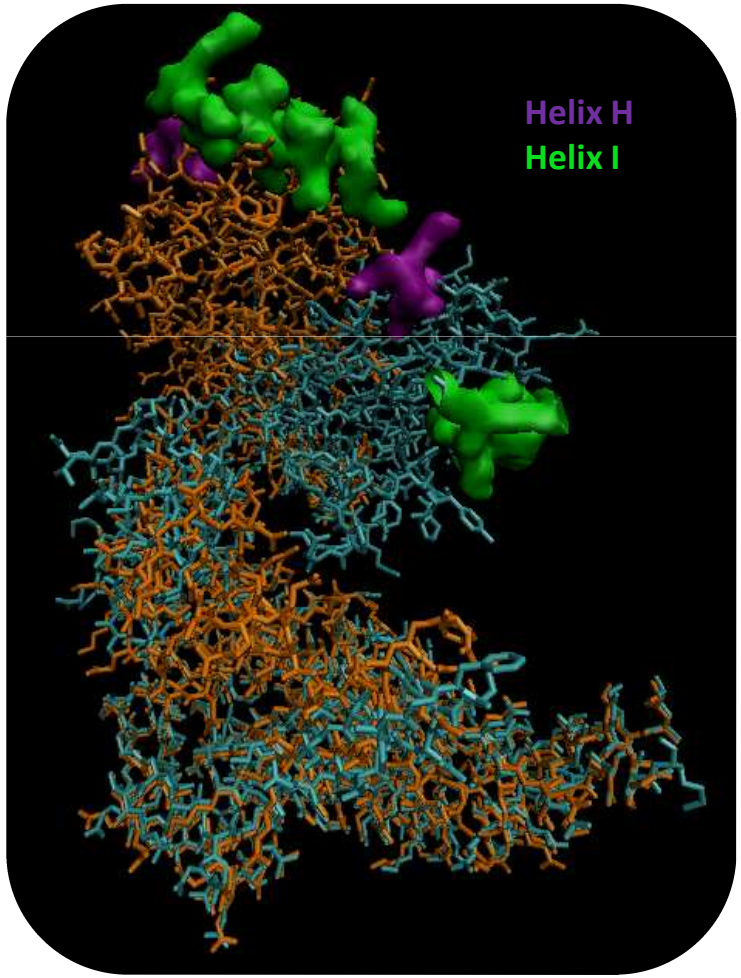


Fig78. STAMP GroEL ATP_7 (1SX3), GroEL-ATP_7-GroES (1SVT).

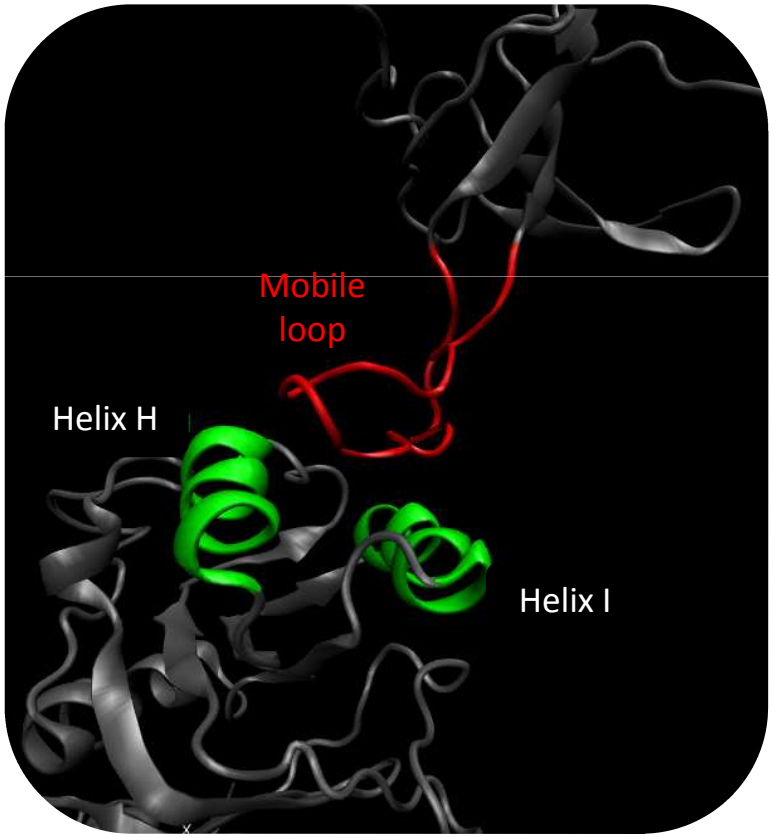


Fig79. GroEL-GroES chain A and O, interface zoom (1AON)

GroEL/GroES> **Folding cycle >** Phase II

Nucleotide and GroES Binding

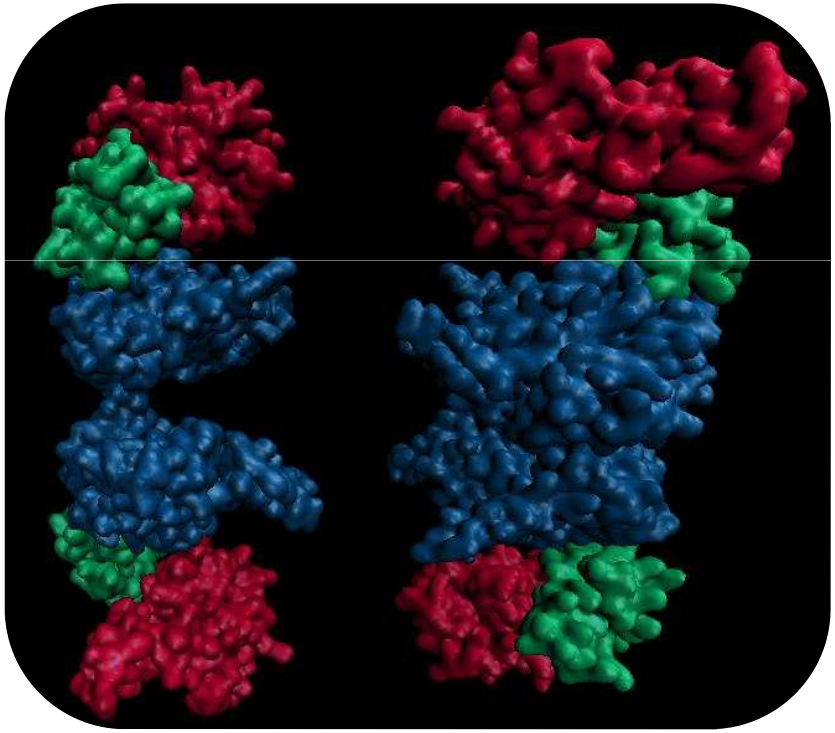


Fig80. GroEL ATP_7 (1SX3)

+ ATP

+ GroES

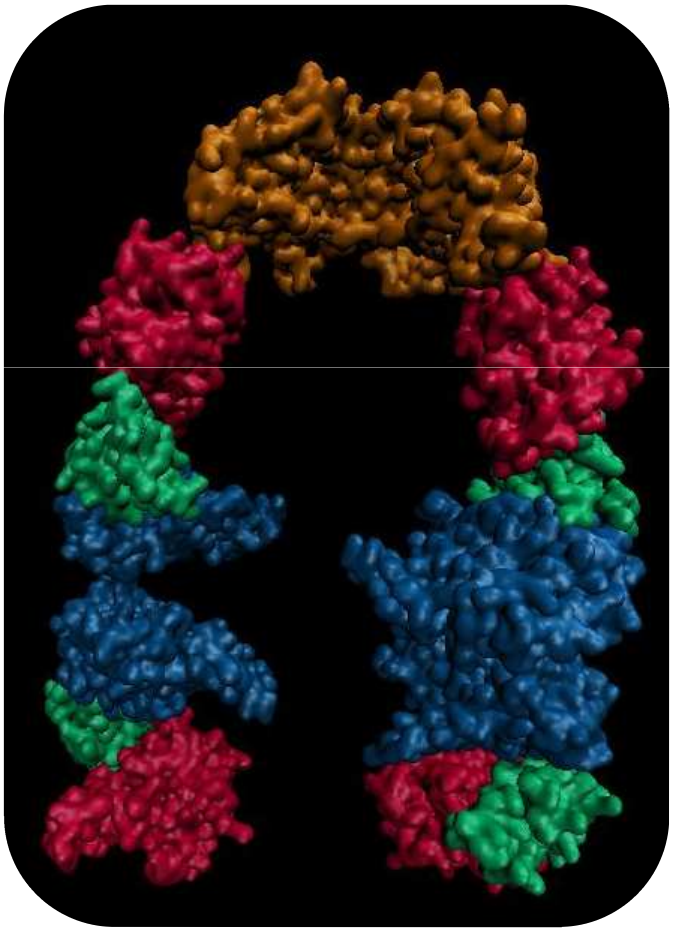


Fig81. GroEL-ATP_7-GroES (1SVT)

GroEL/GroES> **Folding cycle >** Phase II

Nucleotide and GroES Binding

STAMP

GroEL ATP_7 (1SX3) vs

GroEL-ATP_7-GroES (1SVT)

RMSD 3.03

Sc 1.21

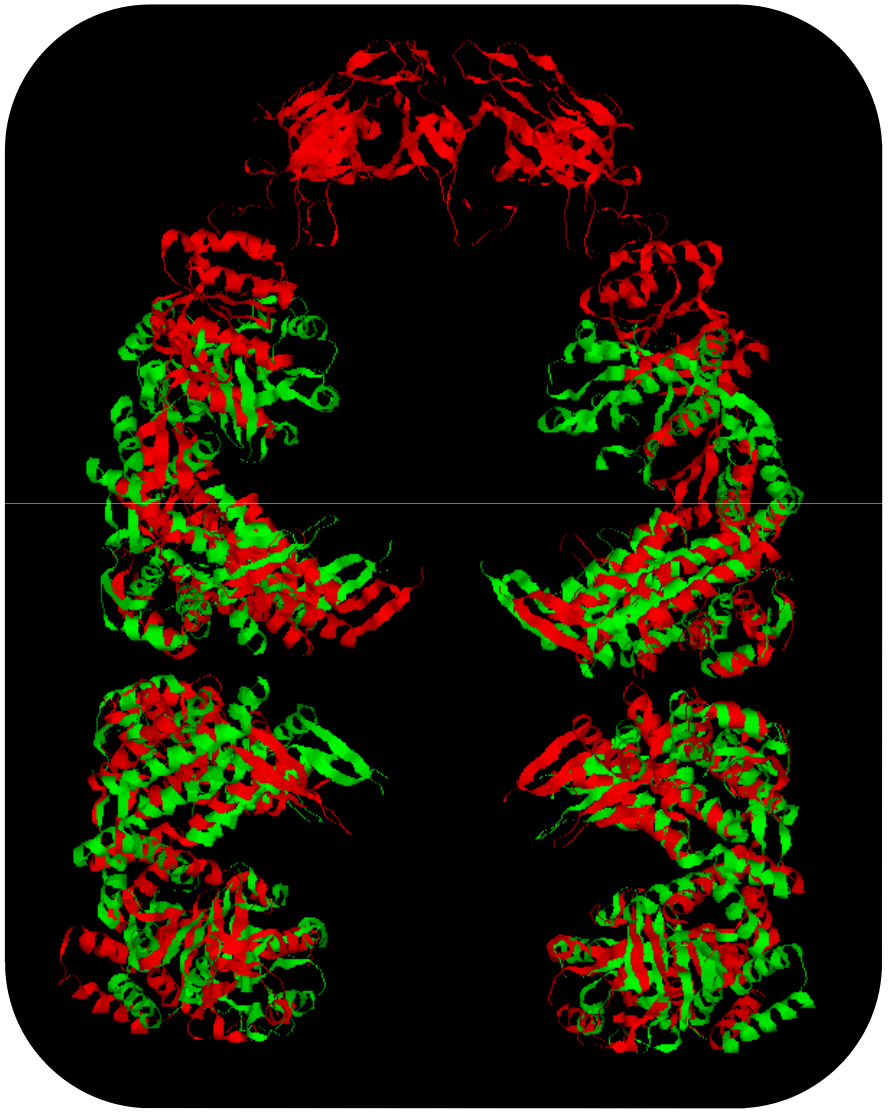


Fig82. STAMP GroEL ATP_7 (1SX3) vs GroEL-ATP_7-GroES (1SVT)

GroEL/GroES> Folding cycle > Phase III

Polypeptide Release and Folding

Hydrophobic residues
Polar residues

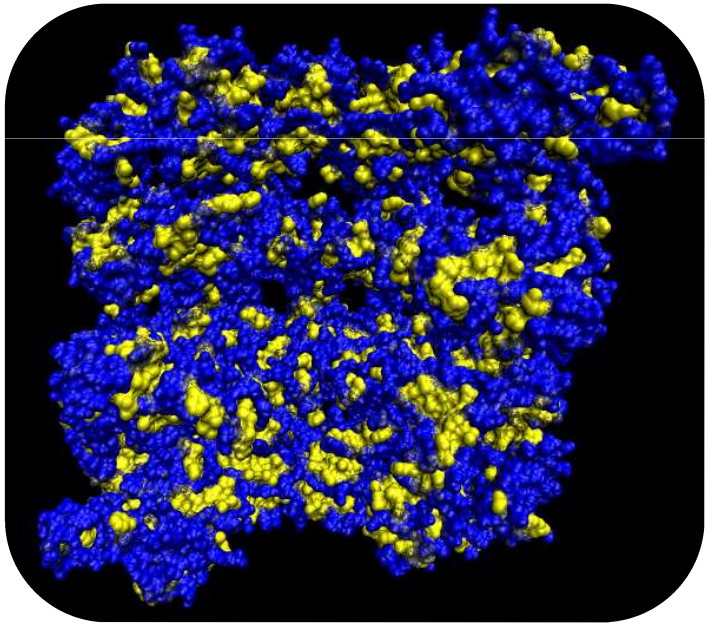


Fig83. GroEL cavities (1MNF)

+ GroEL

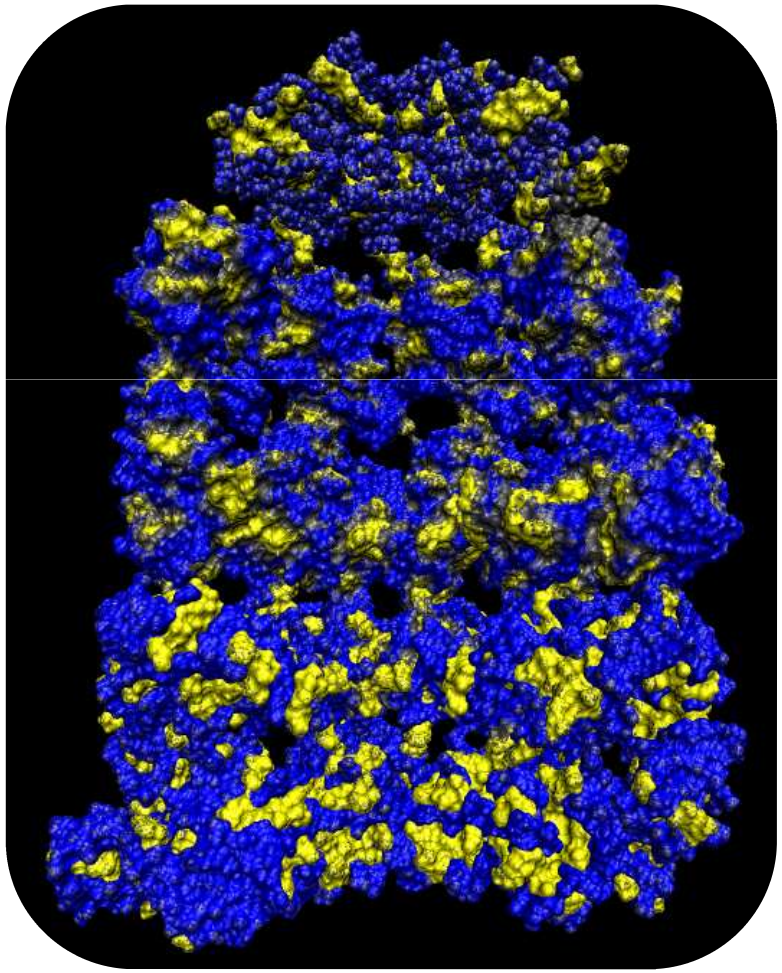
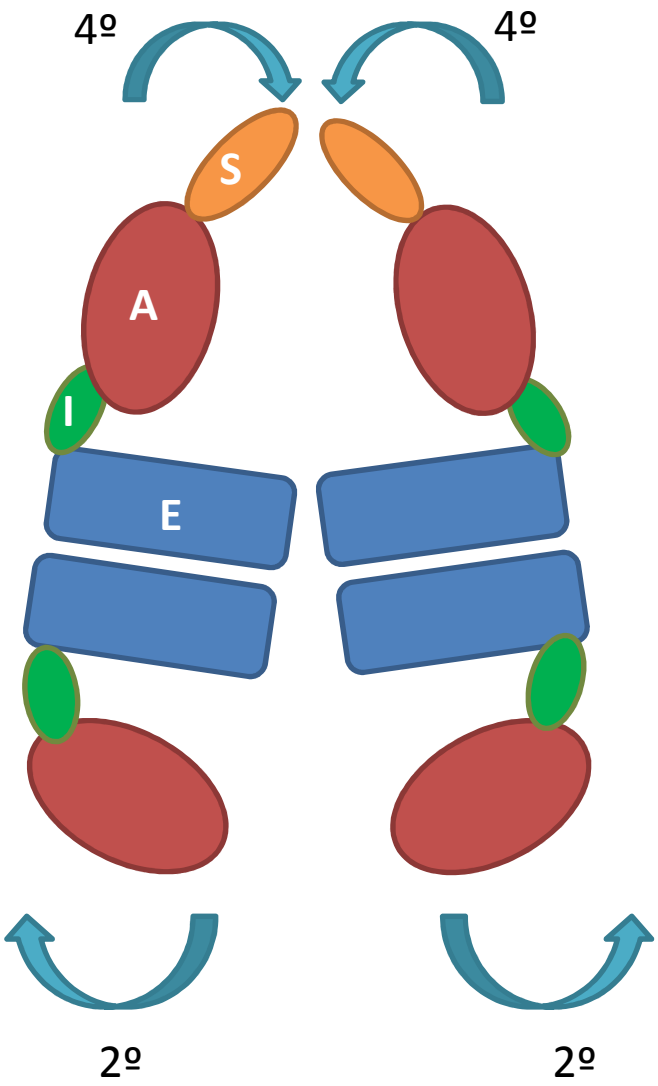


Fig84. GroEL-GroES cavities (1AON)

