

CHAPERONES STRUCTURE

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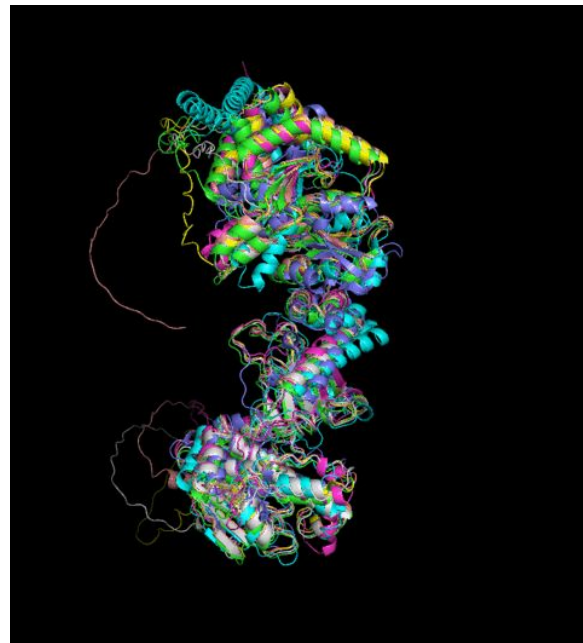
MODELS

PDB



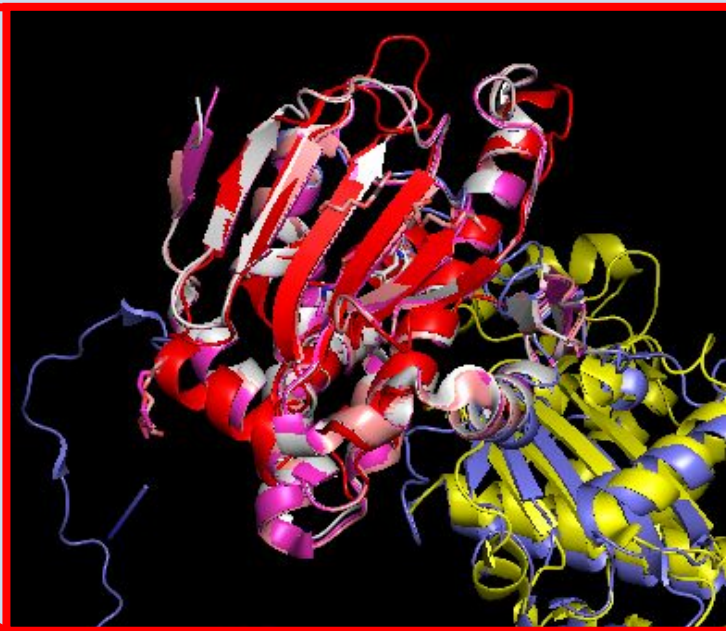
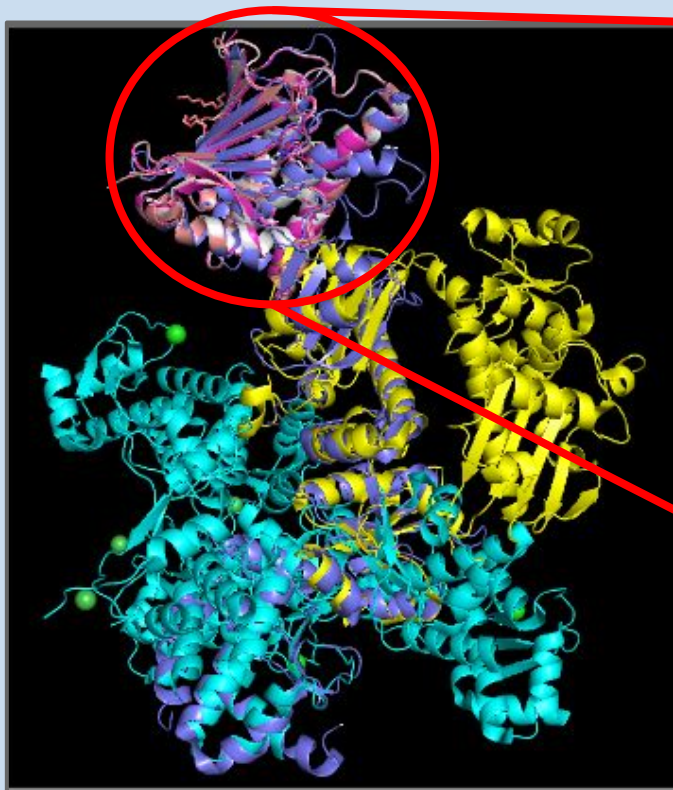
6XG6 1SF8 1QY5 1Y6Z 1YT2
1QY8

