

Supplementary Material

Structural modeling of the N-terminal signal-receiving domain of I κ B α

Samira Yazdi^a, Serdar Durdag^{a,b}, Michael Naumann^c, Matthias Stein ^{a*}

^aMax Planck Institute for Dynamics and Complex Technical Systems, Molecular Simulations and Design Group, Sandtorstrasse 1, 39106 Magdeburg, Germany.

^bCurrent addresss:Department of Biophysics, School of Medicine, Bahcesehir University, Istanbul, Turkey.

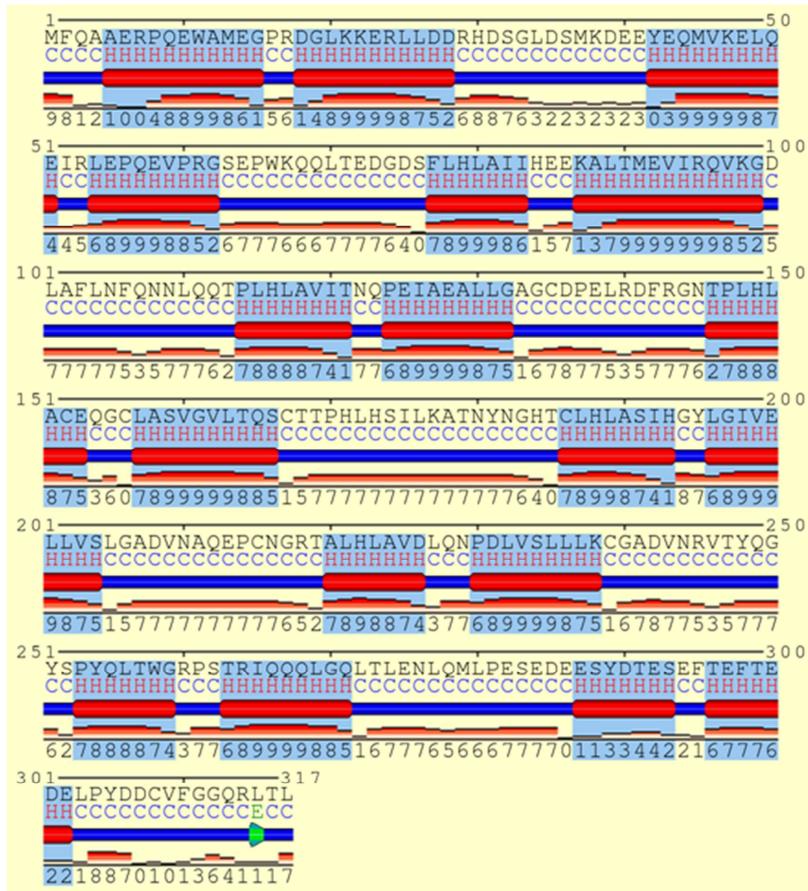
^cInstitute of Experimental Internal Medicine, Medical Faculty, Otto von Guericke University, Leipziger Strasse 44, 39120 Magdeburg, Germany.

* Correspondence: Corresponding Author, Dr. Matthias Stein, Molecular Simulations and Design Group, Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstrasse 1, 39106 Germany. Fax +49-391-6110403.
Email matthias.stein@mpi-magdeburg.mpg.de

Supplementary Data

- **Supplementary Figure 1.** A comparison of secondary structure predictions of the full length I κ B α using different methods.
- **Supplementary Figure 2.** Results from JPRED3 analysis of the full 317 amino acid residues from human I κ B α with confidence scores.
- **Supplementary Figure 3.** pDomThreader prediction results.
- **Supplementary Figure 4.** The total energy variation of the three system replicas for the initial (A) and final (B) 100ns simulation.
- **Supplementary Figure 5.** Temperature of the three system replicas for the initial 100 ns (A) and the final 100ns (B).
- **Supplementary Figure 6.** RMSD of the complexed I κ B α /NF- κ B protein backbone against the starting structure of the three system replicas for the initial 100 ns (A) and the final 100ns (B).
- **Supplementary Figure 7.** Root mean square fluctuations of amino acid residues mapped onto C α -backbone atoms of I κ B α .
- **Supplementary Figure 8.** (A) The total energy variation of the three system replicas for the free I κ B α simulations.(B) Temperature of the three system replicas for the free I κ B α simulations

Supplementary Figure 1. A comparison of secondary structure predictions of the full length I κ B α using different methods.