GroEL/GroES> **Folding cycle >** Phase IV

Protein Folding and Release of Ligands



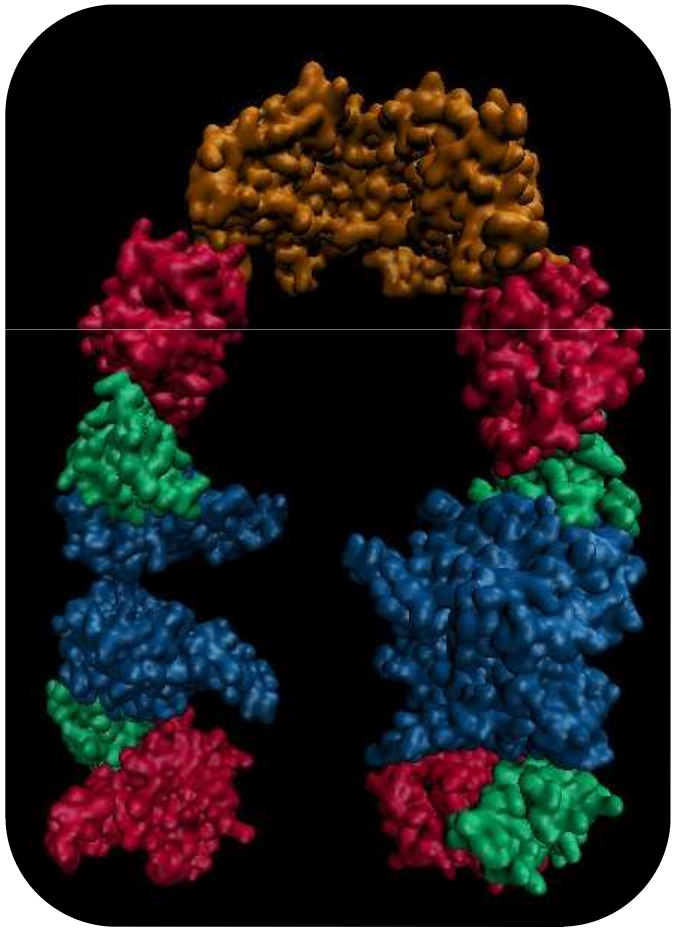
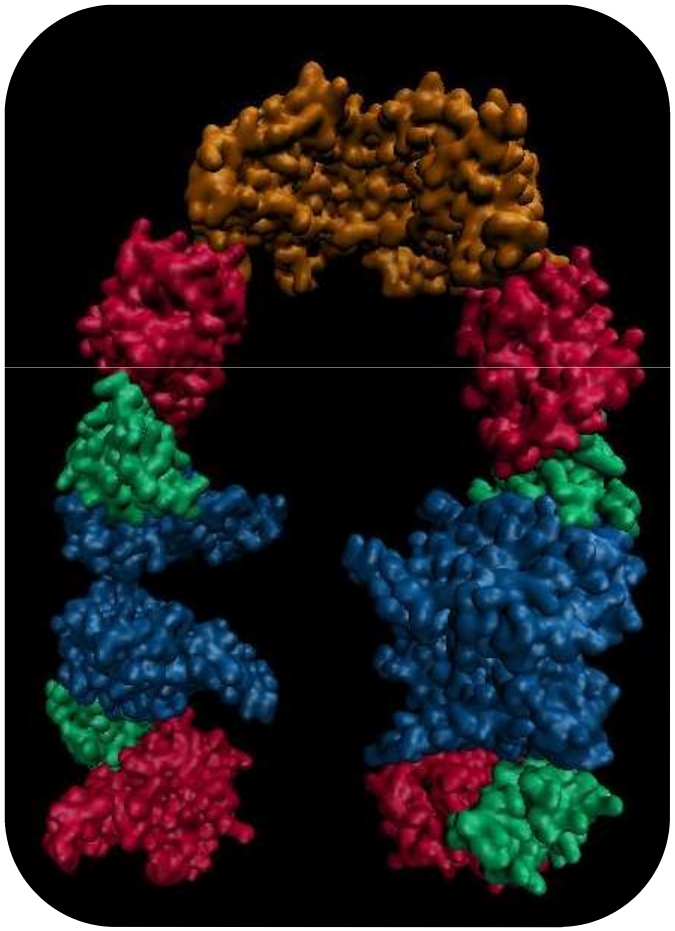


Fig85.GroEL-ATP$_7$-GroES (1SVT)

GroEL/GroES> **Folding cycle >** Phase IV

Protein Folding and Release of Ligands



- Pi

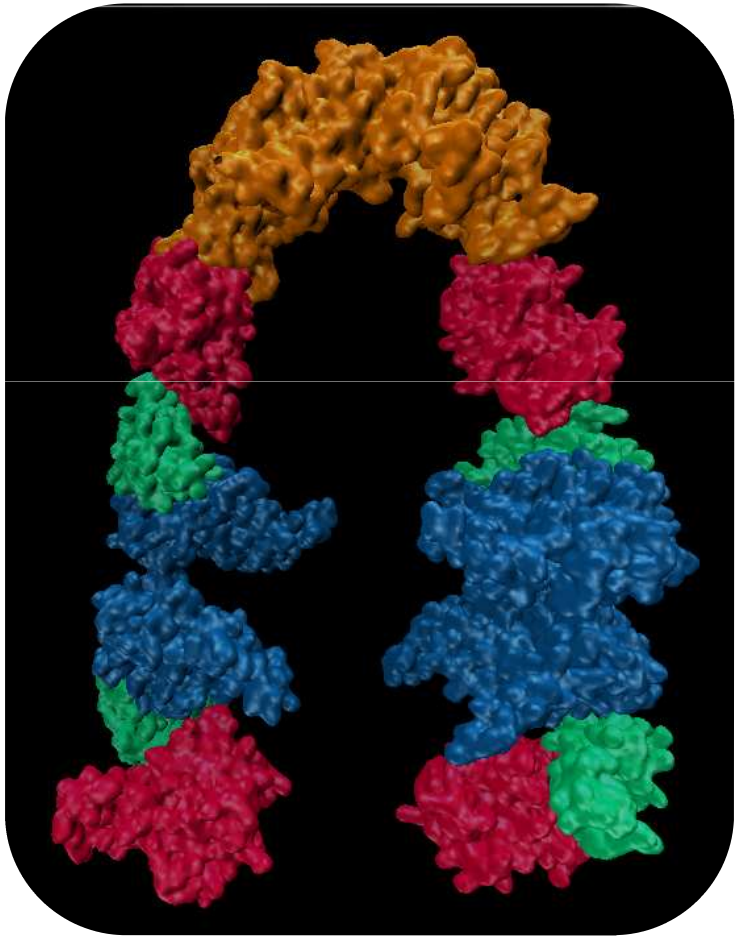


Fig86. GroEL-ATP$_7$-GroES (1SVT)

Fig87. GroEL-ADP$_7$-GroES (1SX4)

GroEL/GroES> **Folding cycle >** Phase IV

Protein Folding and Release of Ligands

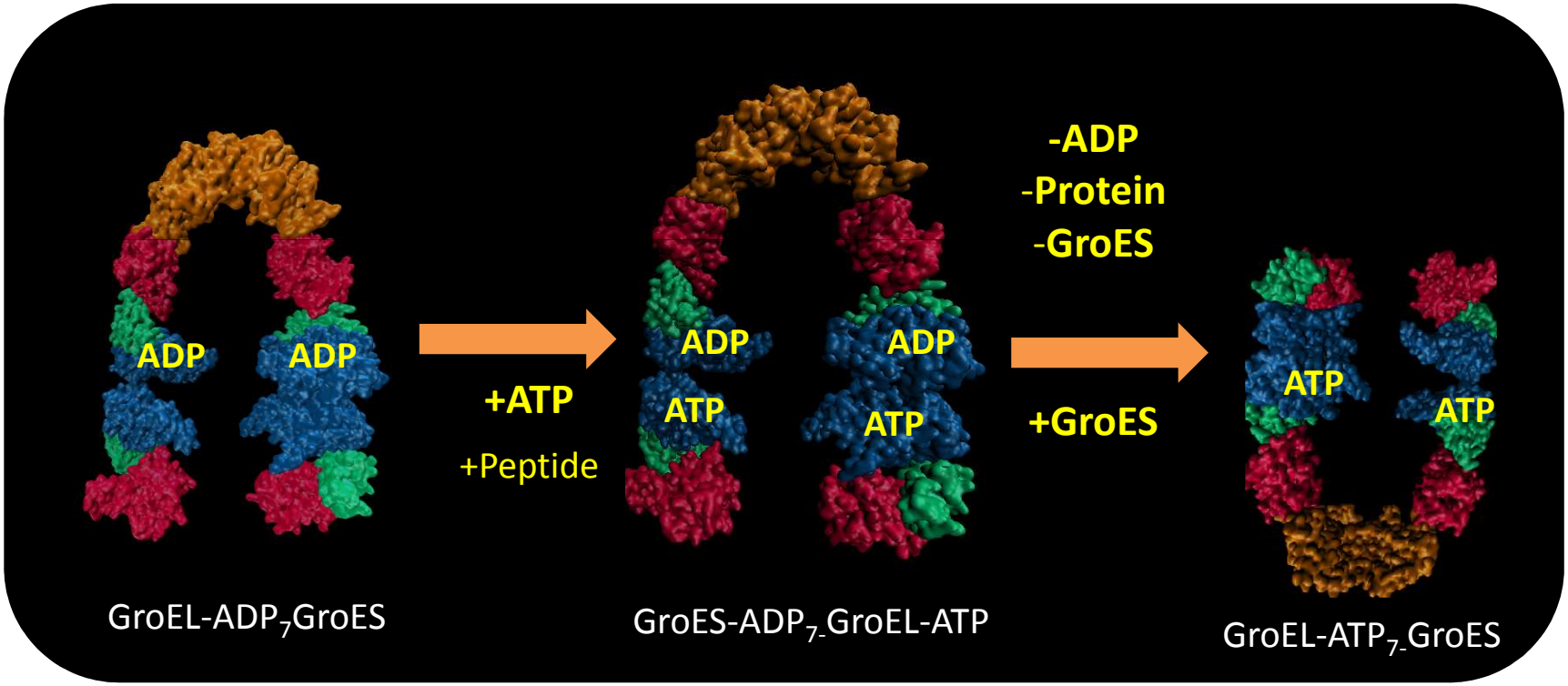


Fig88. Release of Ligands (1SX4, 1GRU, 1SVT)

GROUP II CHAPERONINS

Group II > Main characteristics

Archaea (Thermosome) and Eukaryotes (TRiC/CCT)

Two hetero or homo rings with 8 to 9 subunits

Major structural difference: “Build-in lid”

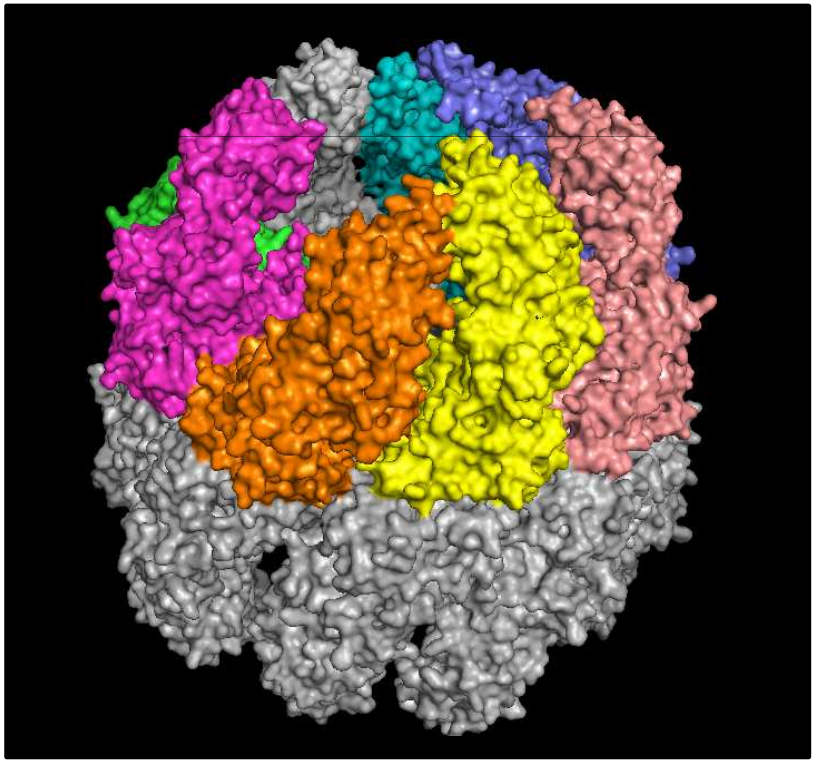


Fig89. TRiC/CCT, eukaryote chaperonin (4A0O)

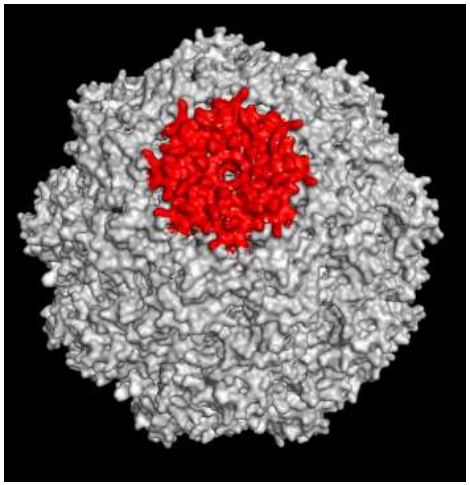


Fig90. Lids closing the chamber (3LOS)

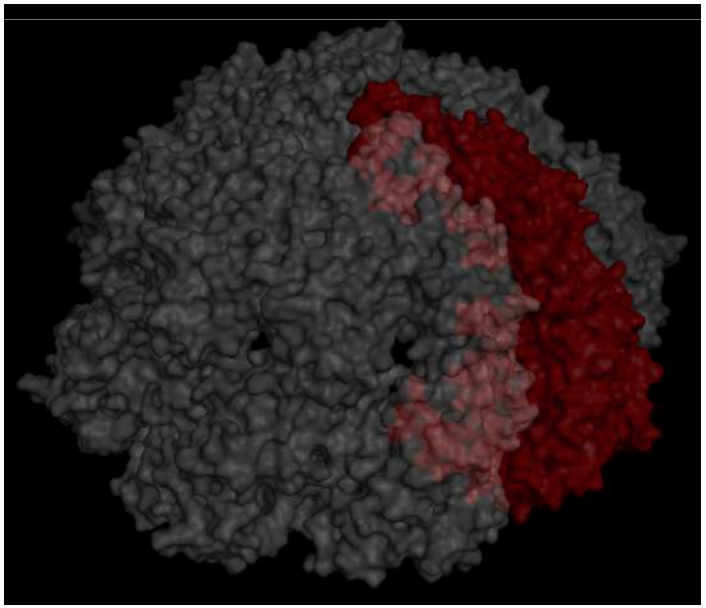


Fig91. Single subunit of MmCpn (3LOS)