ALPHA FOLD



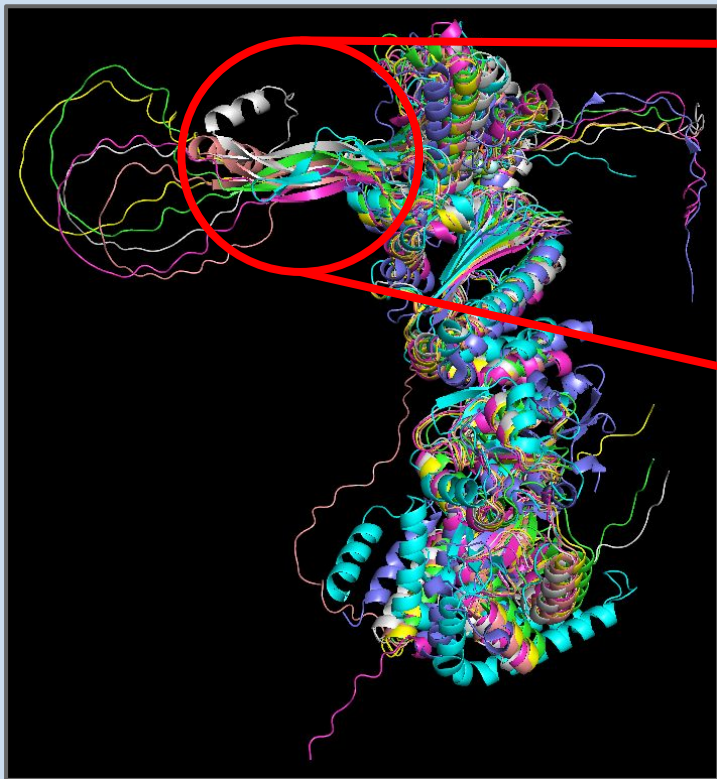
6XG6 P24724 P04809 P06660
Q8SSE8 P36181 POC938

PDB SUPERIMPOSITION



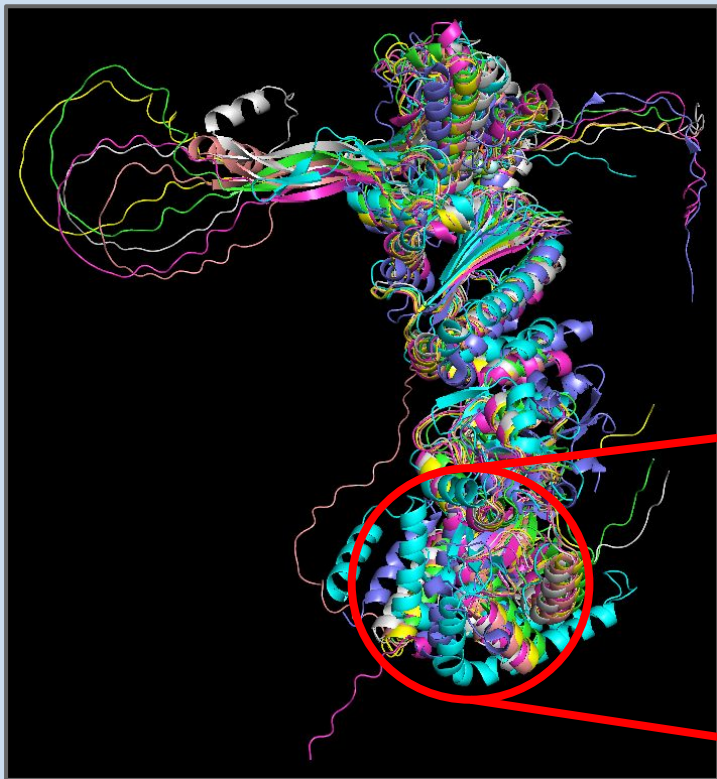
The **N-terminal domain**, what is mainly superposed in all the sequences, yet there is a lot of variability in the superposing of the different selected proteins