Supplementary Figure 2. Results from JPRED analysis of the full 317 amino acid residues from human I κ B α . Two helix-coil-helix motifs can be recognized between residues 5-62 which is indicative of an ankyrin repeat-like organization of the SRD.

domTHREADER PREDICTION RESULTS:
 HTML formatted results can be found at:
<http://bioinf.cs.ucl.ac.uk/psipred/result/333460>
 You can also view the results in a machine printable format at:
http://bioinf.cs.ucl.ac.uk/genthreader_output/333460.html

- Key -----
 Conf = Description of confidence level
 Score = Raw score from SVM
 p-val = Probability of false positive
 Epair = Pairwise energy for model
 Esolv = Solvation energy for model
 AlnSc = Sequence alignment score
 Alen = Length of alignment
 Dlen = Length of PDB entry
 Tlen = Length of target sequence
 Start = Start position of the domain
 Stop = End position of the domain
 PDB_ID = PDB identifier (+ chain code + domain code in CATH format)

 Confidence levels:
 CERT p-value < 0.0001
 HIGH p-value < 0.001
 MEDIUM p-value < 0.01
 LOW p-value < 0.1
 GUESS p-value >= 0.1

 CERT 11.734 2e-08 -287.9 1.6 549.5 216 216 317 73 293 liknD00
 CERT 11.479 2e-08 -291.4 -1.3 473.4 126 126 317 108 242 ln0rA00
 CERT 11.232 3e-08 -203.6 -0.7 408.8 93 93 317 141 242 ln0qB00
 CERT 11.142 3e-08 -262.6 0.3 627.0 272 404 317 1 286 ln1lA00
 CERT 10.815 4e-08 -295.3 -6.7 364.0 153 153 317 108 270 lawcB00
 CERT 10.750 5e-08 -373.3 -7.6 470.0 216 228 317 72 317 lk1aA00
 CERT 10.541 6e-08 -240.0 -0.6 327.0 131 131 317 100 237 lympA00
 CERT 10.521 6e-08 -336.6 -6.9 415.0 200 285 317 73 287 lwdyA00
 CERT 10.505 6e-08 -279.6 -3.1 409.0 152 155 317 112 270 2bkgA00
 CERT 10.471 7e-08 -380.9 -5.8 406.0 214 223 317 36 271 luohA00
 CERT 10.469 7e-08 -389.9 -4.5 405.0 204 209 317 55 272 2f8yB00
 CERT 10.053 1e-07 -401.7 -4.9 351.0 215 226 317 35 274 2dznA00
 CERT 9.872 1e-07 -301.0 -0.3 324.0 155 156 317 73 240 lbd8A00
 CERT 9.872 1e-07 -244.9 2.0 320.0 150 162 317 83 242 ls70B01
 CERT 9.559 2e-07 -189.0 0.7 299.0 122 124 317 136 267 3c5rA00
 CERT 9.433 2e-07 -228.6 -2.2 298.0 123 128 317 114 242 lycsB01
 CERT 9.431 2e-07 -186.3 -0.6 259.0 125 125 317 109 241 lbi7B00
 CERT 9.029 4e-07 -110.3 -2.1 244.0 93 93 317 40 136 ln0qB00
 CERT 9.016 4e-07 -144.4 2.2 267.0 125 129 317 112 243 ls70B02
 CERT 7.289 3e-06 -208.8 -3.0 205.0 215 254 317 15 259 lsw6A00
 HIGH 5.818 2e-05 -137.0 -3.9 164.0 96 124 317 35 136 3c5rA00
 HIGH 5.697 2e-05 36.1 4.7 164.0 98 126 317 4 108 ln0rA00
 HIGH 5.411 2e-05 37.7 7.9 157.0 105 155 317 1 112 2bkgA00
 HIGH 4.308 9e-05 22.1 1.4 132.0 103 129 317 6 112 ls70B02
 MEDIUM 4.165 1e-04 0.2 1.0 129.0 99 128 317 8 114 lycsB01
 MEDIUM 3.991 1e-04 50.7 7.3 125.0 98 153 317 1 108 lawcB00
 MEDIUM 3.163 3e-04 78.3 2.5 108.0 91 131 317 1 98 lympA00
 LOW 2.171 0.001 51.5 0.8 89.0 80 162 317 1 83 ls70B01
 LOW 1.936 0.001 0.1 2.7 84.1 15 61 317 303 317 2pw8I00
 LOW 1.905 0.001 -28.1 2.8 83.0 34 125 317 72 109 lbi7B00
 LOW 1.464 0.002 -0.0 1.9 75.3 16 132 317 302 317 lgupA02
 LOW 1.131 0.004 80.0 6.0 69.0 70 285 317 1 73 lwdyA00
 LOW 1.061 0.004 -0.0 -0.3 68.7 15 29 317 302 317 lubdC04
 LOW 1.031 0.004 -3.3 -1.0 68.7 14 205 317 301 317 lvgoA01
 LOW 0.905 0.005 58.5 1.5 65.0 69 228 317 1 72 lk1aA00
 LOW 0.770 0.006 1.0 -1.4 64.2 17 115 317 299 317 2r6fa04
 LOW 0.692 0.006 -1.7 -1.6 62.9 15 230 317 303 317 2nvkX01
 LOW 0.686 0.006 60.7 1.3 61.0 70 216 317 1 73 liknD00
 LOW 0.427 0.008 -2.8 2.2 56.0 37 93 317 1 40 ln0qB00
 LOW 0.380 0.009 -204.1 -9.2 53.0 163 196 317 65 244 ltx4A00
 LOW 0.309 0.010 -39.2 -2.1 43.0 72 72 317 62 145 lpveA00
 LOW 0.266 0.010 -32.9 -2.6 43.0 52 52 317 19 75 lrquA01
 GUESS 0.104 0.012 32.9 4.4 50.0 52 209 317 1 55 2f8yB00
 GUESS 0.103 0.012 65.8 5.0 50.0 69 156 317 1 73 lbd8A00
 GUESS 0.018 0.013 -31.6 -5.0 39.0 57 57 317 208 301 ltteA02
 GUESS 0.011 0.013 -16.6 -1.2 38.0 56 56 317 209 284 lh9eA00