Group II > Sequence alignment

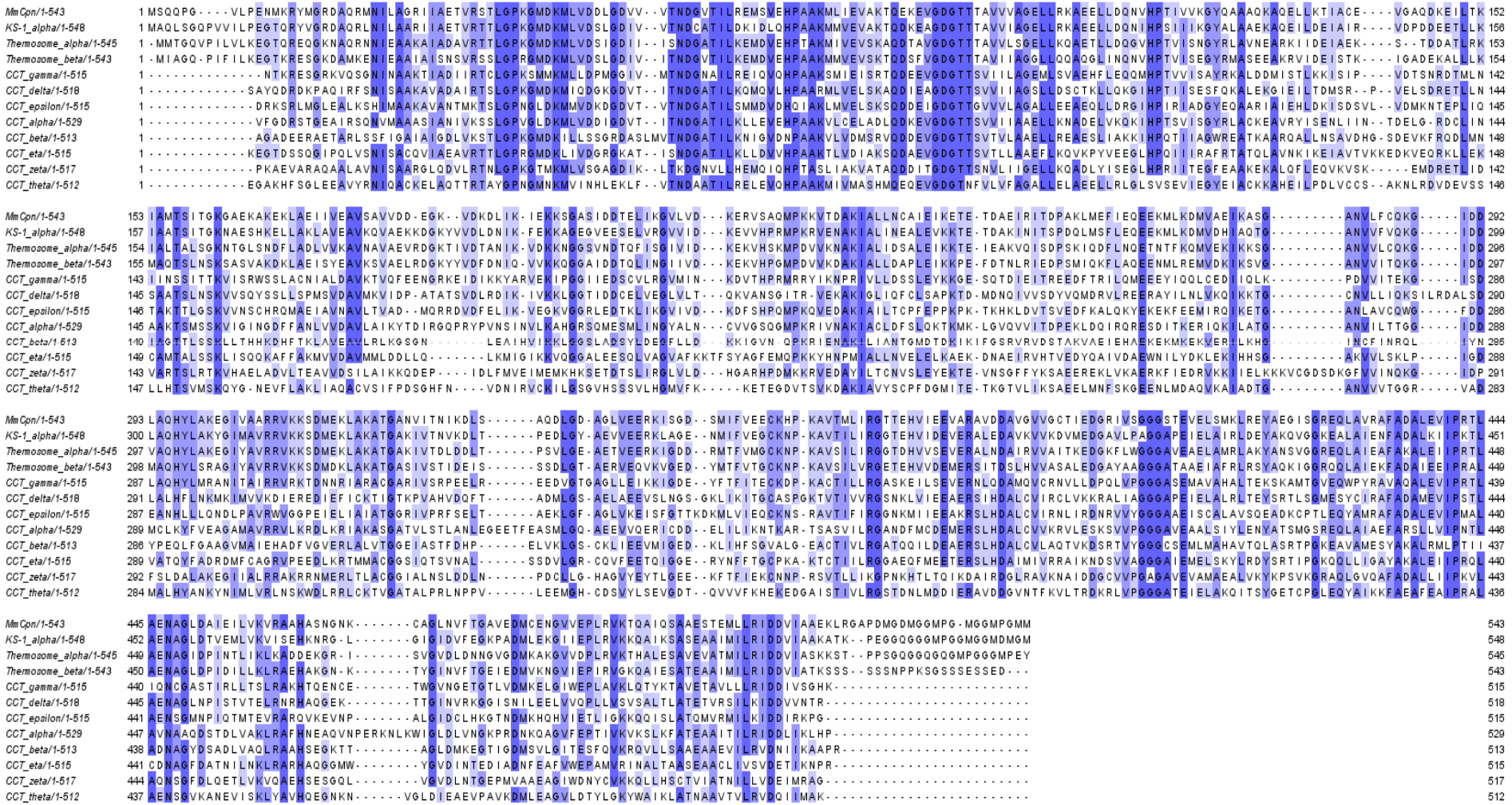


Fig92. Sequence alignment between members of the group II chaperonins

Group II > Structural alignment

The structure is much more conserved that the sequence

Sc 8,17

RMSD 1,56

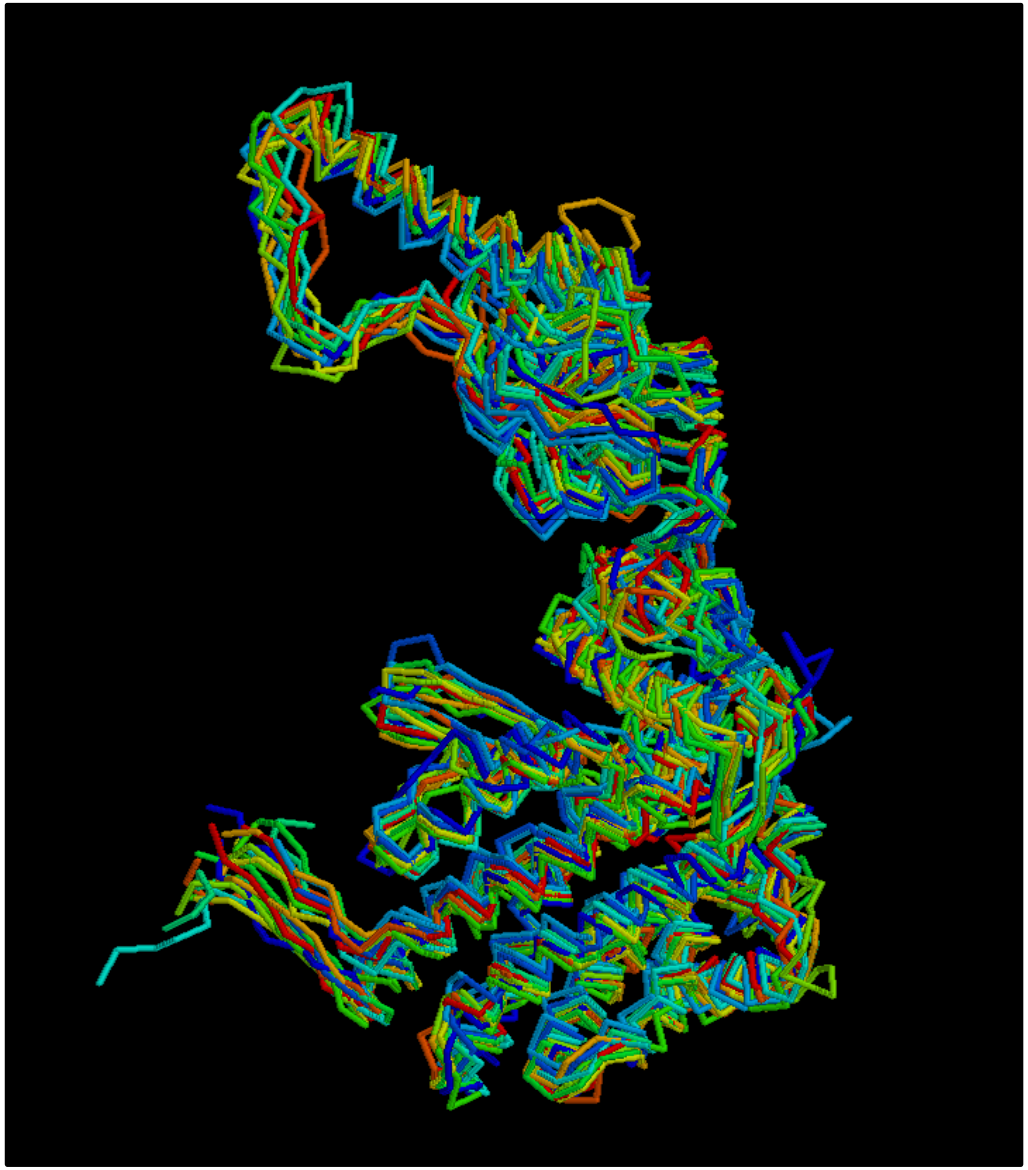


Fig93. Structural alignment between members of the group II chaperonins

MmCpn > General structure

Archaea: *Methanococcus maripaludis*

Homo- octameric ring

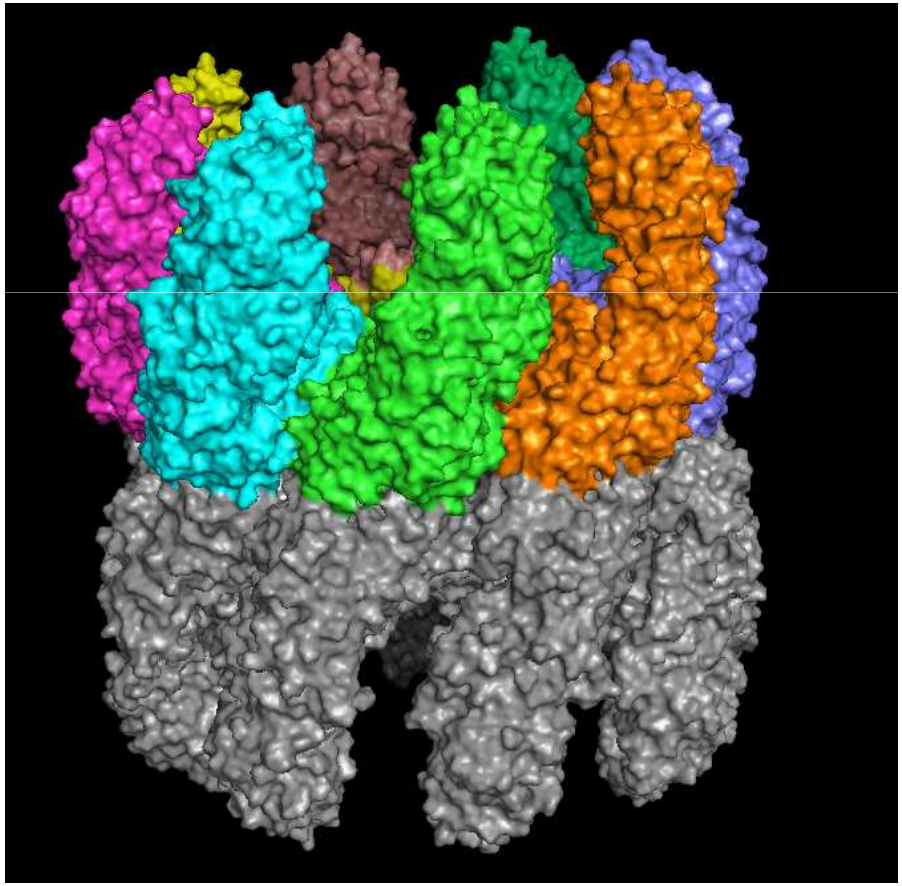


Fig94. Lateral view of MmCpn in open conformation (3IYF)

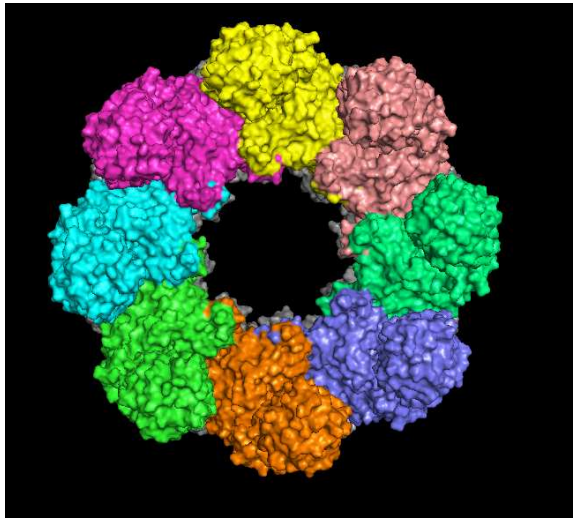


Fig95. Top view of MmCpn in open conformation (3IYF)

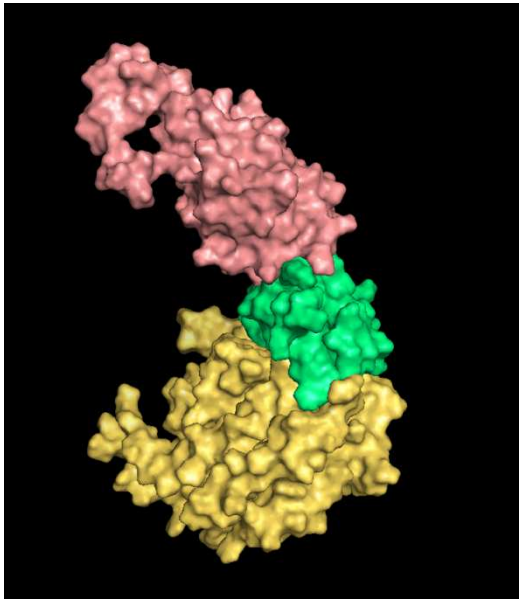


Fig96. Subunit architecture (3KFB)

MmCpn > Cycle overview

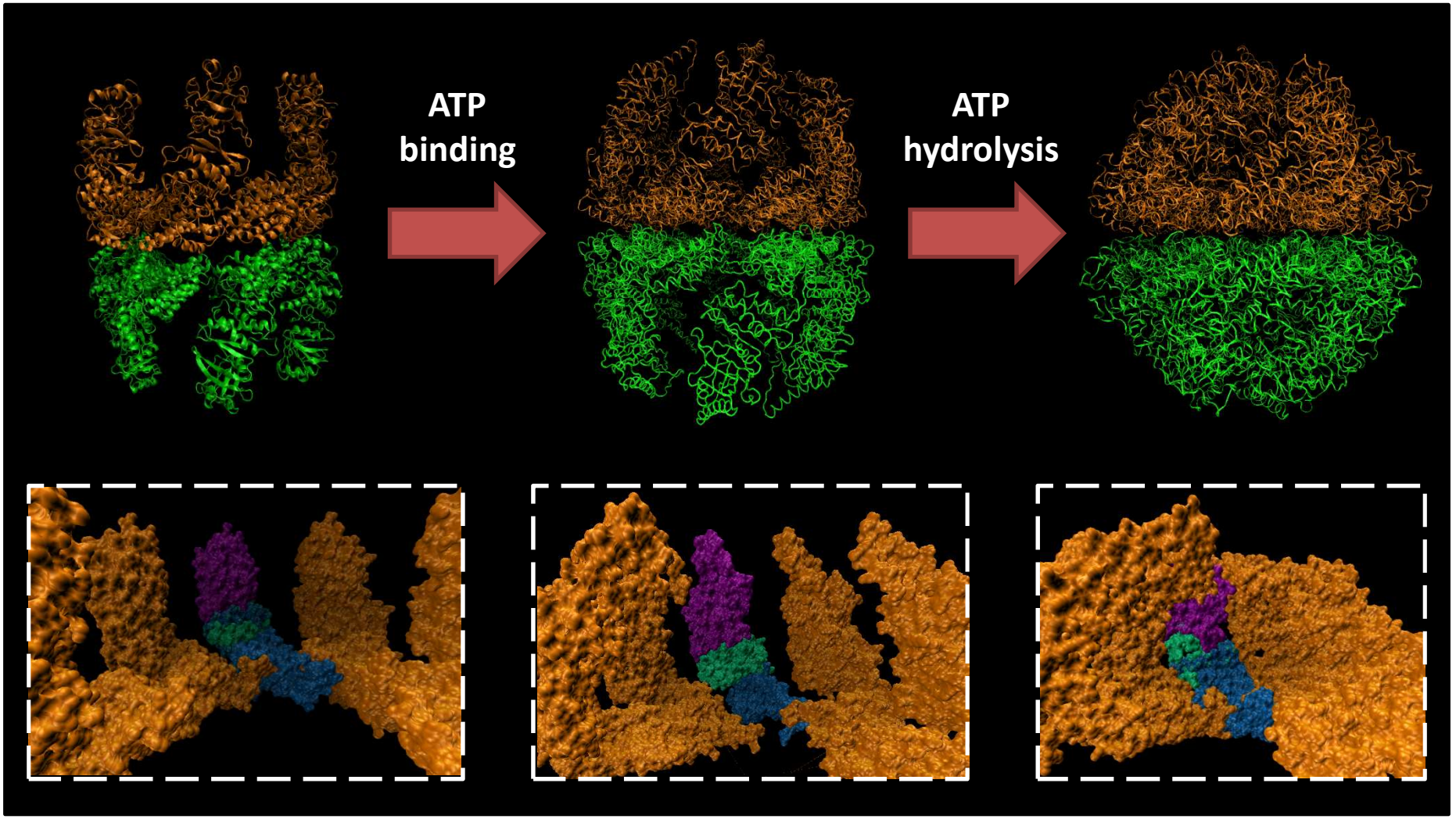


Fig97. Cycle overview (3IYF, 3IZH, 3LOS)

MmCpn > Open state

Contacts
- Inter-ring
- Intra-ring

Substrate binding site

Nucleotide binding site

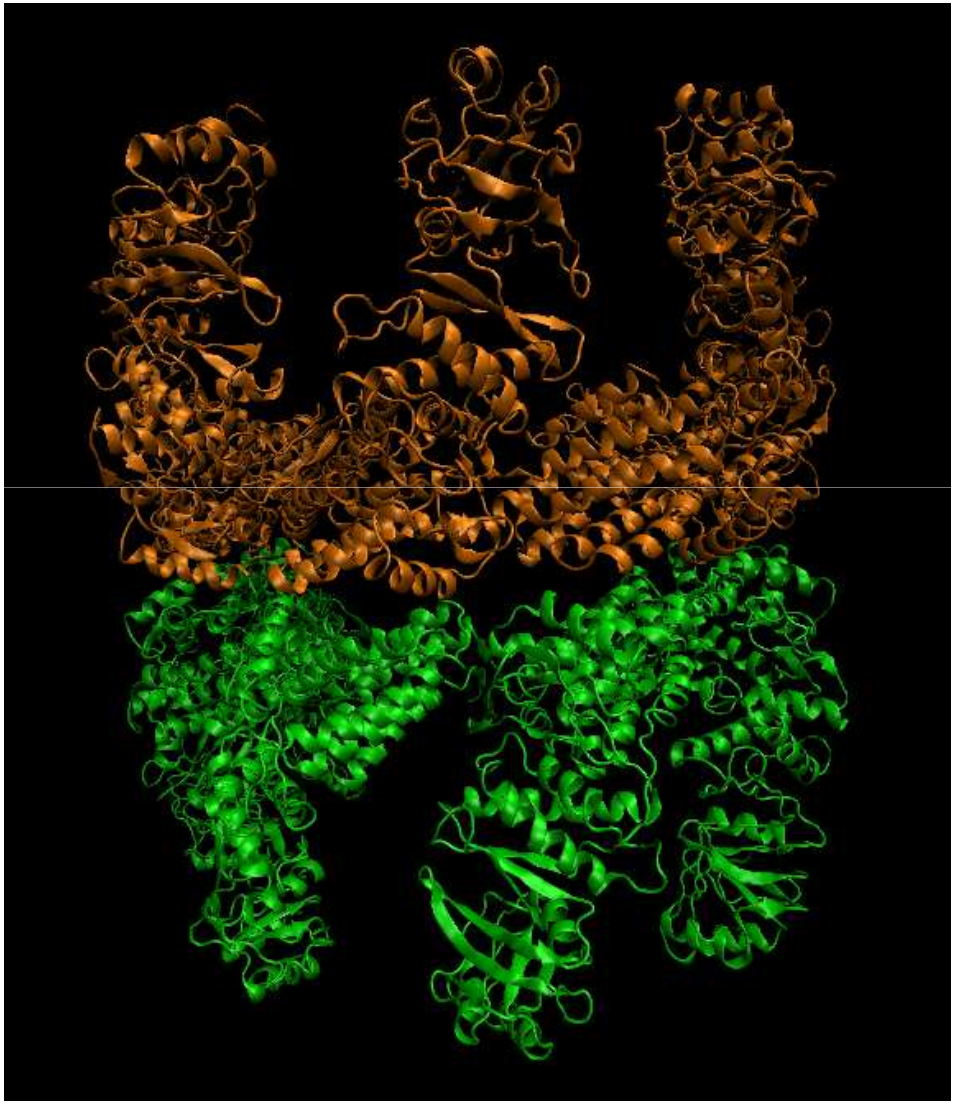


Fig98. MmCpn in open conformation (3IYF)

MmCpn > Open state > Inter-ring interactions

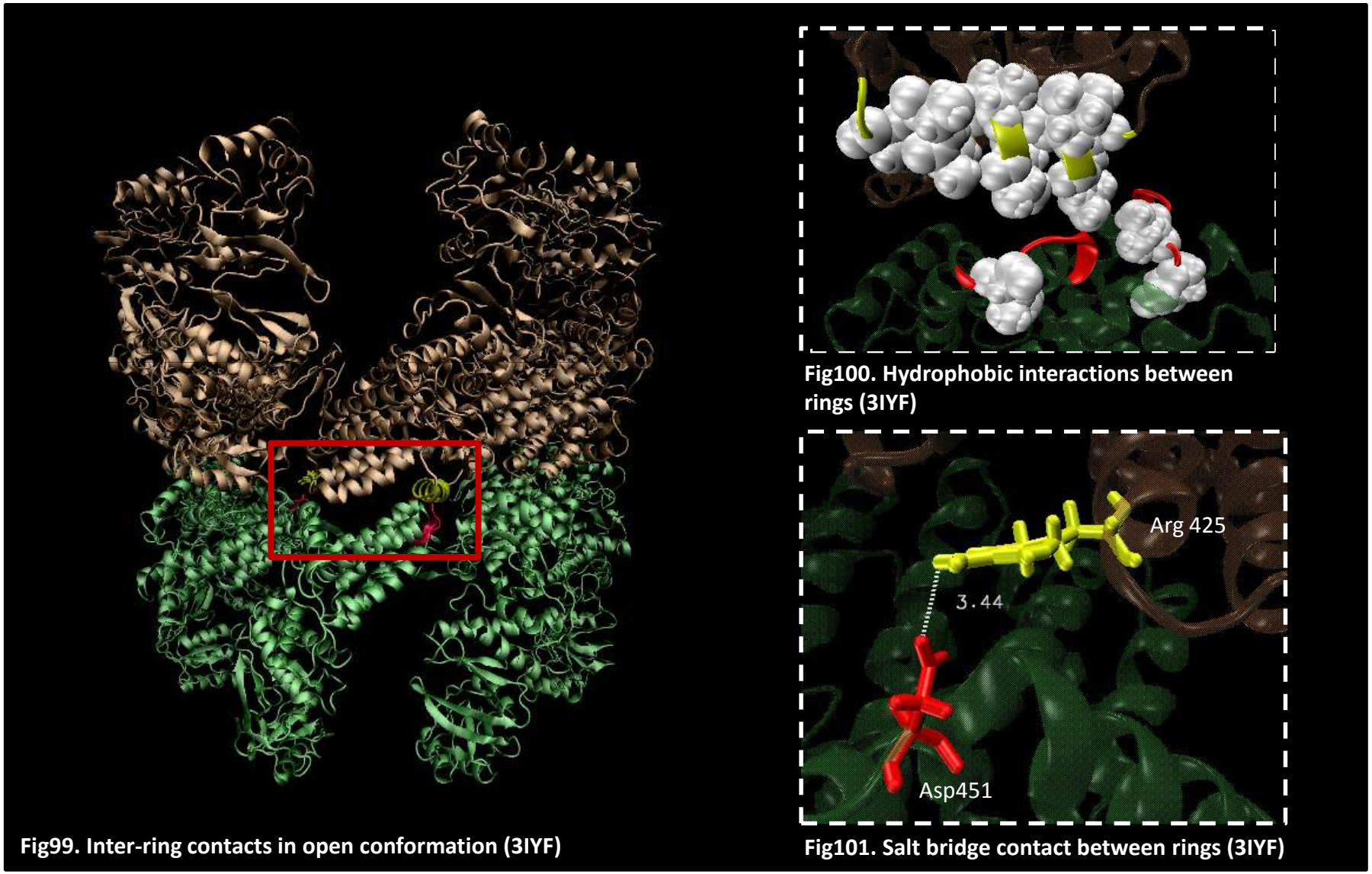


Fig99. Inter-ring contacts in open conformation (3IYF)

Fig100. Hydrophobic interactions between rings (3IYF)

Fig101. Salt bridge contact between rings (3IYF)