ALPHA FOLD SUPERIMPOSITION

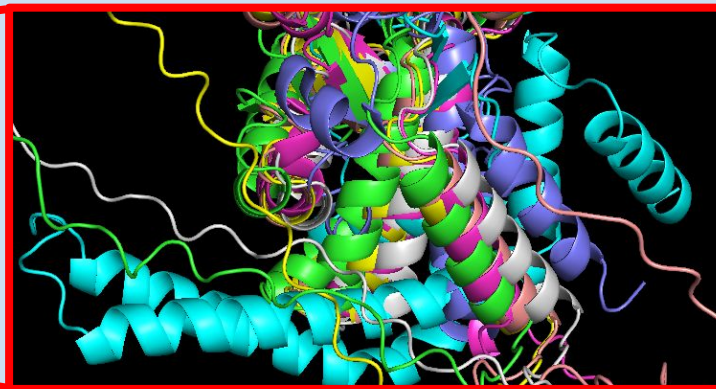


In the N-terminal domain, we can see **variability** between the types of **beta sheets** they have before the loops.

ALPHA FOLD SUPERIMPOSITION



In the **C-terminal** domain, the turquoise blue (p0c938) looks like it's **bigger** than the rest of proteins since it has **more alpha helices**.



ALPHA FOLD CONSERVED REGIONS



```

sp|002705|HS90A_PIG      DISMIGQFGVG FYSAYLVAEKVTITKHND---DEQYAWESSAGGSFTVR
sp|P82995|HS90A_RAT      DISMIGQFGVG FYSAYLVAEKVTITKHND---DEQYAWESSAGGSFTVR
sp|P11501|HS90A_CHICK     DISMIGQFGVG FYSAYLVAEKVTITKHND---DEQYAWESSAGGSFTVR
sp|Q76LV1|HS90B_BOVIN     DISMIGQFGVG FYSAYLVAEKVVITKHND---DEQYAWESSAGGSFTVR
sp|Q69QQ6|HSP82_ORYSJ     DVSMIGQFGVG FYSAYLVAERVVTTKHND---DEQYVWESQAGGSFTVT
sp|P14625|ENPL_HUMAN      TSELIGQFGVG FYS AFLVADKIVITSKHNN---DTQHIWESDSN-EFSVI
sp|A4SLY0|HTPG_AERS4      DSQ LIGQFGVG FYS AFIVADKVTTVSRAAGTAPEQGVQWESEGEGSFTVA
sp|P0A6Z3|HTPG_ECOLI      DSQ LIGQFGVG FYS AFIVADKVTVRTRAAGEKPENG VFWESAGEGEYTVA
6XG6_1|Chains             -SKIIGQFGVG FYS AFMVADRVEVYSRSAAPG-SLGYQWLSDGS GVF EIA
sp|Q12931|TRAP1_HUMAN     -SKIIGQFGVG FYS AFMVADRVEVYSRSAAPG-SLGYQWLSDGS GVF EIA
sp|Q24VT7|HTPG_DESHY      DVN LIGQFGVG FYS AFMVADKVS LTRSRSYEPD-AQGYRWESDGRG SYSIS
.:***** ***::***:* : : : * * . : :
    
```

```

116 121
-SMIGQFGVG
1 116
-AIGHFGLG
136 141
-SNLIGQFGLG
116 12
I-SMIGQFGVG
16 121
-SMIGQFGVG
21 126
I-SMIGQFGVG
196 201
-SKIIGQFGVG
    
```

N-terminal domain

Structurally not variable

Flexible since it is a loop

Conserved → related to the **ATP binding site**
(important to for the function of the protein)