>>> Alignment with liknD00:
 10 20 30 40 50 60
 CCCCCCHHHHCCCCCCCCCCCCCCCCCCCCCCCCHHHHHHCCCCHHHHCCCCCCCC
 liknD00 DGDSFLHLALIHEEKALTMEVIRLAFLNQNLQQTPLHLAVITNQPEIAEALLGAGCDP
 Query -----

```

70          80          90          100         110
CCCCCCCCCHHHHHHHCCHHHHHHHHCCCCCCCCCCCCCCCCHHHHHHCC--  

1iknD00    ELRDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSILKATNYNGHTCLHLASIHY--  

Query      -----MFQA---AERPQEWAPEGPRDG  

-----CCCC---CCCCHHHHHCCCCC  

10

120         130         140         150         160         170
-HHHHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHH  

1iknD00    -LGIVELLVSLGADVNAAQEPNCNGRTALHLAVDLQNPDLSLLKCGADVNRVTYQGYSPY  

Query      |  
LKKEERLLDDRRHDGLDS-MKDDEEYEQMVKELQEIIRLEPQEVPGRGSEPWKQQLTED----  
|  
HHHHHHHHHHCCCCCCC-CCCCCHHHHHHHHHCCCCCCCCCCCCCCCCCCCCCCC-----  

30          40          50          60          70

180         190         200         210
HHCCCCCCCCHHHHHHHHCCCCCCCCCCCCCCCCCCCC  

1iknD00    QLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTE-  

Query      -----

```

Percentage Identity = 1.9.

```

>>> Alignment with 1n0qB00:
          10      20      30      40      50
CCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCHHHHHCC - HHHHHHHHHC-
1n0qB00 NGRTPHLAARNGHLEVVKLLLEAGADVNAKDKNGRTPLHLAARNGH - LEVVKLLLEA-
Query -----MFQAAERPQEWAEGPRDGLKKERLLDDRH
-----CCCCCCCCCHHHHHCCCCCCCCHHHHHHHHHC
          10      20      30
          60      70      80      90
CCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCC
1n0qB00 GADVNAKDKNGRTPLHLAARNGHLEVVKLLLEAGAY
Query DSGLDSMKE-----
CCCCCCCCCC-----
          40

```

Percentage Identity = 5.4.

```
>>> Alignment with 1tx4A00:
```

	110	120	130	140	150	
1tx4A00	H H H H C C C C C H H H H H H H H C C C C H H H H H H H H H C H H H C C C H H H H					
	Y P H V V G F L N I D E S Q R V P A T L Q V L Q T L P E E N Y Q V L R F L T A F L V Q I S A H S Q D N K M T N T N L A V					
Query	--S I L K A T N Y N --G H T C L H L A S I H G ---Y L G I V E L V L S L G A D V N A Q O E P C N G R T A L H L A V					
	--C C C C C C C C --C C H H H H H H C C --C H H H H H H C C C C C C C C C C C C C H H H H H H H H					
		180	190	200	210	220

170 180 190
 HHHHHHCCCCHHHHHHCHHHHHHHHHHHHHHHHHHHH-----
 1tx4A00 VFGPNLLWAKDAAITLKAINPINTFTKFLLDHQGELF-----
 | |
 Query DLQNPDL-----VSLLLKGADVNDRVTVYQGYSPYQLTWGRPSTRIQQ
 HCCCCHHH-----HHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHHH
 230 240 250 260

1tx4A00 -----
 Query QLGQLTLENLQMLPESEDEESYDTESEFTEFTEDELPYDDCVFGQRLTL
 HHHHCCCCCCCCCCCCCCCCCCCCHHCCCCCCCCCCCCCCCCCCCC
 270 280 290 300 310

Percentage Identity = 14.3.