MmCpn > Open state > Intra-ring interactions

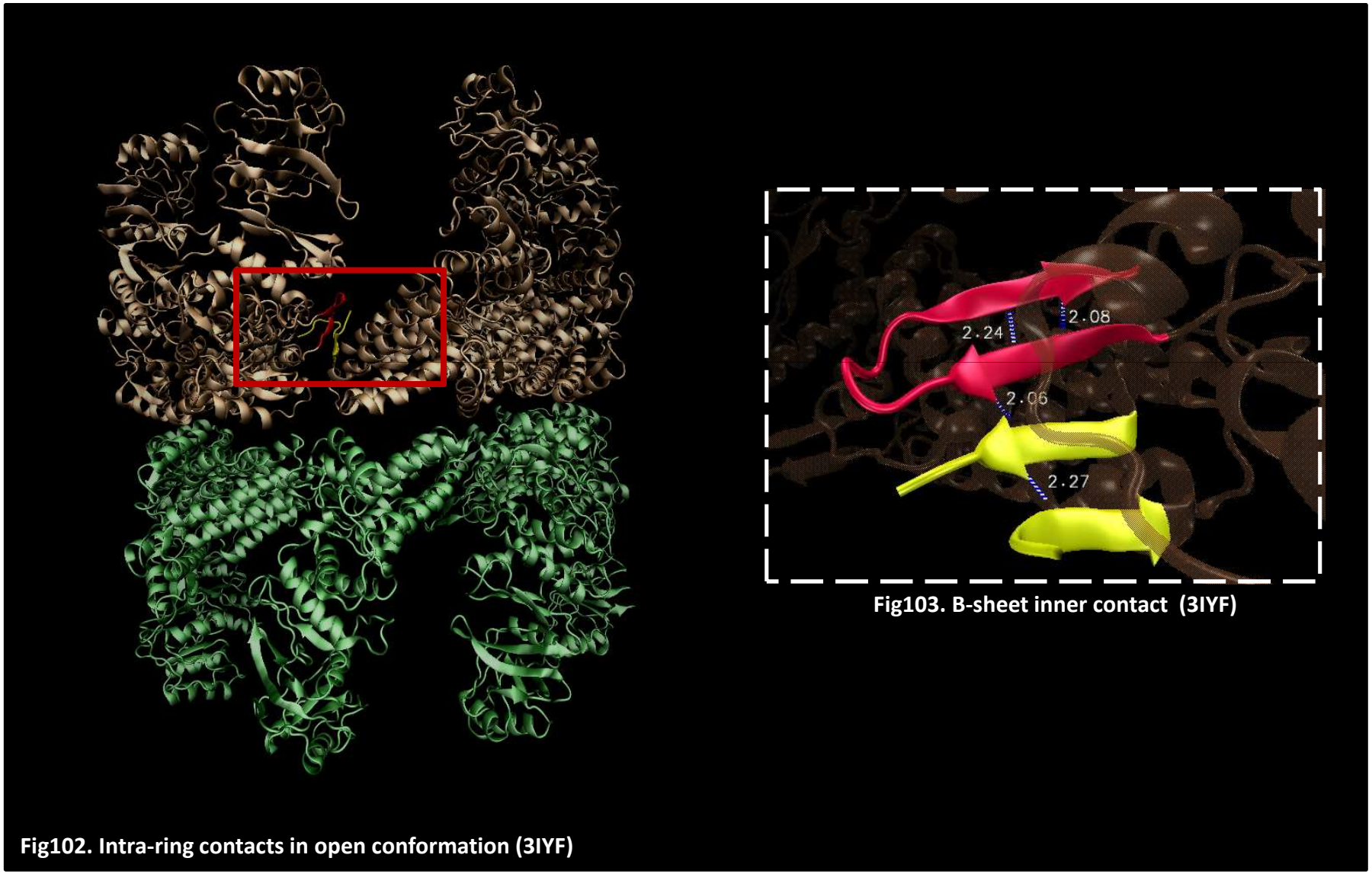


Fig103. B-sheet inner contact (3IYF)

Fig102. Intra-ring contacts in open conformation (3IYF)

MmCpn > Open state > Substrate binding site

Hydrophobic patch in the apical domain

Interface between helices H10 and H11

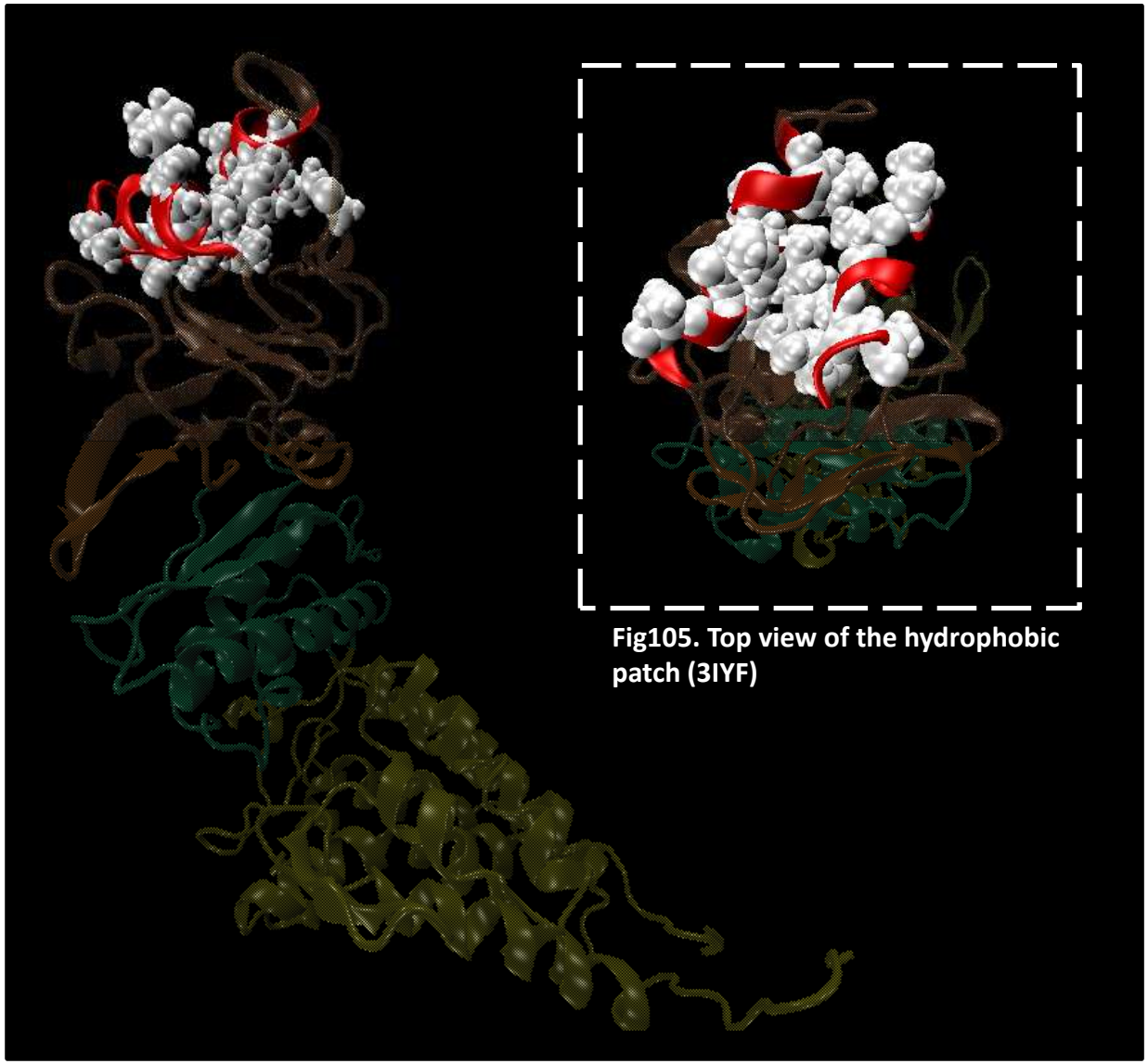


Fig105. Top view of the hydrophobic patch (3IYF)

Fig104. Hydrophobic patch between H10 and H11 (3IYF)

MmCpn > **Open state >** Nucleotide binding site

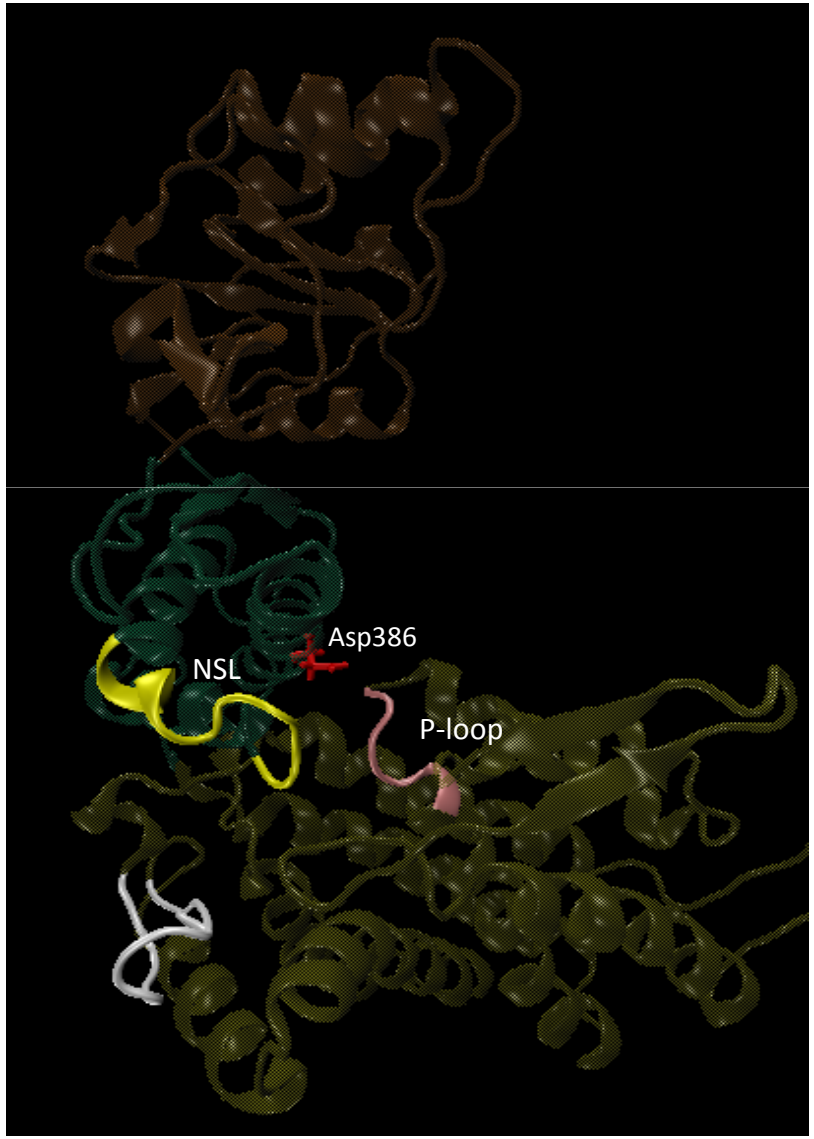


Fig108. Important residues in the Nucleotide binding site (3IYF)

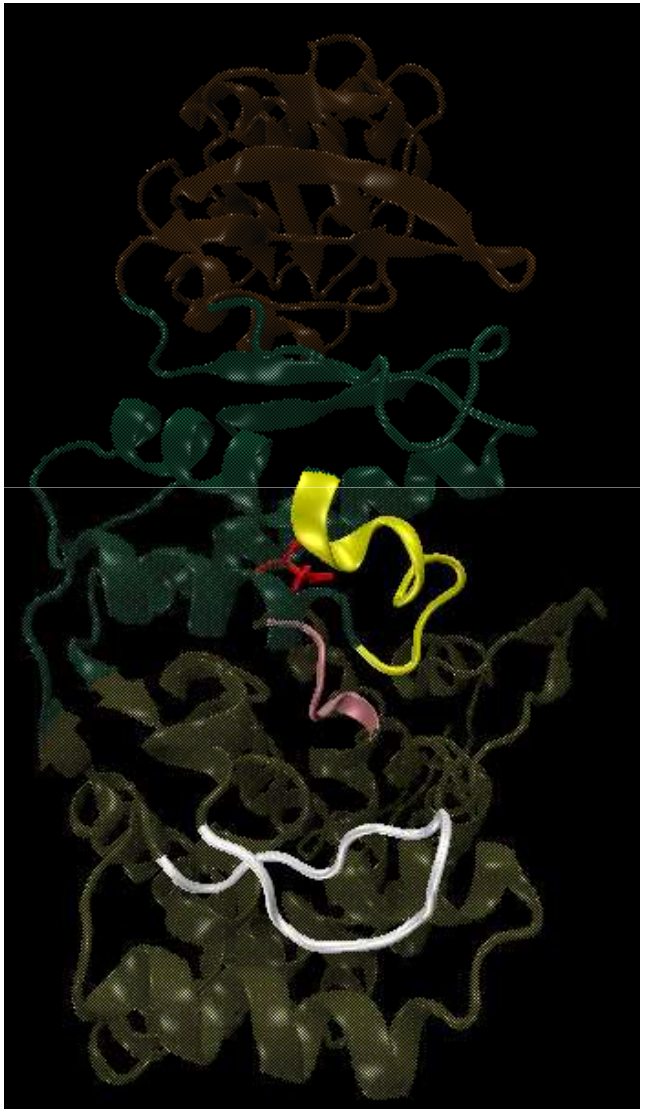


Fig109. Rear view of the Nucleotide binding site (3IYF)

MmCpn > Prehydrolysis state

ATP binds to the nucelotide binding site.

Large *en bloc* movement of the domains in each subunit:

- **Apical**
- **Intermediate**

Fig110. MmCpn in Prehydrolysis conformation (3IZH)

MmCpn > Prehydrolysis state > General movement

Apical and intermediate domains tilt toward the equatorial domain

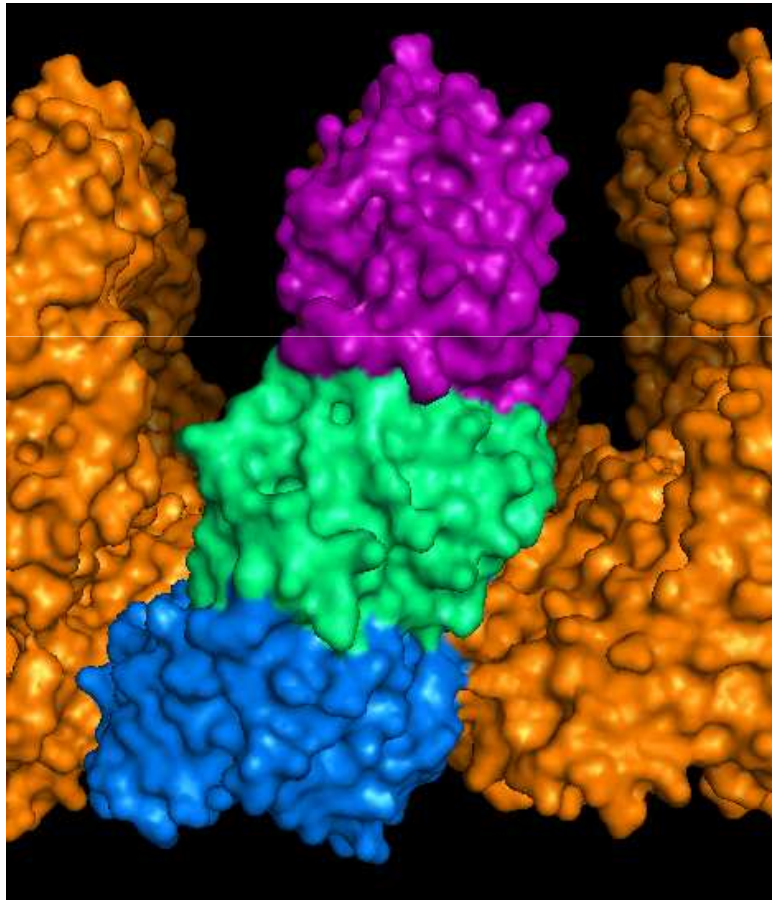


Fig111. Single subunit in open conformation (3IYF)

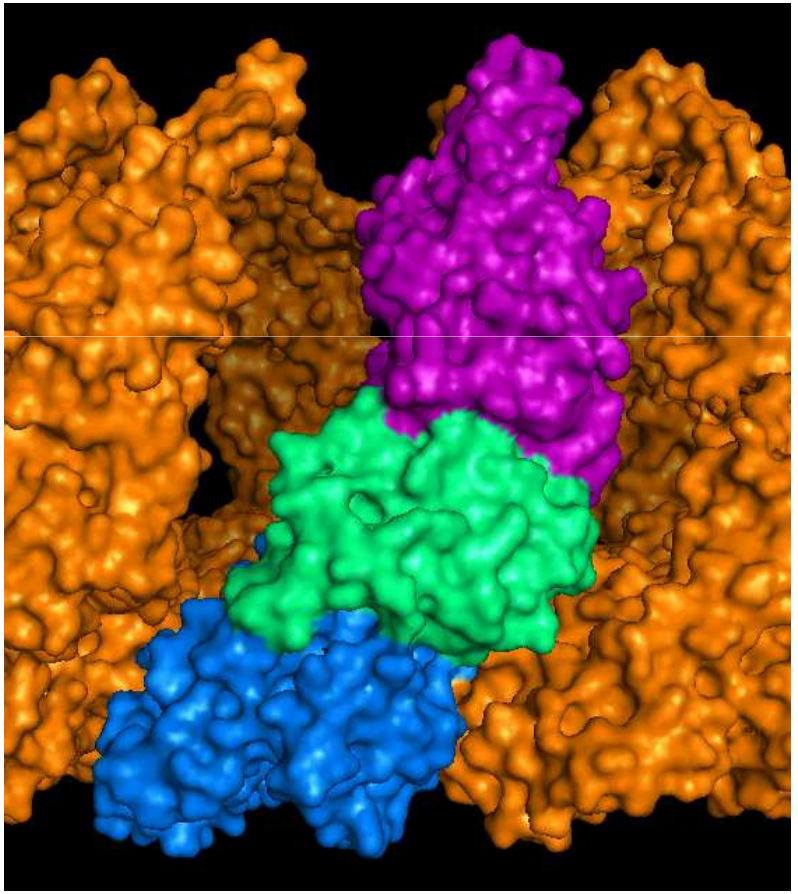


Fig112. Single subunit in Prehydrolysis conformation (3IZH)

MmCpn > Prehydrolysis state > Apical movement

Counter-clockwise rotation of the apical domains

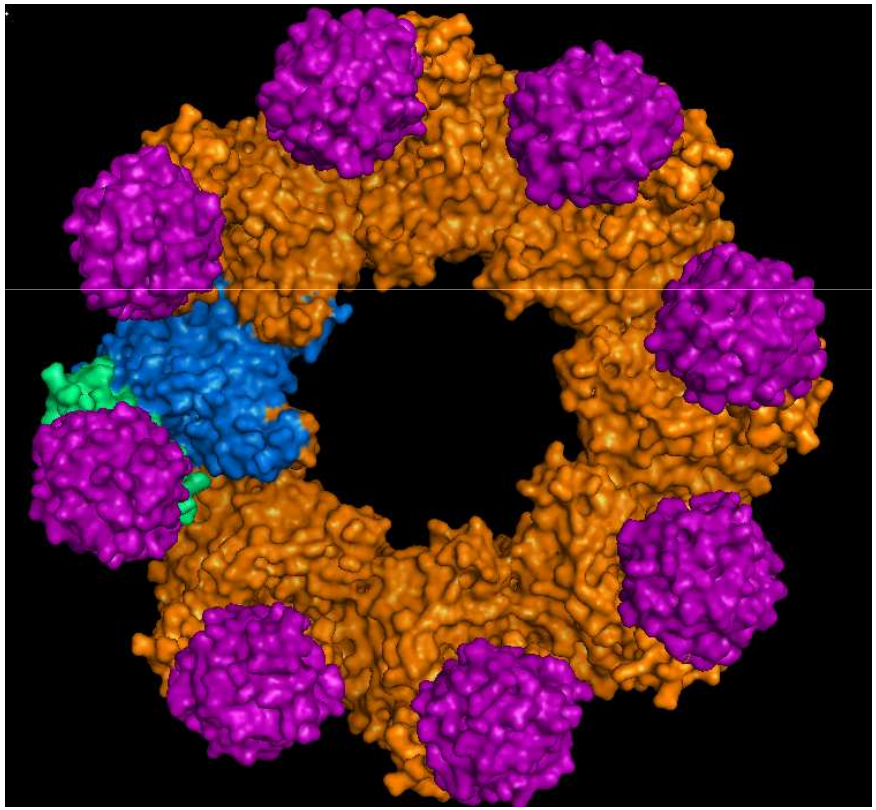


Fig113. Apical domains in open conformation (3IYF)