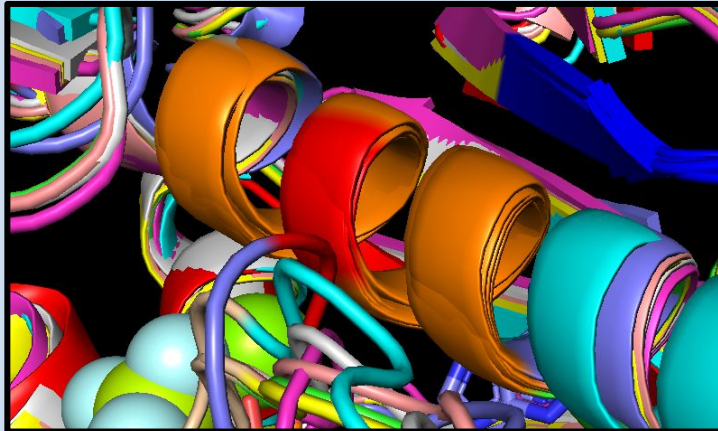
ALPHA FOLD CONSERVED REGIONS

```

sp|002705|HS90A_PIG      IINTFYSNKEIFLRELISNSSDALDKIRYESLTDPS-KLDSGKELHINLI
sp|P82995|HS90A_RAT      IINTFYSNKEIFLRELISNSSDALDKIRYESLTDPS-KLDSGKELHINLI
sp|P11501|HS90A_CHICK    IINTFYSNKEIFLRELISNSSDALDKIRYESLTDPS-KLDSGKDLKINLI
sp|Q76LV1|HS90B_BOVIN    IINTFYSNKEIFLRELISNASDALDKIRYESLTDPS-KLDSGKELKIDII
sp|Q69QQ6|HSP82_ORYSJ    IINTFYSNKEIFLRELISNSSDALDKIRFESLTDKS-KLDAQPELFIHIV
sp|P14625|ENPL_HUMAN     IINSLYKNKEIFLRELISNASDALDKIRLISLTDEN-ALSGNEELTVKIK
sp|A4SLY0|HTPG_AERS4     MAHSLYSNKEVFLRELISNASDAADKLRFKALSDAS-LFENDGQLRVRLV
sp|P0A6Z3|HTPG_ECOLI     MIHSLYSNKEIFLRELISNASDAADKLRFRALSNPD-LYEGDGELRVRS
6XG6_1|Chains            VARSLYSEKEVFIRELISNASDALEKLRHKLVS----DGQALPEMEIHLQ
sp|Q12931|TRAP1_HUMAN    VARSLYSEKEVFIRELISNASDALEKLRHKLVS----DGQALPEMEIHLQ
sp|Q24VT7|HTPG_DESHY     VINSLYTDREIFLRELISNAADASEKVRYMQLSGQNVKDQELP-LEIRIT
: .:*.:*:*:*****:*: *:* : : . : :
    
```

```

31      36      41
FLR-E-L-IS-N-S-SD-A-L-DK
      31      36
-I-F-L-RE-I-V-SN-A-V-DA-
46      51      56
LR-E-L-VS-N-S-SD-A-C-DK-
      31      36
-E-I-F-LR-E-L-IS-N-S-SD-
31      36      41
-I-F-L-RE-L-I-SN-A-S-DA-
36      41      46
-I-F-L-RE-L-I-SN-A-S-DA-
111     116     121
-V-F-I-RE-L-I-SN-A-S-DA-
    
```