>>> Alignment with 1pveA00:

1pveA00 -----
 Query MFQAAERPQEWAEGPRDGGLKKERLLDDRHDGLDSMKDEEYEQMVKEIIRLEPQEVP
 CCCCCCCCCHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCCCCC
 10 20 30 40 50 60

10 20 30 40
 1pveA00 -CCCCCCCCCCCCCCCCHHHHHCCCCHHHHHHHHHHHHC-----CCHHHHHHH
 | | | | | |
 GSHMPLEFLRNQPQFQQMRQIIQQNPSLLPALLQQIGR-----ENPQLLQQI
 | | | | | |
 Query RGSEPWKQQLTEDGDSFLHLIAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
 CCCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHH
 70 80 90 100 110 120

50 60 70
 1pveA00 HCCCCHHHHHHHHCCCCHHHHHCCCC-----
 | | | | | |
 SQHQEHFIQMLNEPVQEAGGQGGGG-----
 | | | | | |
 Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASGVVLTQSCTTPHLHSILKATN
 CCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCC
 130 140 150 160 170 180

1pveA00 -----
 Query YNGHTCLHLASIHYGLGIVELLVSLG
 CCCCCHHHHHHHHCCCCHHHHHHHHCC
 190 200

Percentage Identity = 18.1.

>>> Alignment with 1rquA01:

10 20 30
 1rquA01 -----CCCHHHHHHHHC-----CCCHHHHHHHHHHHCCCCCCCC
 | | | | | |
 SITKDQIIIEAVA-----AMSVMDVVELISAMEEKFGVSAAAA
 | | | | | |
 Query MFQAAERPQEWAEGPRDGGLKKERLLDDRHDGLDSMKDEEYEQMVKEIIRLEPQEVP
 CCCCCCCCCHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCCCCC
 10 20 30 40 50 60

40 50
 1rquA01 CCCCCCCCCCCCCC-----
 | | | | | |
 VAVAAGPVEAAEEKT-----
 | | | | | |
 Query RGSEPWKQQLTEDGDSFLHLIAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
 CCCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHH
 70 80 90 100 110 120

1rquA01 -----
 Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASGVVLTQSCTTPHLHSILKATN
 CCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCC
 130 140 150 160 170 180

```

1rquA01 -----
Query YNGHTCLHLASIHYLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSLLKCG
CCCCHHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCC
190      200      210      220      230      240

1rquA01 -----
Query ADVNRVTYQQGSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTEFTE
CCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCCHHCCCCC
250      260      270      280      290      300

1rquA01 -----
Query DELPYDDCVFGQRRLTL
CCCCCCCCCCCCCCCC
310

Percentage Identity = 7.7.

>>> Alignment with 2f8yB00:
          10      20      30      40      50      60
CCCCHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHHH
2f8yB00 AVISDFIYQGASLHNQTDRTGETALHLAARYSRSDAAKRLLEASADANIQDNMGRTPLHA
Query -----
          70      80      90      100      110      120
HHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCC
2f8yB00 AVSADAQGVFQILIRNRAVDLADMHDGTTPLILAARLAVEGMLEDLINSHADVNAVDDL
Query -----MFQA
-----CCCC

          130      140      150      160      170
CCCCHHHHHC---CCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCC
2f8yB00 GKSALHWAAAV---NNVDAAVVLLKNGANKDMQNNRETPFLAAREGSYETAKVLLDHF
Query AERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEIRLE
-----CCCCHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCC
          10      20      30      40      50

          180      190      200
CCCCCCCCCCCCHHHHHHCCCHHHHHHHCC
2f8yB00 ANRDITDHMDRLPRDIAQERMHHDIVRLLE
Query -----


Percentage Identity = 2.9.

>>> Alignment with 1bd8A00:
          10      20      30      40      50      60
CHHHHHHHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCC
1bd8A00 RAGDRLSGAARGDVQEVRLLHRELVHPDALNRFGKTAQVMMFGSTAIALELLKQGAS
Query -----
          70      80      90      100      110
CCCCCCCCCCCCHHHHHHCC---HHHHHHHHCCCCCCCCCCCCCHHHHHHHHHCC
1bd8A00 PNVQDTSGTSPVHDAARTGF---LDTLKVLVEHGADVNPDGTVGALPIHLAVQEGHTAVV
Query ---MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEIRLEPQ
---CCCCCCCCHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCC
          10      20      30      40      50

          120      130      140      150
HHHHC---CCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCC
1bd8A00 SFLAA-ESDLHRRDARGLTPLELALQRGAQDLDILQGHM