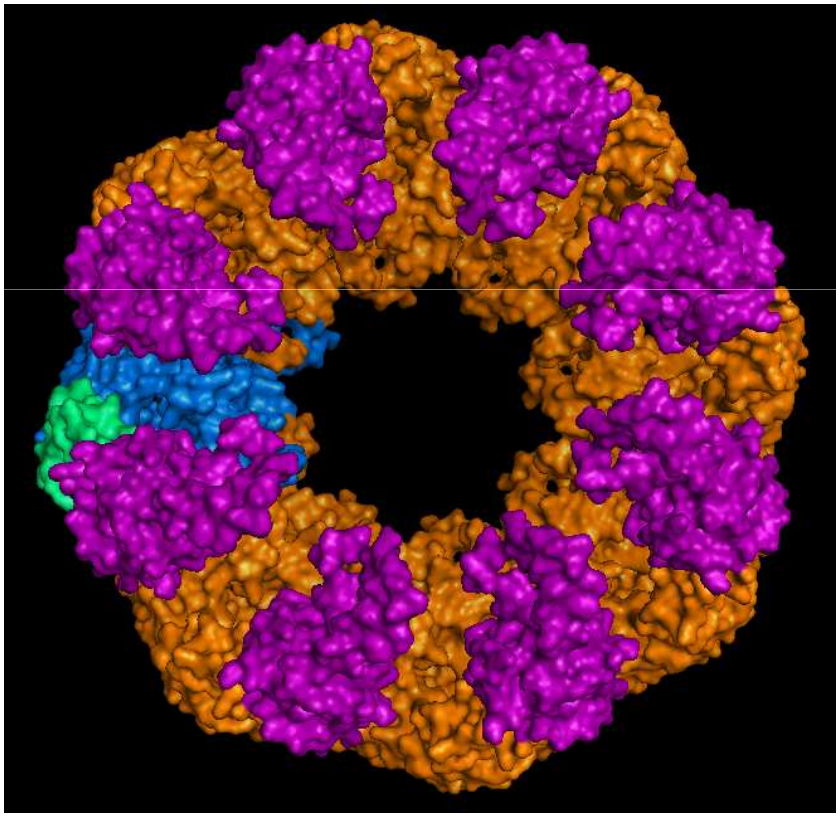


Fig114. Apical domains in Prehydrolysis conformation (3IZH)

MmCpn > Prehydrolysis state > Intermediate movement

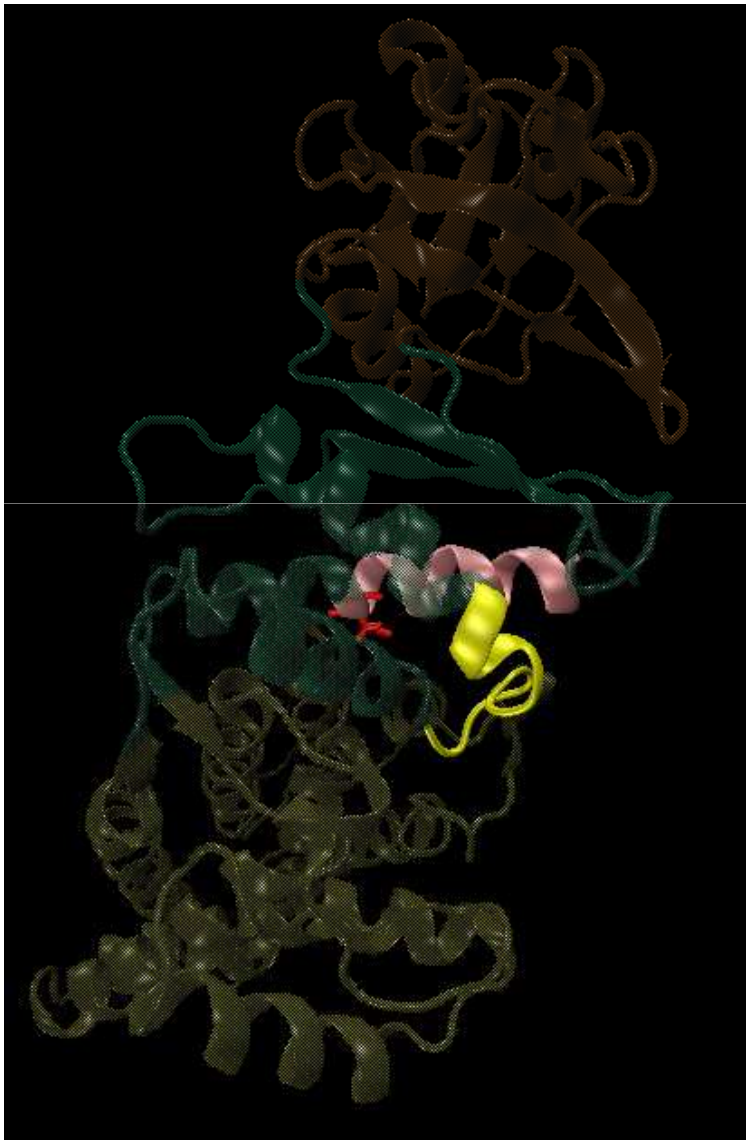


Fig115. NSL and Asp386 in open state (3IYF)

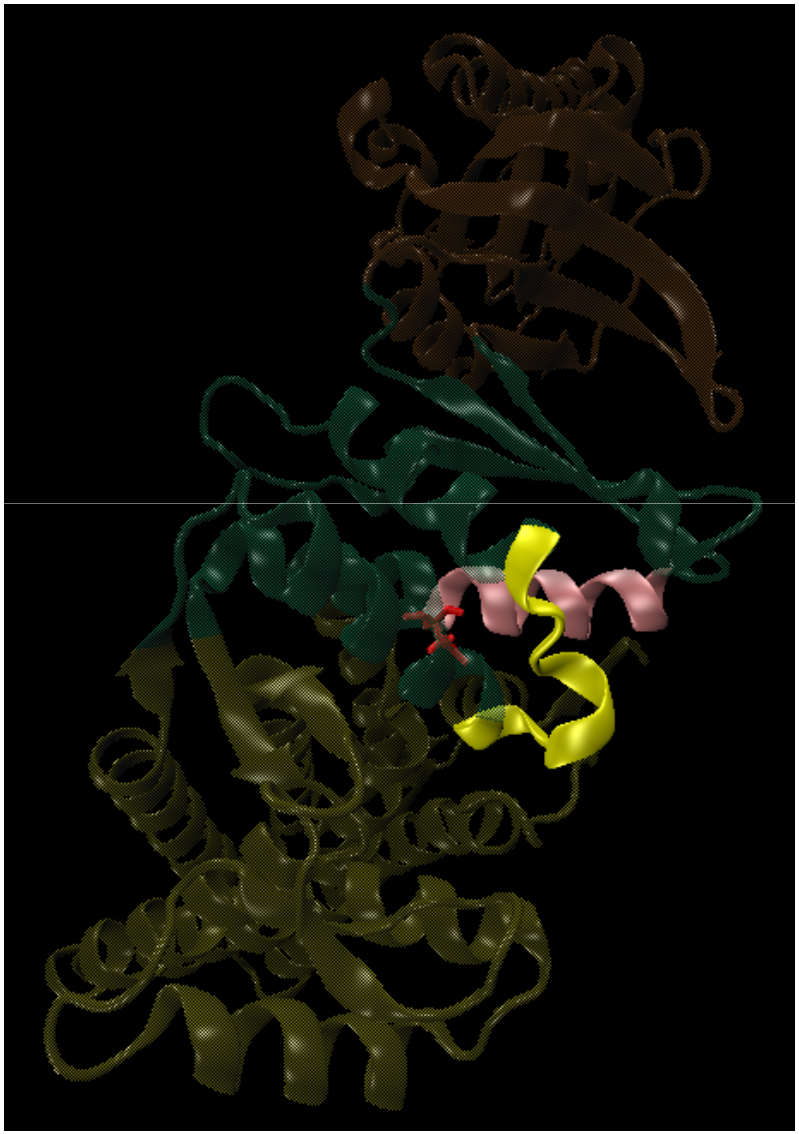


Fig116. NSL and Asp386 in Prehydrolysis state (3RUV)

MmCpn > Prehydrolysis state > Nucelotide binding site

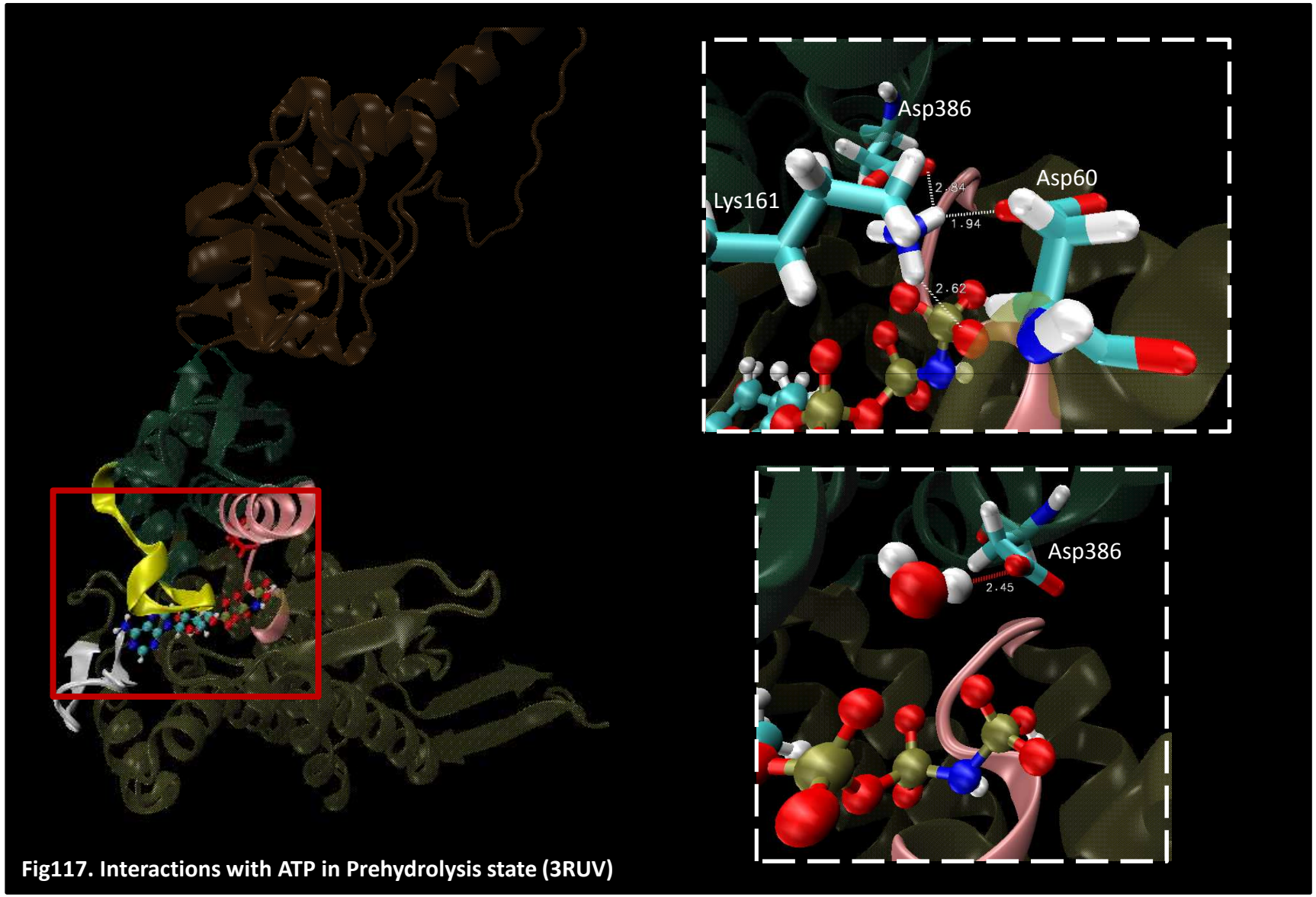


Fig117. Interactions with ATP in Prehydrolysis state (3RUV)

MmCpn > Prehydrolysis state > Nucelotide binding site

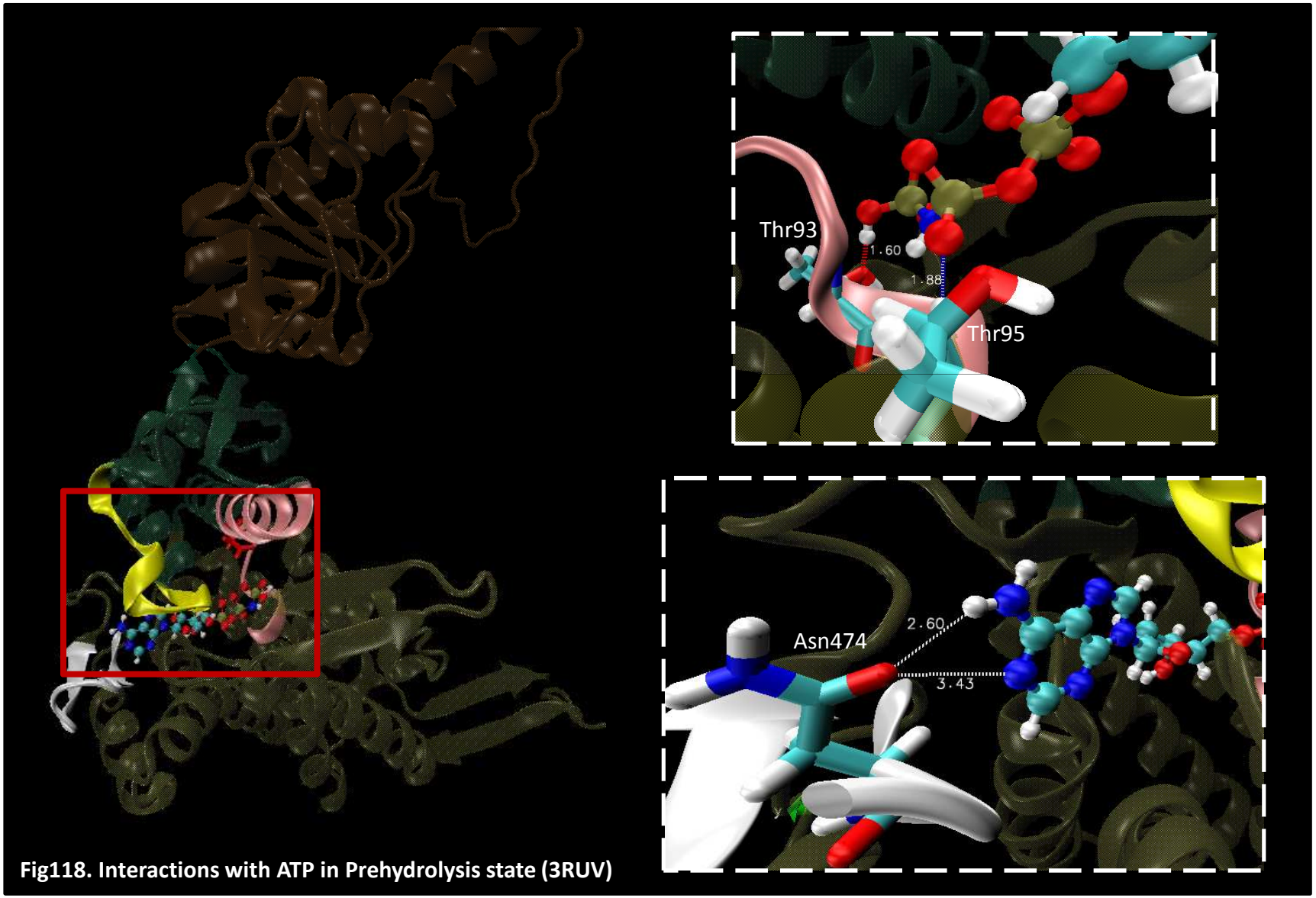


Fig118. Interactions with ATP in Prehydrolysis state (3RUV)

MmCpn > Prehydrolysis state > Nucelotide binding site

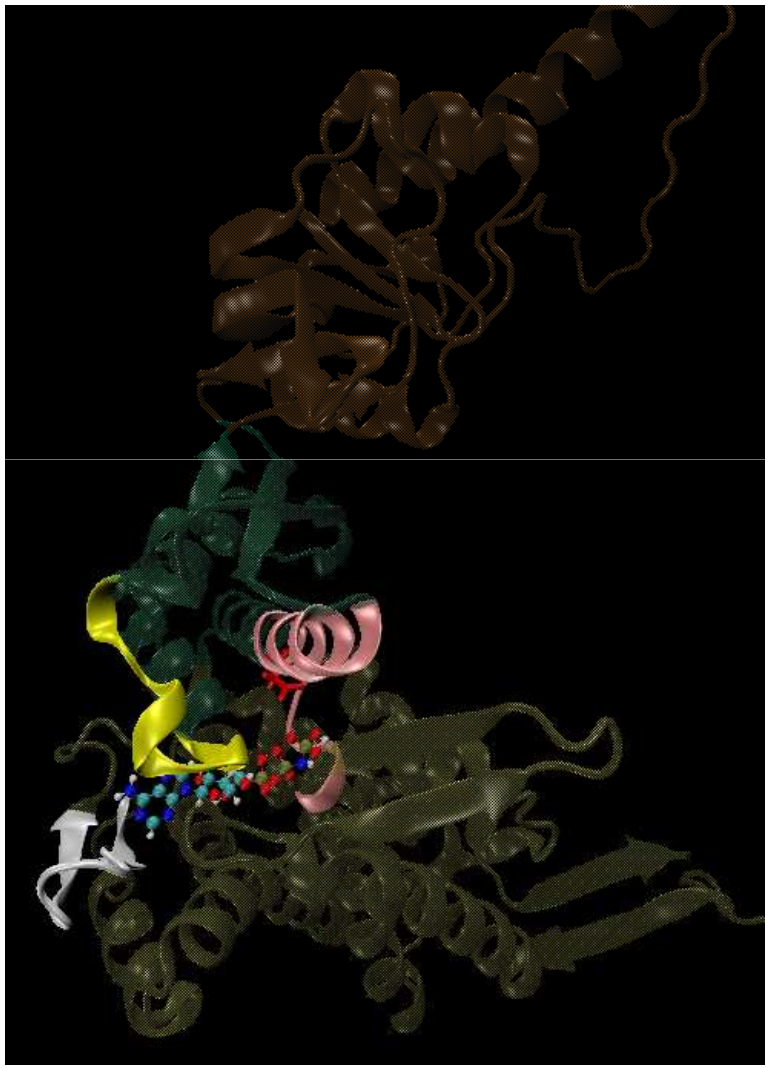


Fig119. Lateral view of the nucleotide binding pocket (3RUV)