Structurally not variable

Not flexible since it is an helix

Conserved in general

There is a **serine** [S] that is an **ADP binding site**

ALPHA FOLD CONSERVED REGIONS

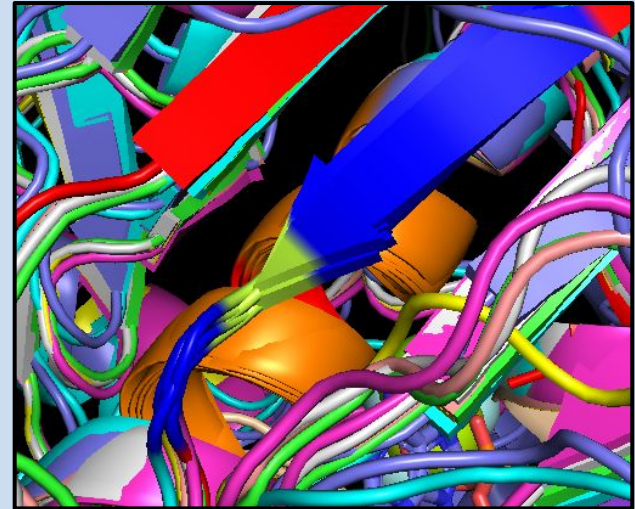
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sp|P82995|HS90A_RAT      PNKQDRTLTIIVDTGIGMTKADLINNLGTIAKSGTKAFMEALQAGAD----
sp|P11501|HS90A_CHICK    PNKHDRTLTIIVDTGIGMTKADLVNNLGTIAKSGTKAFMEALQAGAD----
sp|Q58FF7|H90B3_HUMAN    PNPQERTLALVDTGIGMTKADLINNLRTIAKSGTKACMEALQA-----
sp|Q76LV1|HS90B_BOVIN    PNPQERTLTLVDTGIGMTKADLVNNLGTIAKSGTKAFMEALQAGAD----
sp|Q69QQ6|HSP82_ORYSJ    PDKASNTLSIIDSGVGMTKSDLVNNLGTIARSGTKEFMEALAAGAD----
sp|P14625|ENPL_HUMAN     CDKEKNLLHVTDTGVGMTREELVKNLGTIAKSGTSEFLNKMTEAQEDGQS
sp|A4SLY0|HTPG_AERS4     VDKENRTLISDNGIGMTRDQVIEHLGTIAKSGTAEFFKSLNKGSDQG---R
sp|P0A6Z3|HTPG_ECOLI     FDKDKRTLTIISDNGVGMTRDEVIDHLGTIAKSGTKSFESLGSQA---K
6XG6_1|Chains            TNAEKGTITIQDTGIGMTQEELVSNLGTIARSGSKAFDLALQNQAEAS--
sp|Q12931|TRAP1_HUMAN    TNAEKGTITIQDTGIGMTQEELVSNLGTIARSGSKAFDLALQNQAEAS--
sp|Q24VT7|HTPG_DESHY     PDENAKTLTIADAGIGMTKEDLIENIGTIAHSGSKAFVQRLAEAGDKKD-
:      : : * :***: :::: : ***:**:  .. :
```

76 81
FLTIIDSGI
L 76
FITVSDRGV
L 96
FLTIKONGI
76 8
FLTVEDTGI
76 81
FLTIIDTGI
31 86
FLTIEDSGI