```

Query EVPRGSEPWKQQLTED-----
CCCCCCCCCC-----

Percentage Identity = 3.8

>>> Alignment with `ltteA02`:

1tteA02 -----
Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEIRLEPQEVP
CCCCCCCCHHHHHCCCCCCCCHHHHHHHHHHCCCCCCCCCCCCHHHHHHHHHHCCCCCCCC
10 20 30 40 50 60

1tteA02 -----
Query RGSEPWKQQLTEDGDSFLHLIAI1HEEKALTMEVIRQVKGDLAFLNFFQNNLQQTPLHHLAVI
CCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCCCCCCCCCCCCCHHHHHHH
70 80 90 100 110 120

1tteA02	-----
Query	TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSILKATN CCCCHHHHHHHHHCC 130 140 150 160 170 180

		10		20		
	-----	CCC-CCCCCCC-	-----	CHHHHHHHHHHHC		
ltteA02	-----	NVE-ESDLYGI-----	-----	DHDLIDEFESQG		
Query	YNGHTCLHLASIHGYLGIVELLVSLGADVNQAEPGNCRTALHLAVDLQNPDVLSSLKCG					
	CCCCHHHHHHHHCCCHHHHHHHHHCCCCCCCCCCCCCCCCHHHHHHHHCCCHHHHHHHHHCC					
	190	200	210	220	230	240

	30	40	50			
1tteA02	-----CCHHHHHHHHHHHCCC-----	-----CCCCCCCCHHHHHHHHHHC				
	-----FEKDKI V EVLRRLGV-----	KSLDPDNNTANR1I E ELL				
Query	ADVNDRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDE S YDTE E SEFTEFTFE					
	CCCCCCCCCCCCHHHHHHHHCCC H HHHHCCCCCCCCCCCCCCCCCCCCHHCCCCCCCC					
	250	260	270	280	290	300

1tteA02 C-----
Query DELPYDDCVFGGQRLTL
CCCCCCCCCC
310

Percentage Identity = 21.1.

>>> Alignment with 1b9e700:

1h9eA00 -----
Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEIRLEPQEVP
CCCCCCCCHHHHCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
10 20 30 40 50 60

1h9eA00 -----
Query RGSEPWKQQLTEDGDSFLHLAI1HEEKALTMEVIRQVKGDLAFLNFFQNNLQQTPLHLAVI
CCCCCCCCCCCCCCCCHHHHHHCCCHHHHHHHHHCCCCCCCCCCCCHHHHHHHH
70 80 90 100 110 120

1h9eA00 -
Query TNOPEIAEALLGAGCDPELRDFRGNTPLHLACEOGCLASGVGLTOSCTTPHLHSILKATN

```

CCCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCC
 130      140      150      160      170      180

```

```

1h9eA00      -----          10          20
              CCCCCCCCCCCC-----CCHHHHHHHHCC
-----PEFLEDPVSILT-----KDKLKSELVANN
Query YNGHTCLHLASIHGYLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSSLKCG
CCCCHHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCC
 190      200      210      220      230      240

```

```

1h9eA00      30          40          50
              CCCCCCCC-----CCCHHHHHHHHHCCCCCCCCCCCC-----C
VTLPAGEQ-----RKDVYVQLYQLQHLTARNRPPPLPAGT-----
Query ADVNRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTEFTE
CCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCCHHHCCCC
 250      260      270      280      290      300

```

```

1h9eA00      -----
Query DELPYYDDCVFGGQRRLTL
CCCCCCCCCCCCCCCC
 310

```

Percentage Identity = 23.2.

>>> Alignment with 1vg0A01:

```

1vg0A01      -----
Query MFQAAERPQEWAEGPRDGKKERLLDDRHDGLDSMKDEEYEQMVKEIQLRLEPQEVP
CCCCCCCCCHHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCCCCC
 10      20      30      40      50      60

```

```

1vg0A01      -----
Query RGSEPWKQQLTEDGDSFLHLAIIEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
CCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCCCCCCCCCCCCHHHHHHHH
 70      80      90      100      110      120

```

```

1vg0A01      -----
Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASGVVLQSCTTPHLHSILKATN
CCCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCC
 130      140      150      160      170      180

```

```

1vg0A01      -----
Query YNGHTCLHLASIHGYLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSSLKCG
CCCCHHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCC
 190      200      210      220      230      240

```

```

1vg0A01      -----
Query ADVNRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTEFTE
CCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCCHHHCCCC
 250      260      270      280      290      300

```

```

1vg0A01      10          20          30          40          50
              CCCCCCCCCEECC---CHHHHHHHHHCCCCCEECCCCCCCCCCCCHHHHHHH
DNLPDFDVIVIGT---GLPESIIAACSRSGQRVLHVDSRSYYGGNWASFSGLLSWL
| ||| | | | | |
Query DELP--YDDCVFGGQRRLTL-
CCCC--CCCCCCCCCCCC
 310