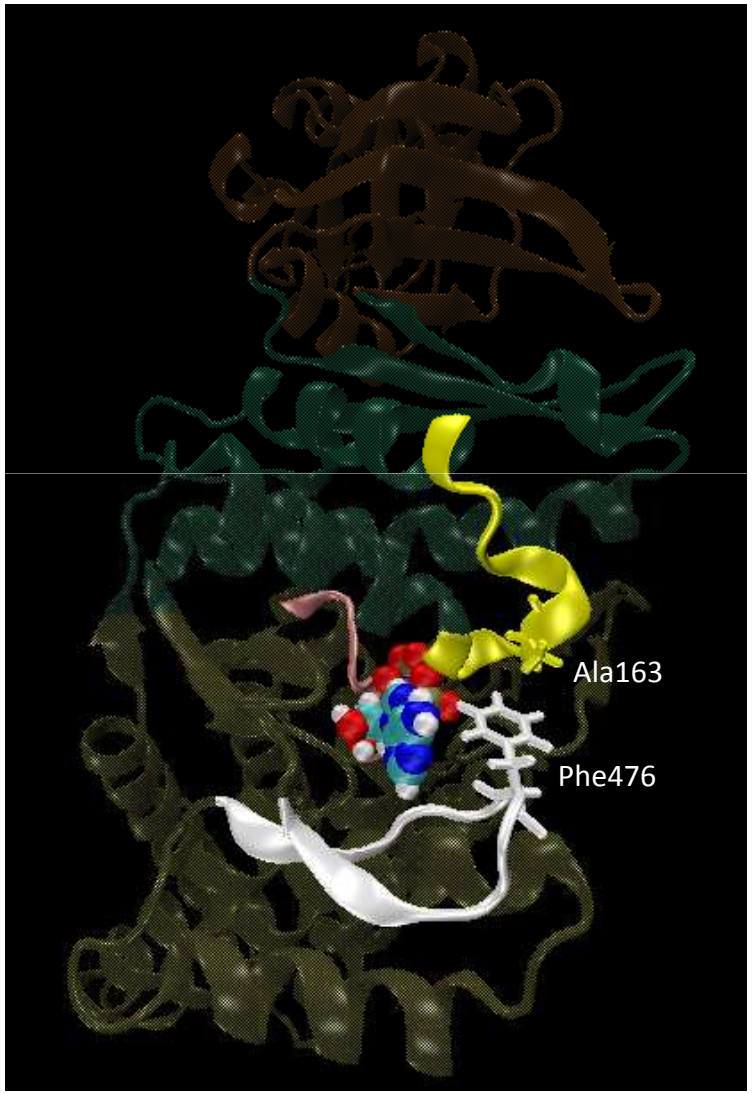


Fig120. Rear view of the nucleotide binding pocket (3RUV)

MmCpn > Closed state

ATP is hydrolyzed in the nucleotide binding site

All the three domains suffer a large rocking motion to completely close the chamber

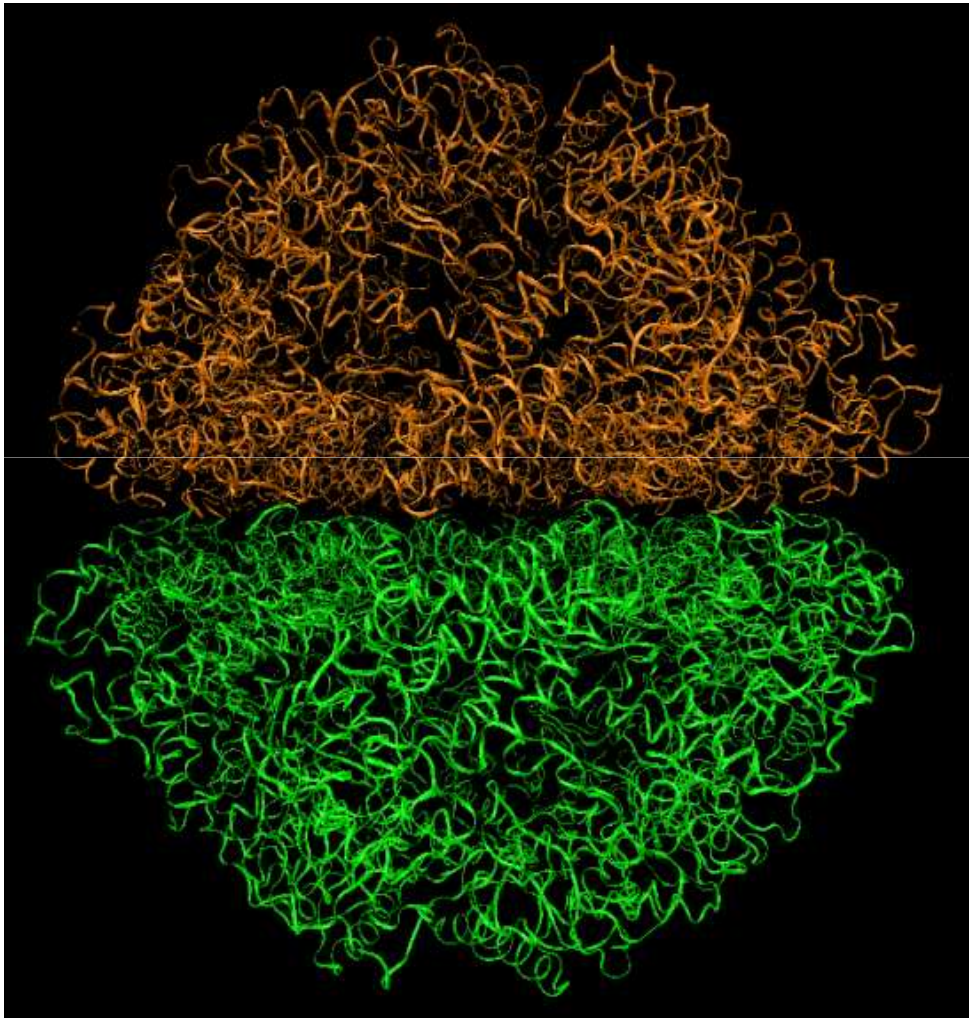


Fig121. MmCpn in Closed confomation (3LOS)

MmCpn > Closed state

Equatorial domains suffers a significant outward and lateral rotation

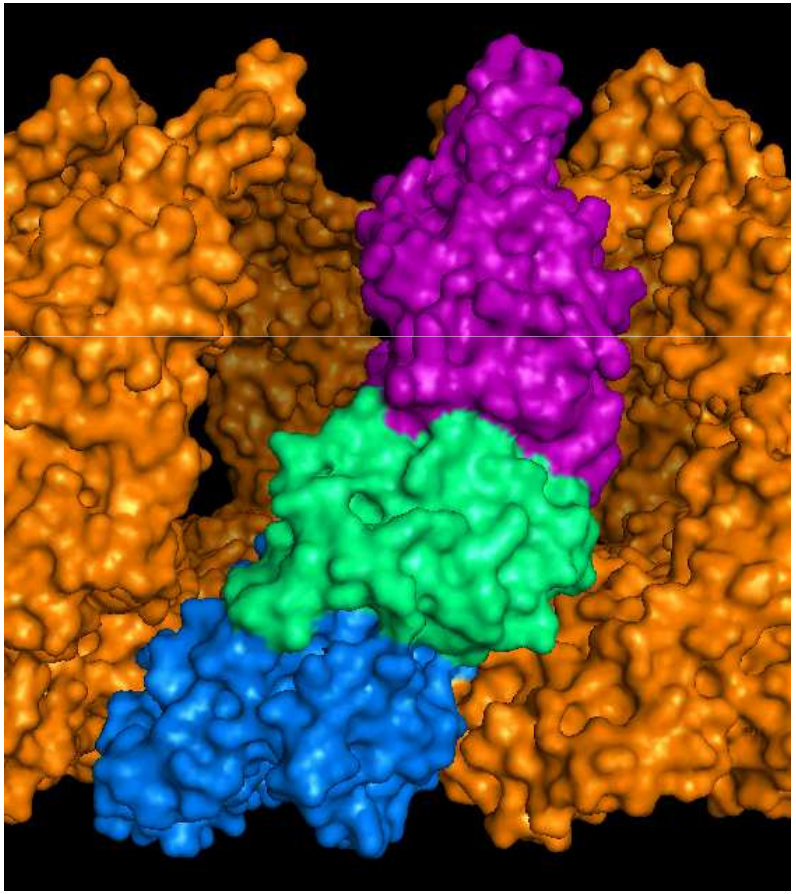


Fig122. Single subunit in Prehydrolysis conformation (3IZH)

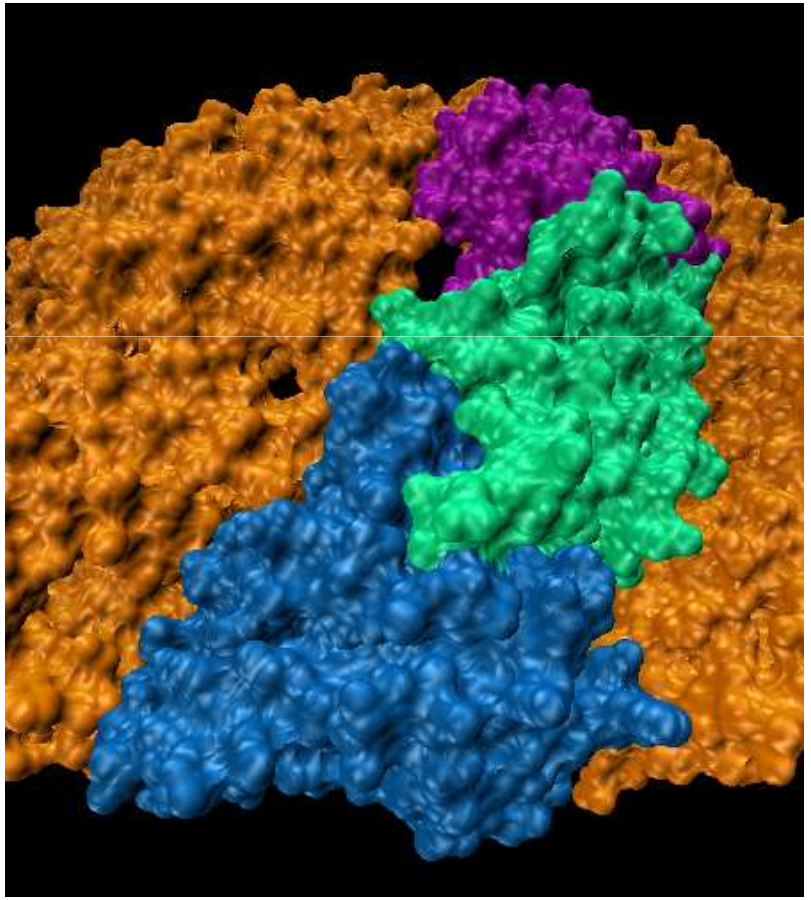


Fig123. Single subunit in Closed confomration (3LOS)

MmCpn > **Closed state >** Closing the chamber

ATP hydrolysis has a dual function:
- Chamber closure
- Substrate release

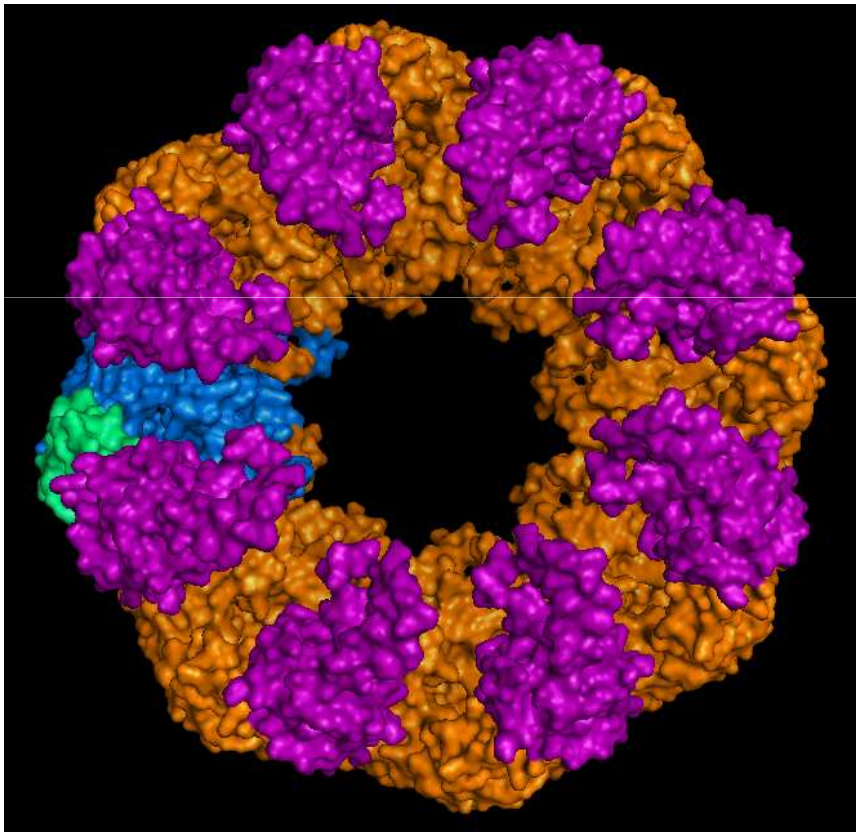


Fig124. Apical domains in Prehydrolysis conformation (3IZH)

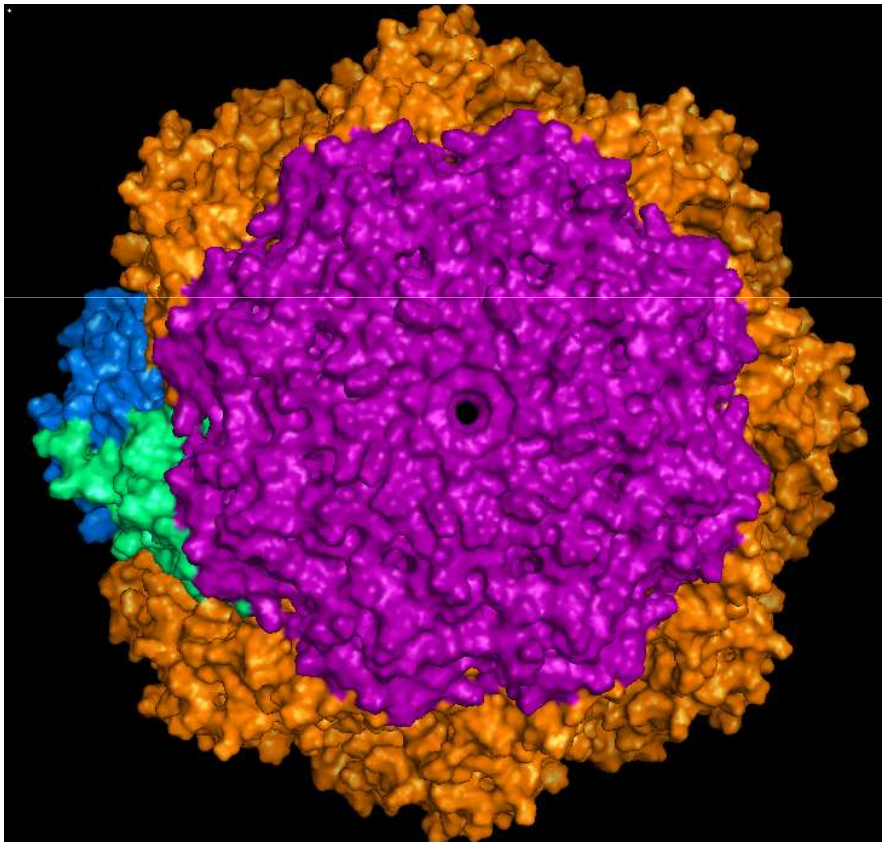


Fig125. Apical domains in Closed conformation (3LOS)

MmCpn > **Closed state >** Closing the chamber

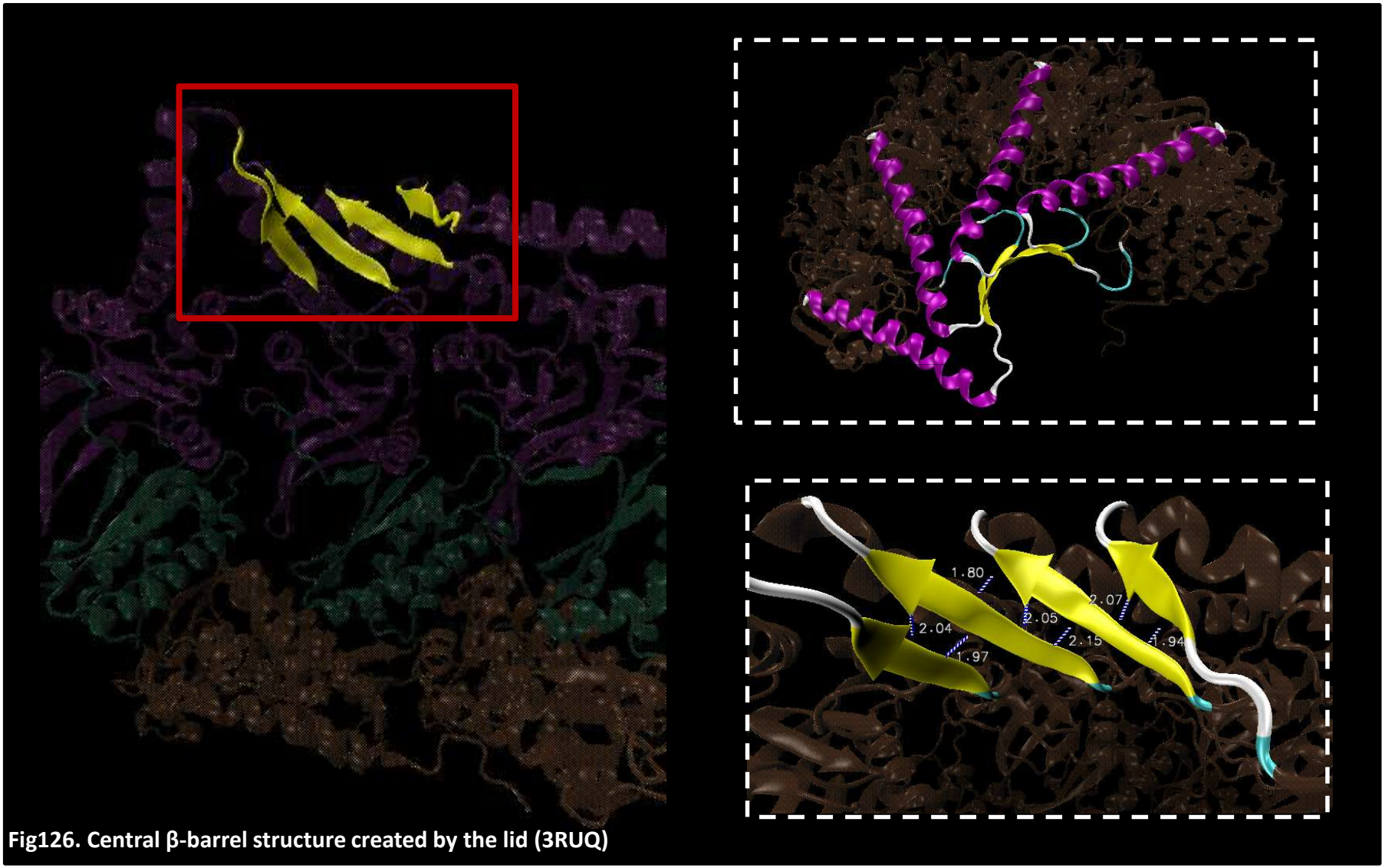


Fig126. Central β-barrel structure created by the lid (3RUQ)