L 156 1
FITIQDTGI

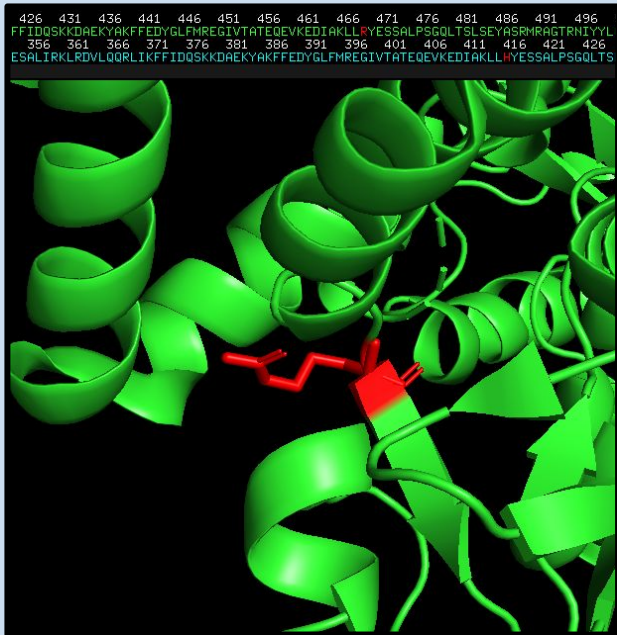
Structurally not variable

Not flexible since it is a beta sheet

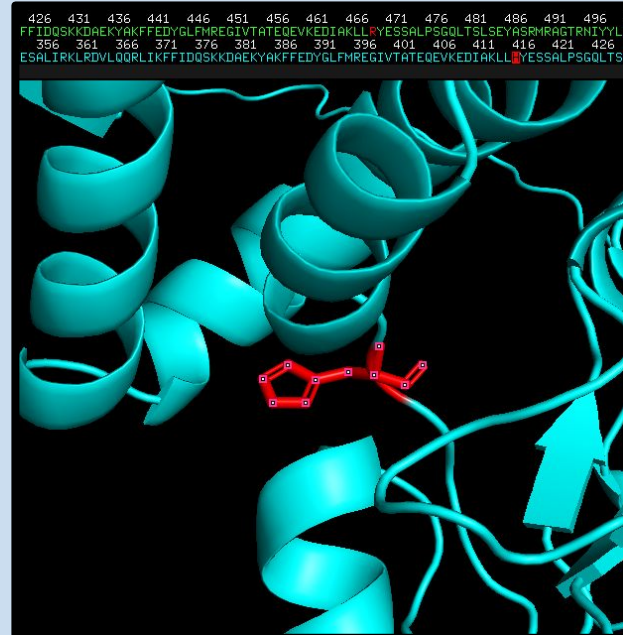
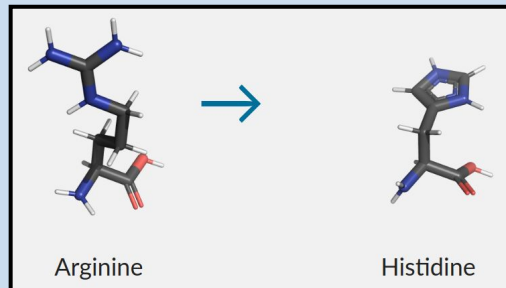
There is an **aspartic acid** [D] that is an **ATP binding site**



PyMOL MUTATION



NOT MUTATED

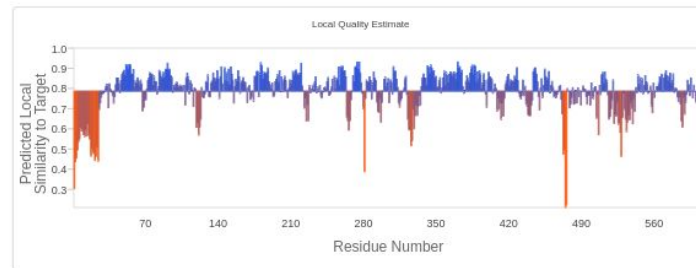


MUTATED

WILD TYPE MODEL

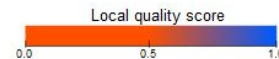
Quality for 6xg6A.pdb

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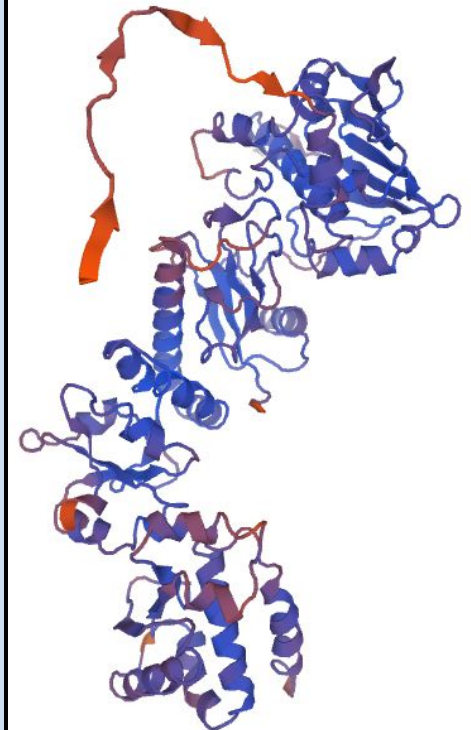


QMEANDisCo Global: **0.79** ± 0.05

Sequence colored by local quality:



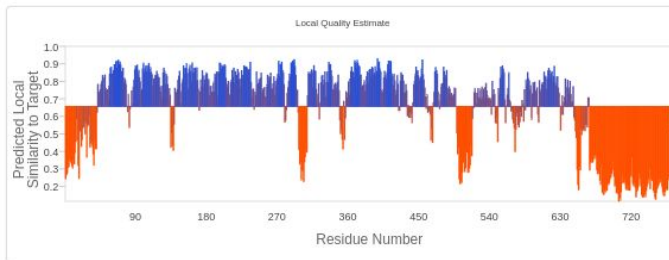
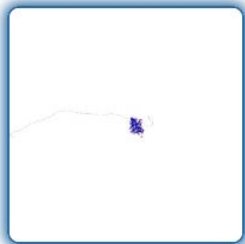
A: **PLHSIISSTESVQGSKHEFQAE**TKKLLDIVARSLYSEKEVFIRELISNASDALEKLRHKLVSDDG**ALPEMEIHLQTNAEKGITITIQDTGIGMT** 95
A: **QEELVSNLGTIARSGSKAFLDALQ**NQAEASSKIIGQFGVGFFYSAFMVADRVEVYSRSAAPGSLGYQWLSDDSGGVFEIAEASGVRTGTGKIIHLKS 190
A: **DCKEFSSEARVRDVVTKYSNFVSFPLYLNGRRMNTLQ**AIWMMDPKDVGGEWQHEEFYRYVAQAHDKPRYTLHYK**TDAPLNIRSIFFVYVDMKPSVAL** 285
A: **YSRKVLITKATDILPKWLR**FIRGVVDSEDIPLNLS**RELLQESALIRKLRDVLQQR**LKFFIDQSKKDAEKYAKFFEDYGLFMREGIVTATEQEV 380
A: **KEDIAKLLRYESSALPSGQLTSLSEYASRMRA**GRTRNIYYLCAPNRHLAEHSPYYEAMKKKDTEVLCFEQ**DFDELTLLHLREFDKKKLISVETDIE** 475