```

60 70 80 90 100 110
 lvg0A01 HHCCCCHHHHCCCCEEEEEECCCCCCCCCCCCHHHHHHHHHHHHCCCCEEECCCCEEEEEE
 KEYQMWMQEQLILENEEAIPLSSKDFLFPFLYQGQGELPQCFCRMCAVFGGIYCLRHSVQCLVV

Query -----

120 130 140 150 160 170
 lvg0A01 ECCCCCEEEECCCCCEECCCEECCCCCCCCCCCCCCCCCCCCCCCCCCCCCEE
 DKESRKCKAVIDQFGQRRIISKHFIIEDSYLSENTCSRVQYSSDISRDCYNDLPSNVYVCS

Query -----

180 190 200
 lvg0A01 CCCCCCCCCHHHHHHHHHHHHHHHCCCCC
 GPDGLGNDNAVKQAETLFQQICPNEDF

Query -----

Percentage Identity = 3.4.

>>> Alignment with 1klaA00:

10 20 30 40 50 60
 1klaA00 CCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHH
 EDGDTPLHIAVVQGNLPAVHLVNLFQQGGRELDIYNRLQTPLHLAVITTLPSVVRLLV

Query -----

70 80 90 100 110 120
 1klaA00 HCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCCCCCHHHHHHH
 TAGASPMALDRHGQTA AHLACEHRSPTCLRALLDSAAPGTLDEARNYDGLTALHVAVNT

Query -----

130 140 150 160 170
 1klaA00 CCHHHHHHHHHCCCCCCCCCCCCHHHHHHCC--CHHHHHHHHC--CHHHHHHHHC
 ECQETVQLLERGADIDAVDIKGSGRSPLIHAVENN--SLSMVQLLLQH-GANVNAQMYSG
 Query -----
 -MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEE
 -----CCCCCCCCHHHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCC
 10 20 30 40

180 190 200 210 220
 1klaA00 CCHHHHHHHHHCCCCCCCCCCCCCCCCCCCCCCCCCHHHHHHHCC
 SSALHSASGRGLLPLVRLVRSRGADSSLKNCHNDTPLMVARSRVIDILRG
 Query YEQMVKELEIRLEPQEVPVRGSEPWKQQLTE-----
 HHHHHHHHHHHCCCCCCCCCCCCCCCCCCCCCCCC
 50 60 70

Percentage Identity = 3.5.

>>> Alignment with 2r6fA04:

2r6fA04 -----

Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEIRLEPQEVP
 CCCCCCCCCHHHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
 10 20 30 40 50 60

2r6fA04 -----

Query RGSEPWKQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
 CCCCCCCCCCCCCCCCCHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHH
 70 80 90 100 110 120

2r6fA04 -----

Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSILKATN
 CCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCC
 130 140 150 160 170 180

2r6fA04 -----

Query YNGHTCLHLASIHYGLGIVELLVSLGADVNQEPNCNGRTALHLAVDLQNPDLVSLLLKGCG
 CCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCC
 190 200 210 220 230 240

2r6fA04 -----CE-----AK

Query ADVNRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTEFTE
 CCCCCCCCCCCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCCCCCHHCCCCCCC
 250 260 270 280 290 300

2r6fA04 -----
 ECC--CHHHHCCCCCCCCCCCCCCCCCCCCCHHHHHHHHHHHHHCCCCCCCCCCCCHHHHHHHH
 LEV--DLDLVIPNDELTILKEHAIAPWEPPYPQLLEAVCRHYGIPDPVKDLPKEQLDKIL
 | | | |||
 Query DELPYD-DCVFGGQRLLT-----
 CCCCCC-CCCCCCCCCCCC-----
 310

2r6fA04 -----
 HCCCCCCCCCCCCCCCCCCCCCCCCCCCCCHHHHHHHHHHHHHCCCCCCCCCCCCCEEC
 YGSGGEPIYFRTNDFGQVREQYIAFEGVIPNVERRYRETSSDYIREQEKYAEQP

Query -----

Percentage Identity = 6.1.