MmCpn > **Closed state >** Closing the chamber

Hydrophilic residues exposed inside the closed chamber

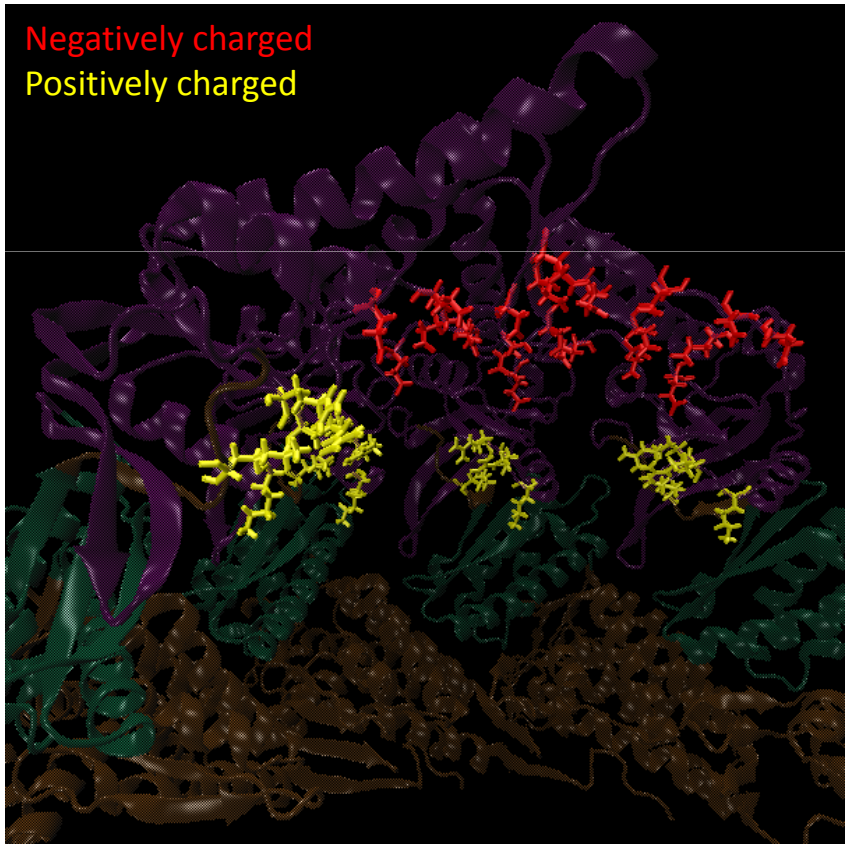


Fig127. Polar residues inside the closed chamber (3RUQ)

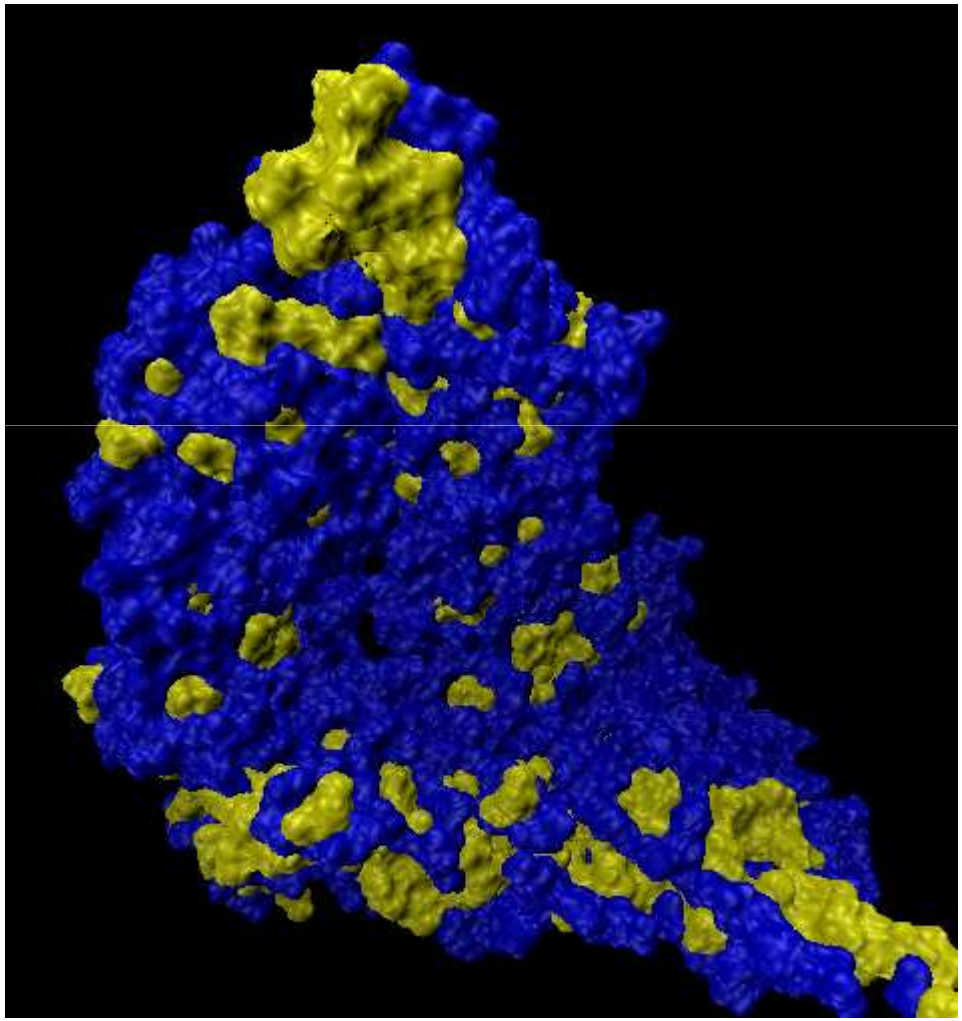


Fig128. Hydrophilic inner surface of the closed chamber (3RUQ)

MmCpn > Closed state > Intra-ring interactions

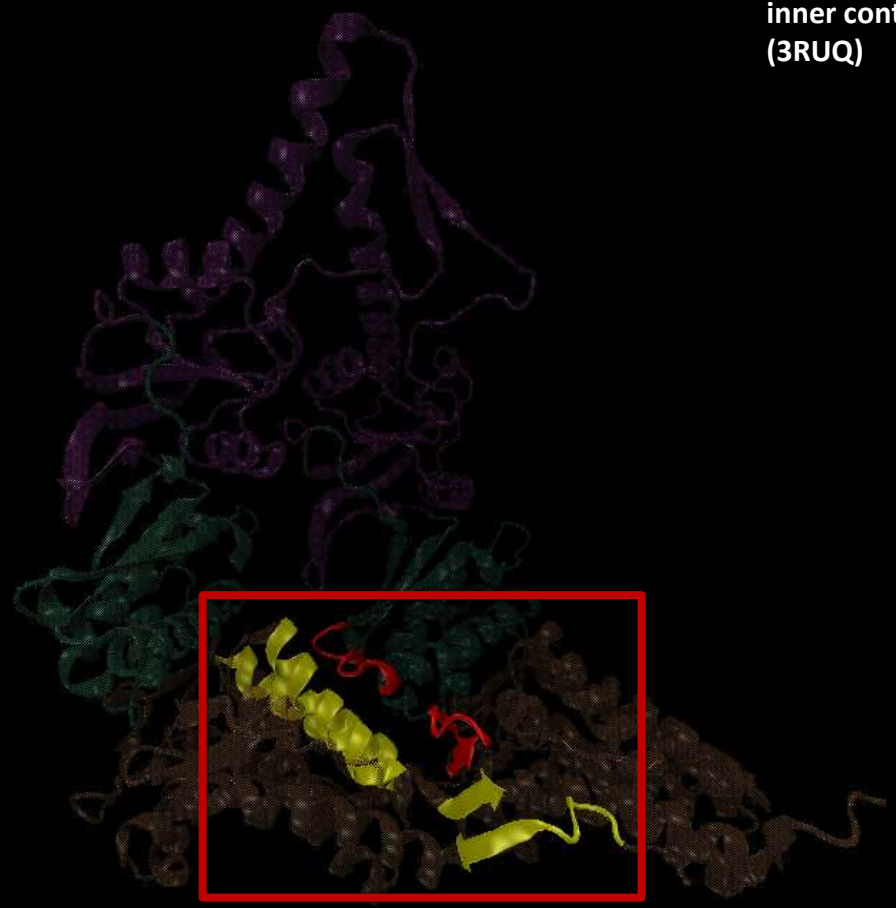
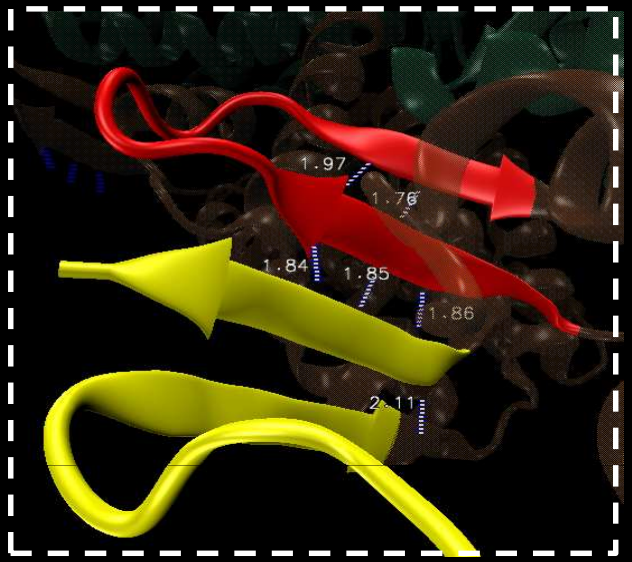


Fig129. Equatorial and intermediate inter subunit contacts (3RUQ)

Fig130. B-sheet inner contact (3RUQ)



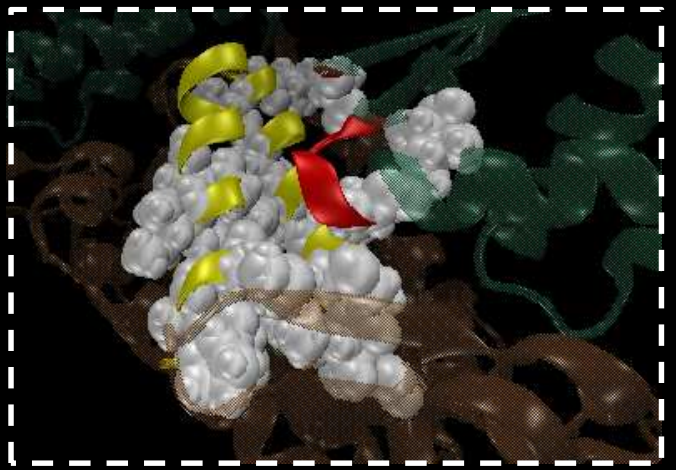


Fig131. Hydrophobic contacts between intermediate and equatorial domains (3RUQ)

MmCpn > Closed state > Inter-ring

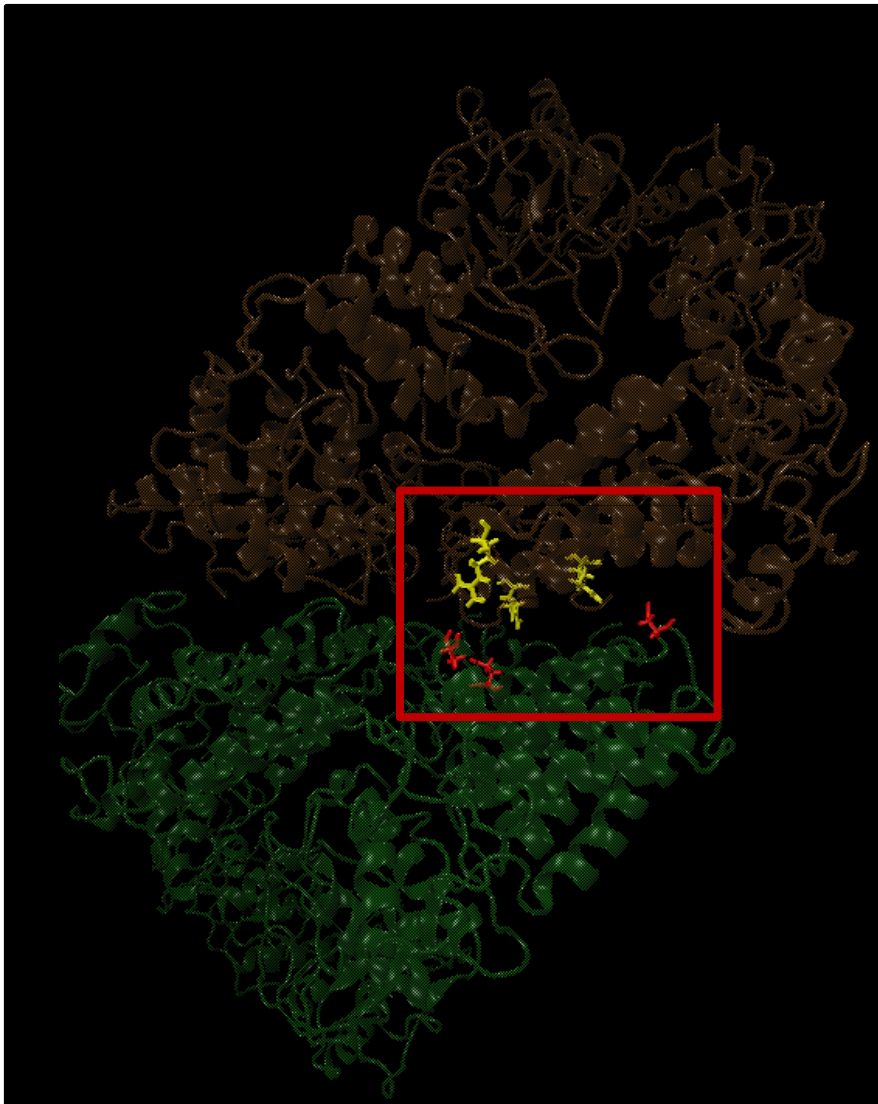


Fig132. Inter-ring contacts in Closed state (3LOS)

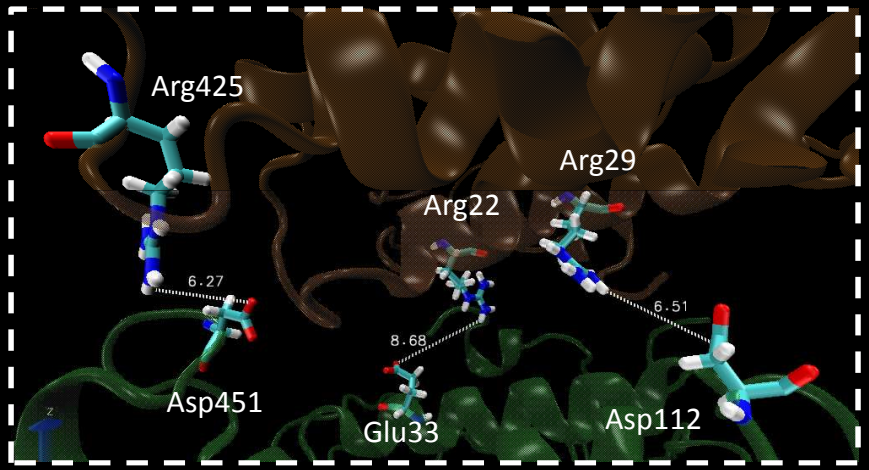


Fig133. Salt bridges between in the interface ring- ring (3LOS)

MmCpn > **Closed state >** Nucleotide binding site

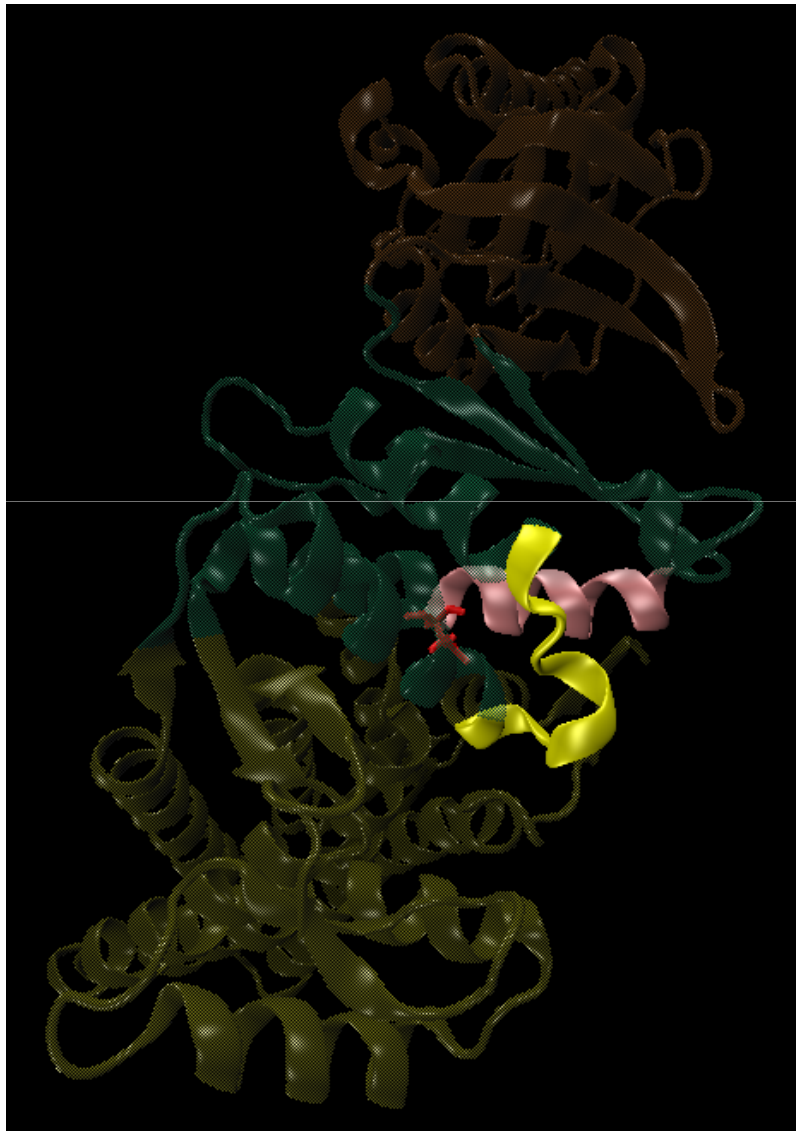


Fig134. NSL and Asp386 in Prehydrolysis state (3RUV)