A: **CLSEKETEE**LMAMMRNVLGSRVTNVKVT**LRLD**THPAMVTVLEMGAARHFLRM**QQLAKTQEERAQL**LPTLEINPRHALIKKLNQLRASE**PGLAQL** 570
A: **LVDQIYENAMIAAGLVDDPRAMVGR**LNELLVKAL**ERH** 607



MUTATED MODEL I

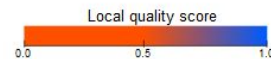
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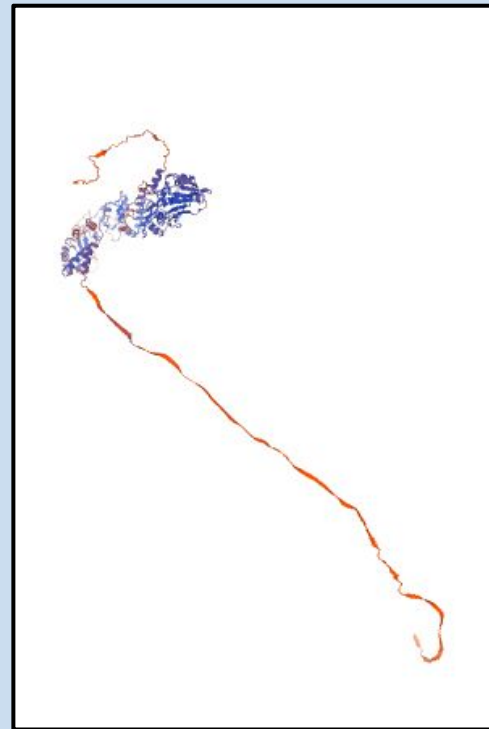


QMEANDisCo Global: **0.66** ± 0.05 ⓘ

ⓘ Sequence colored by local quality:



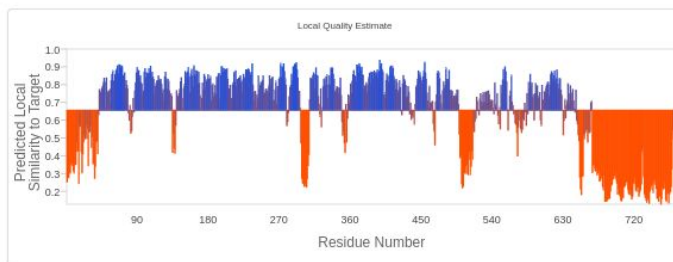
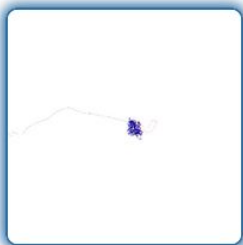
A: GIDPFTSTQTAEDKEEPLHSIISSTESVQGSTSKHEFQAETKKLLDIVARSLYSEKEVFIRELISNASDALEKLRHKLVSDDGQALPEMEIHLQTN 95
 A: AEKGITITIQDTGIGMTQEELVSNLGTIARSGSKAFDALQNAEASSKIIGQFGVGFFSAFHVADRVEVYSRSAAPGSLGYQLSDGSGVFEIAE 190
 A: ASGVRTGKIIHLKSDCKEFSSSEARVQDVVTKYSNFVSFPLYLNGRRMNTLQAIWMMDPKDVGGEWQHEEFYRYVAQAHDKPRYTLHYKTDAPLN 285
 A: IRSIFYVPDMKSPMFDVSRLEGSSVALYSRKVLITKATDILPKWLRFRIGVVDSEDIPLNLSRELLQESALIRKLRDVLQQRLIKFFIDQSKKD 380
 A: AEKYAKFFEDYGLFMREGIVTATEQEVKEDIAKLLHYESSALPSGLTSLSEYASRMRAGTRNIYYLCAPNRHLAEHSPYYEAMKKKDEVLFCF 475
 A: EQFDELTLHLREFDKKKLISVETDIIVVDHYKEEFEDRSPAEECLSEKETEELMAWMRNVLGSRVTNVKVTLRLDTHPAMVTVLEMGAAHFLR 570
 A: MQQLAKTQEERAQLQPTLEINPRHALIKKLNQLRASEPGLAQLLVDDQIYENAMIAAGLVDDPRAMVGRNLNELLVKALERHGGSGSGSSAMVDTL 665