>>> Alignment with 2nvkX01:

2nvkX01 -----

Query MFQAAERPQEWAEGPRDGGLKKERLLDDRHDSGLDSMKDEEYEQMVKELQEIRLEPQEVP
 CCCCCCCCCHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
 10 20 30 40 50 60

2nvkX01 -----

Query RGSEPWKQQLTDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
 CCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCCCCCCCCCCCCHHHHHHHH
 70 80 90 100 110 120

2nvkX01 -----

Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSILKATN
 CCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCC
 130 140 150 160 170 180

2nvkX01 -----

Query YNGHTCLHLASIHYGLGIVELLVSLGADVNQEPNCNGRTALHLAVDLQNPDLVSLLLKGCG
 CCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCC
 190 200 210 220 230 240

2nvkX01 -----

Query ADVNRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTEFTE
 CCCCCCCCCCCCCHHHHHHCCCHHHHHCCCCCCCCCCCCCCCCCCCCHHCCCCCCC
 250 260 270 280 290 300

Query DELPYDDCVFGGQRQLTL
CCCCCCCCCC
310

Percentage Identity = 99.1.

>>> Alignment with 1n0rA00:

1n0rA00 -----
 Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEQEIRLEPQEVP
CCCCCCCCHHHHHCCCCCCHHHHHHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
10 20 30 40 50 60

1n0rA00 -----
 Query RGSEPWKQQLTEDGDSFLHLIAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLALVI
CCCCCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHH
70 80 90 100 110 120

1n0rA00 -----
 Query HCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCHHHHHHHHCCCCCCC
NGHLEVVKLLEAGADVNAKDKNGRTPHLAARNGHLEVVKLLEAGADVN-----AKD
130 140 150 160 170 180

1n0rA00 -----
 Query TNQPEIAEALLGAGCDPELRDFRGNTPHLACEQGCLASGVVLTOSCTTPHLHSILKATN
CCCCHHHHHHHHCCCCCCCCCCCCCCCCHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCC
190 200 210 220 230 240

1n0rA00 -----
 Query CC-----
AY-----
Query ADVNRVTYQGYSPYQLTWGRPSTRIQQLQQLTLENLQMLPESEDESESYDTESEFTEFTE
CCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCCCCCCHHCCCCCCC
250 260 270 280 290 300

1n0rA00 -----
 Query DELPYDDCVFGGQRQLTL
CCCCCCCCCC
310

Percentage Identity = 46.0.

>>> Alignment with 1n0qB00:

1n0qB00 -----
 Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEQEIRLEPQEVP
CCCCCCCCHHHHHCCCCCCHHHHHHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
10 20 30 40 50 60

1n0qB00 -----
 Query RGSEPWKQQLTEDGDSFLHLIAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLALVI
CCCCCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHH
70 80 90 100 110 120

1n0qB00 -----
 Query TNOPEIAEALLGAGCDPELRDFRGNTPHLACEQGCLASGVVLTOSCTTPHLHSILKATN
10 20 30
-----C--CCCHHHHHHHCCCCHHHHHHHHCCCCCCC
-----N--GRTPHLAARNGHLEVVKLLEAGADVN-----AKD

CCCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCC
 130 140 150 160 170 180

40 50 60 70 80 90
 1n0qB00 CCCCCHHHHHHCCCHHHHHHHCCCCCCC-CCCCCCHHHHHHHCCCHHHHHHHCC
 KNGRTPLHLAARNGHLEVKLLLEAGADVNAK-DKNGRTPLHLAARNGHLEVKLLLEAG
 ||| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
 Query YNGHTCLHLASIHYGLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSLLKCG
 CCCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCC
 190 200 210 220 230 240

1n0qB00 CC-----
 AY-----
 |
 Query ADVNRVTYQQSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTFTE
 CCCCCCCCCCCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCCCCCHHCCCC
 250 260 270 280 290 300

1n0qB00 -----
 Query DELPYYDDCVFGQRLTL
 CCCCCCCCCCCCCCCC
 310

Percentage Identity = 47.3.

>>> Alignment with 1n11A00:
 10 20 30 40 50 60
 1n11A00 CCCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCC
 LTPLHVASFHMGHLPIVKNLLQRGASPNSVKVETPLHMAARAGHTEVAKYLLQNKA
 KV
 Query -----

70 80 90 100 110 120
 1n11A00 CCCCCCCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHH
 AKAKDDQTPLHCAIRIGHTNMVKLLENNANPNLATTAGHTPLHIAAREGHVETVL
 ALLE
 Query -----

130 140 150 160 170
 1n11A00 CCCCCCCCCCCCCHHHHHHCCC--HHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCC
 KEASQACMTKKGFTPPLHVAKYGK--VRVAELLERDAHPNAAGKNGLTPLHVAVHHNN
 |
 Query ---MFQAAERPQEWAEGPRDGLKKERLLDDRHDGSDLSMKDEEYEQMVKELQEIR
 ---CCCCCCCCHHHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHHHCCCC
 10 20 30 40 50

180 190 200 210 220 230
 1n11A00 HHHHHHHHHCCCCCCCCCCCCHHHHHHCCC---HHHHHHHHCCCCCCCCCCCC
 LDIVKLPLRGSPHSPAUNGTYPLHIAAKQNZ---VEVARSLLQYGGSANAESVQGVT
 |
 Query LEPQEVPRGSEPWKQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQT
 CCCCCCCCCCCCCCCCCCCCCCCCCHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCC
 60 70 80 90 100 110