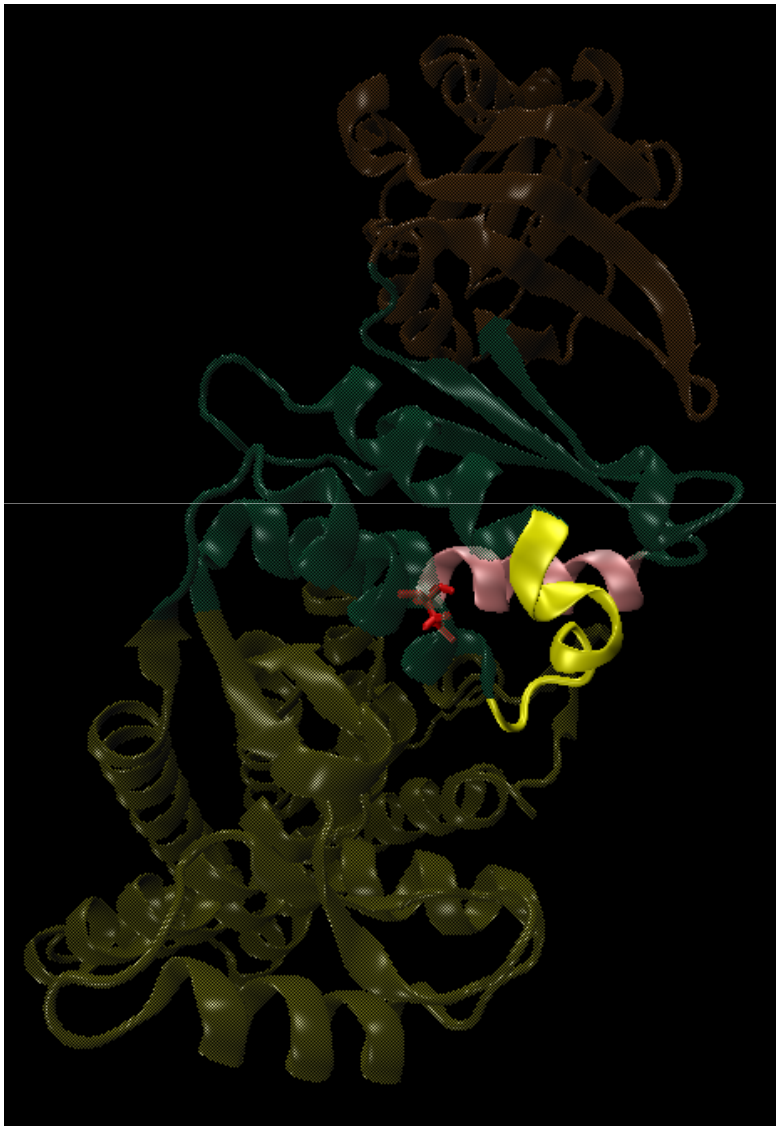
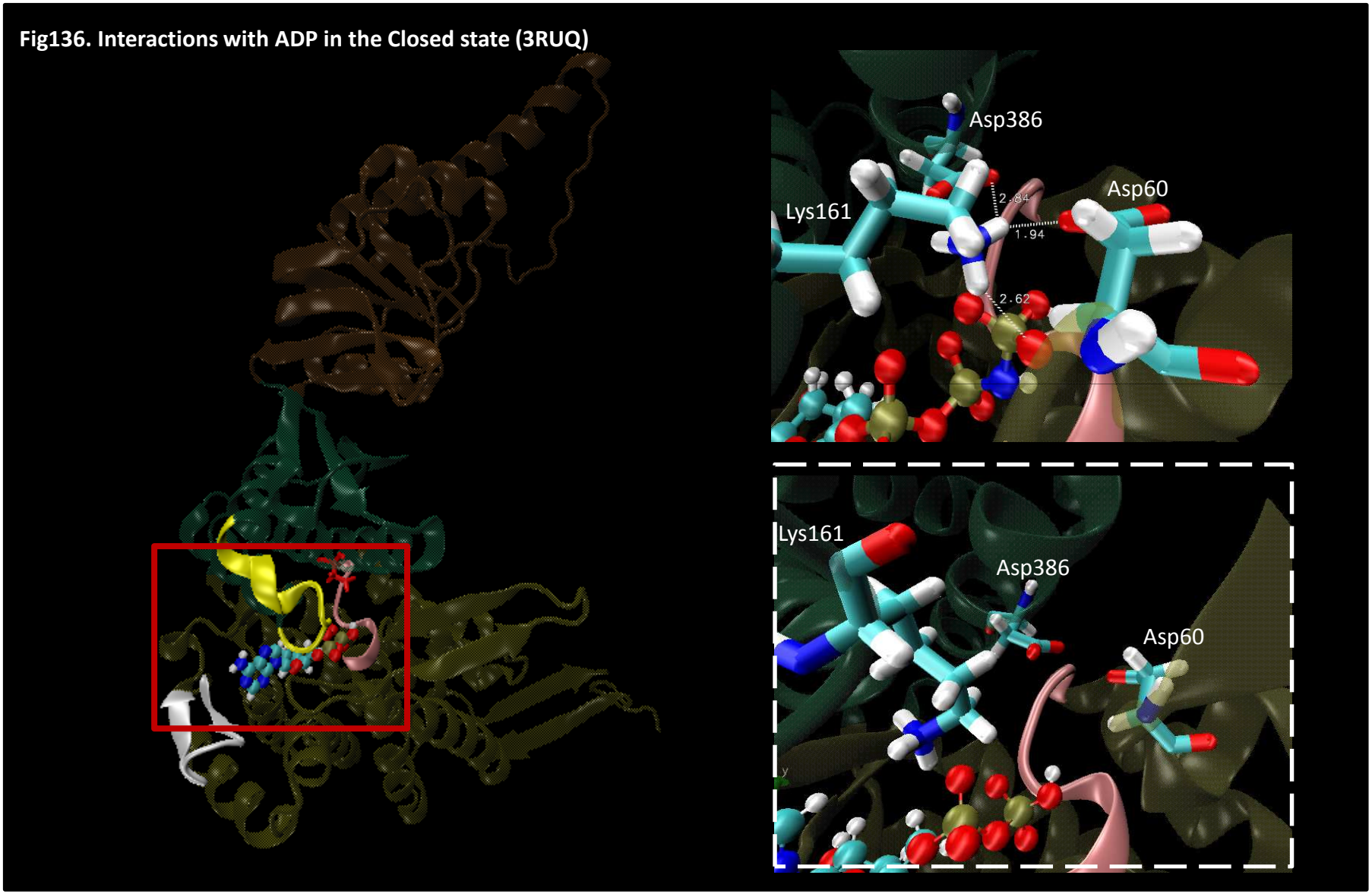


Fig135. NSL and Asp386 in Closed state (3RUQ)

MmCpn > **Closed state >** Nucleotide binding site

Fig136. Interactions with ADP in the Closed state (3RUQ)



MmCpn > **Closed state >** Nucleotide binding site

PREHYDROLYSIS STATE

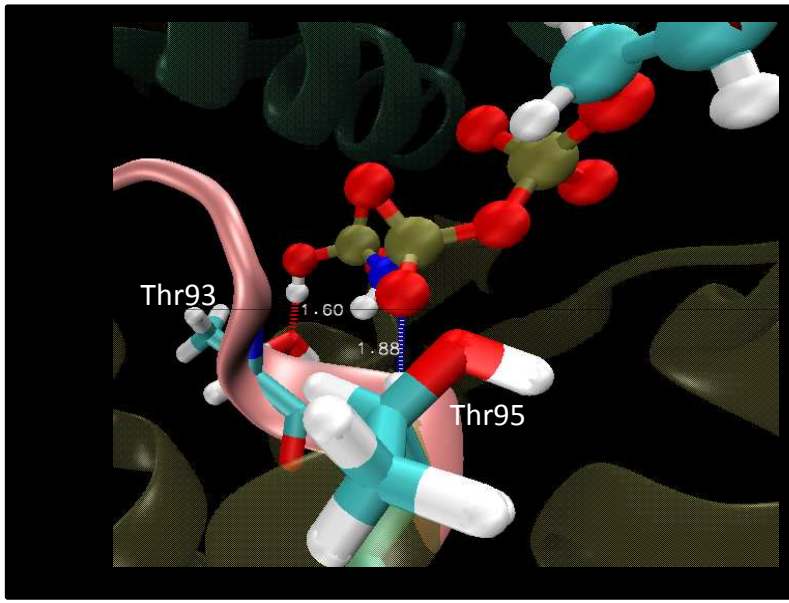


Fig137. P-loop interaction with the gamma and beta phosphate in Prehydrolysis state (3RUV)

CLOSED STATE

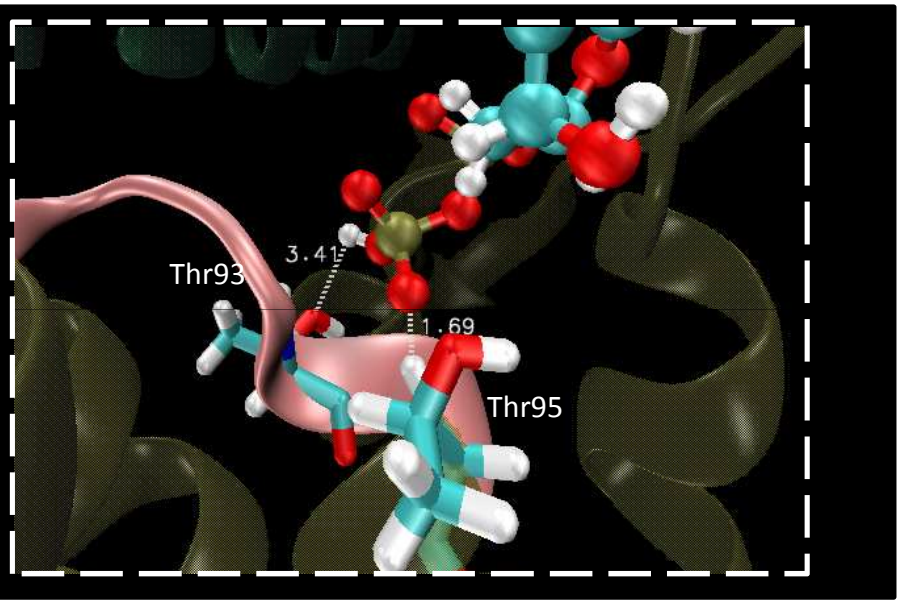


Fig138. P-loop interaction with the beta phosphate in Closed state (3RUQ)

MmCpn > Closed state > Nucleotide binding site

PREHYDROLYSIS STATE

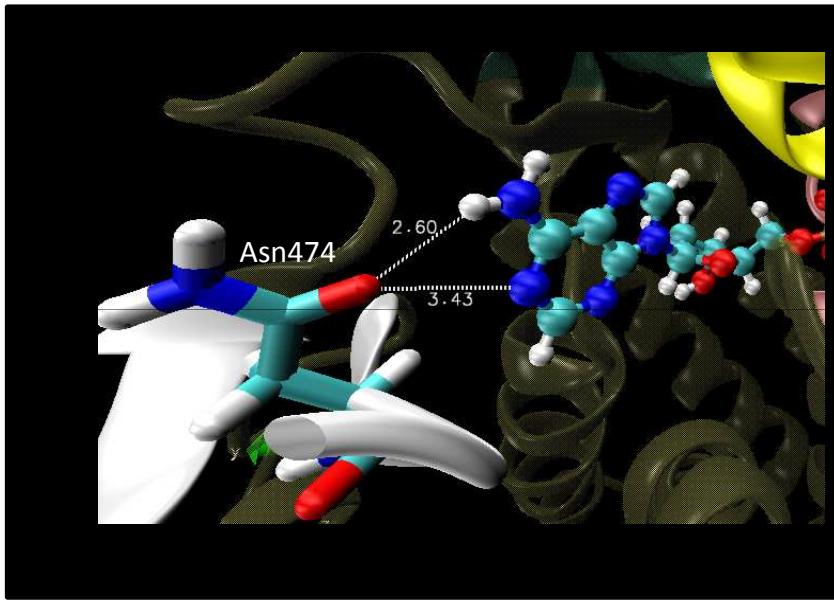


Fig139. Asn474 interaction with the adenine base of ATP (3RUV)

CLOSED STATE

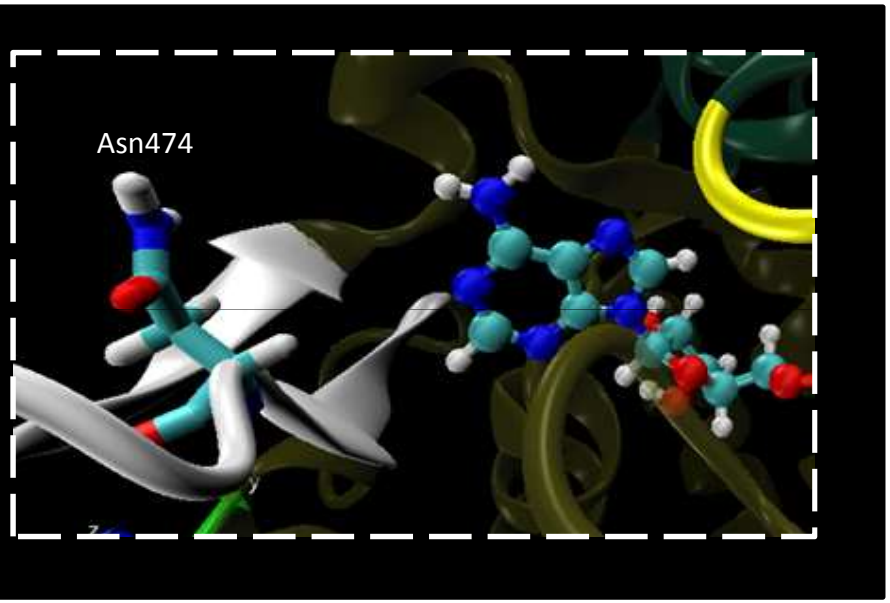


Fig140. Asn474 disposition in Closed state (3RUQ)

MmCpn > **Closed state >** Nucleotide binding site

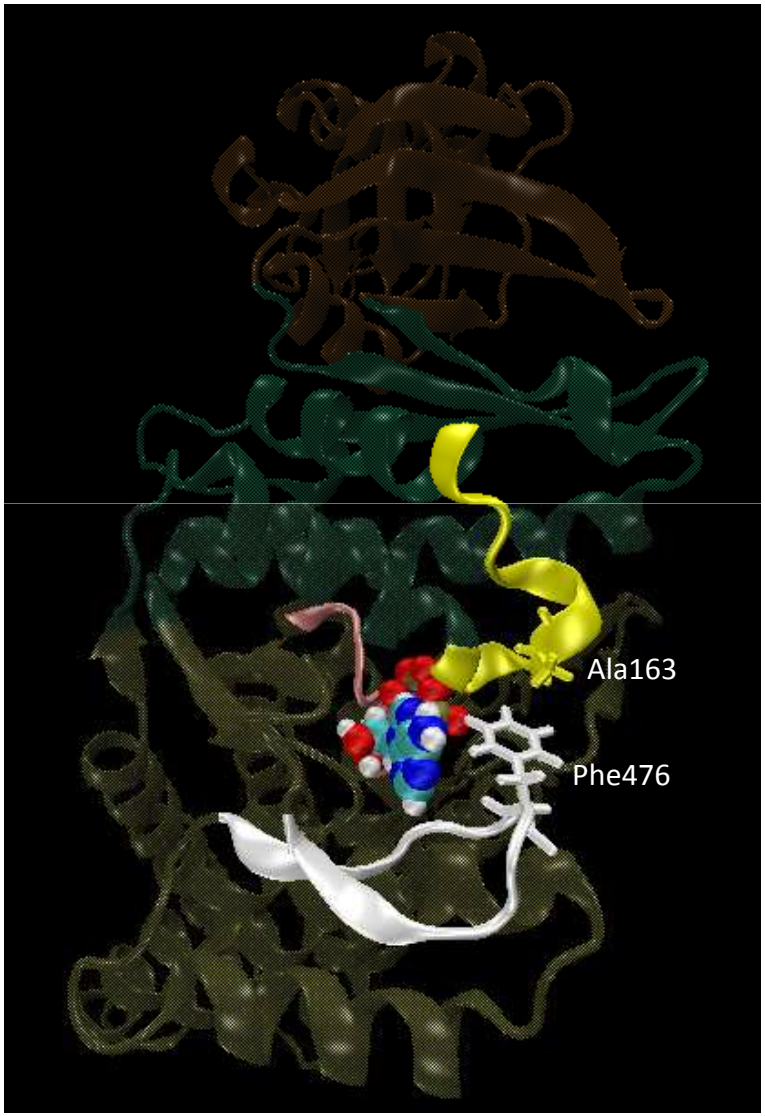


Fig141. Rear view of the nucleotide binding pocket in Prehydrolysis state (3RUV)

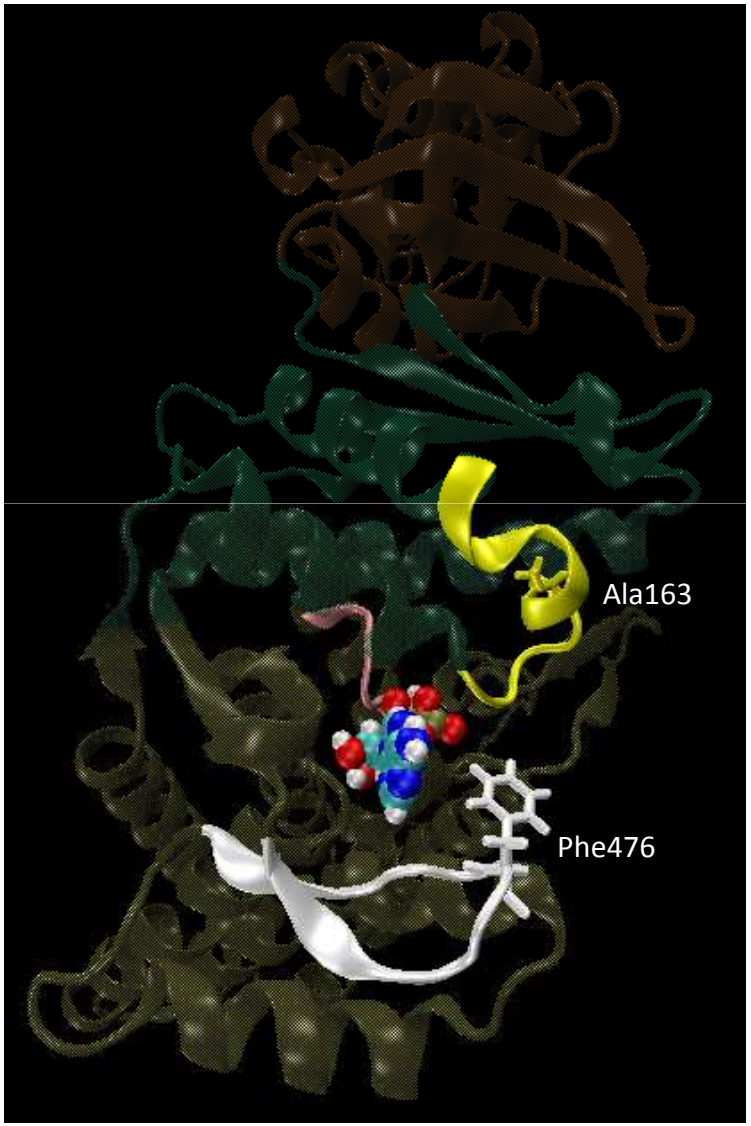


Fig142. Rear view of the nucleotide binding pocket in Closed state (3RUQ)

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USED PROGRAMMES

PDBs:

- 1AON
- 1DKD
- 1GRU
- 1MNF
- 1SS8
- 1SVT
- 1SX3
- 1SX4
- 2C7C
- 3IYF
- 3A0O
- 3KFB
- 3IZH
- 3RUV
- 3RUQ

PROGRAMMES:

- VMD
- PYMOL
- ChemScketch
- ProSA
- Jalview
- Rasmol
- STAMP