 A: SGLSSEQGSGDMTIEEDSATHIKFSKRDEDGKELAGATMELRDSSGKTIISTWISDGQVKDFYLYPGKYTFVETAAPDGYEVATAITFTVNEQGG 760
 A: VTVNGKATKGAHI 774



MUTATED MODEL 2

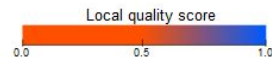
Quality for 6xg6_mutated.B99990002.pdb

Downloads ▾

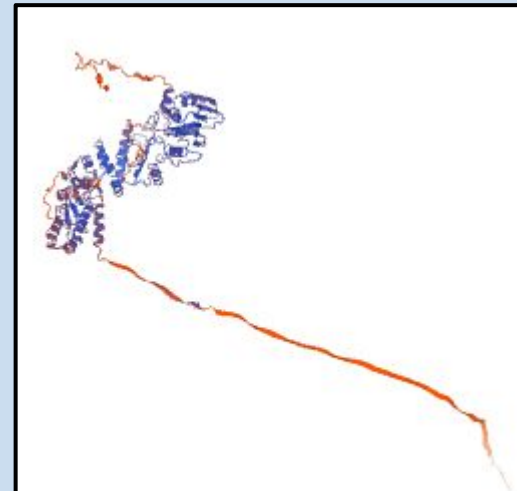


QMEANDisCo Global: **0.66** ± 0.05

Sequence colored by local quality:



A: **GIDPFTSTQTAEDKEEPLHSIISSTESVQGSTSKHEFQAETKKLLDIVARSLYSEKEVFIRELISNASDALEKLRHKLVS****DGQALPEMEIHLQTN** 95
A: **AEKGTITIQDTGIGMTQEELVSNLGTIARSGSKAFD****ALQNAEASSKIIGQFGVGFYSAFMVADRVEVYSSAAPGSLGYQLSDGSGVFEIAE** 190
A: **ASGVRTGTKIIHLKSDCKEFSSEARVDVTKYSNFVSFPLYLNGRRMNTLQAIWMMDPKDVGGEWQHEEFYRYVAQAHDKPRYTLHYKTDAPLN** 285
A: **IRSIIFYVPDMKPSMFDVSRELGSVALYSRKVLITKATDILPKWLRFIGVVDSEDIPLNLSRELLQESALIRKLRDYLQQRLIKFFIDQSKKD** 380
A: **AEKYAKFFEDYGLFMREGIVTATEQEVKEDIAKLLHYESSALPSGQLTSLSEYASRMRAGTRNIYYLCAPNRHLAEHSPYYEAMKKKDTEVLFCE** 475
A: **EQFDELTLHLREFDKKKLISVETDIVVDHYKEEFEDRSPAAECLSEKETEELMAWMNRNVLGSRVTNVKVTLRLDTHPAMVTVLEMGAARHFLR** 570
A: **HQQLAKTQEERAQLLQPTLEINPRHALIKKLNQLRASEPGLAQLLVDDQIYENAMIAAGLVDDPRAMVGRNLNELLVKALERHGGSGSGSSAMVDTL** 665
A: **SGLSSEQGSGDMTIEEDSATHIKFSKRDEDGKELAGATMELRDSGSGKTISTWISDGQVKDFYLYPGKYTFVETAAPDGYEVATAITFTVNEQGG** 760
A: **VTVNGKATKGD****DAHI** 774



THE END!