240 250 260 270 280 290
 1n11A00 HHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCC
 PLHLAAQEGHAEVMALLSKQANGNLGNKSGLTPLHLVAQEGHVPVADVLIKHGVMVD
 ||||| | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
 Query PLHLAVITNQPEIAEALLGAGCDPELRDFRGNTPPLHLACEQGCLASVGVL
 TQSCTTPHLH
 HHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCC
 120 130 140 150 160 170

300 310 320 330 340
 1n11A00 ----CCCCCCCCHHHHHHCCCCCCCCCCCCCCCCCCCCHHHHHHCCCC
 ----ATTRMGTPLHVASHYGNIKLVLKFLLQHQADVNAKTK-LGYSPLHQAAQGHTDIV
 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
 Query SILKATNYNGHTCLHLASIHYGLGIVELLVSLGADVNAQEPCNGRTALHLAV
 DLQNPDLV
 CCCCCCCCCCCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCHHHHHHCCCHHH
 180 190 200 210 220 230

350 360 370 380 390 400
 HHHHHCCCCCCCCCCCCCCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCC
 --

```

1n11A00  TLLLNGASPNEVSSDGTTPLAIAKRLGYISVTDVLKVTDETSFVLHRMSFPETVDE--
| | | | | | | | | | | | | | | |
Query   SLLLKGADNRVTVYQGSPYQLTWGRPSTRIQQQLGQLTLENLQML-----PESEDEES
HHHHHCCCCCCCCCCCCCCCCHHHHHHCCHHHHHHCCCCCCCCCCC-----CCCCCCCC
240      250      260      270      280

```

```

1n11A00  -----
Query   YDTESEFTEFTEDELPYDDCVFGGQRLTL
CCCHHCCCCCCCCCCCCCCCCCCCCCCCC
300      310

```

Percentage Identity = 23.0.

>>> Alignment with lawcB00:

```

lawcB00  -----
Query   MFQAAERPQEWAEGPRDGKKERLLDDRHDGLDSMKDEEYEQMVKELEIRLEPQEVP
CCCCCCCCHHHHCCCCCCCCHHHHHHCCCCCCCCHHHHHHCCCCCCCCHHHHHHCCCCCCCC
10       20       30       40       50       60

```

```

10
lawcB00  -----C--HHHHHHHHHH
-----D--LGKKLLEAAR
| | |
Query   RGSEPWKQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
CCCCCCCCCCCCCCCCHHHHHHCCHHHHHHHHHHHHHHCCCCCCCCCCCCHHHHHHHH
70       80       90       100      110      120

```

```

20       30       40       50       60
HCCCCHHHHHHHHCCCCC-CCCCCCCCCHHHHHHHHCCCHHHHHHHCCCCCCCC-----CCC
lawcB00  AGQDDEVRIILMANGAPFT-TDWLGTSPHLAAQYGHFSTTEVLLRAGVSRD-----ART
| | | | | | | | | | | | | | | | | | | | | |
Query   TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSILKATN
CCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCHHHHHHHHHCCCCCCCCCCCCCCCC
130      140      150      160      170      180

```

```

70       80       90       100      110      120
CCCCCHHHHHHHCCHHHHHHCCCCCCCCCCCC-CCHHHHHHHCCCHHHHHHHHH
lawcB00  KVDRTPLHMAASEGHANIVEVLLKGADVNAKMLK-MTALHWATEHNHQEVVELLIKYG
| | | | | | | | | | | | | | | | | | | | | |
Query   YNGHTCLHLASIHYGLGIVEPLLVLGADVNAQEPNCNGRALHLAVDLQNPDLVSLLKCG
CCCCHHHHHHHHCCCHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCHHHHHHHHH
190      200      210      220      230      240

```

```

130      140      150
CCCCCCCCCCCCHHHHHHCCCHHHHHHC-
lawcB00  ADVHTQSKFKTAFDISIDNGNEDLAEILQ-----
| | |
Query   ADVNRVTVYQGSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTEFTE
CCCCCCCCCCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCHHCCCCCCCC
250      260      270      280      290      300

```

```

lawcB00  -----
Query   DELPYDDCVFGGQRLTL
CCCCCCCCCCCCCCCC
310

```

Percentage Identity = 29.4.

>>> Alignment with 1k1aA00:

```

1k1aA00  -----
Query   MFQAAERPQEWAEGPRDGKKERLLDDRHDGLDSMKDEEYEQMVKELEIRLEPQEVP
CCCCCCCCHHHHCCCCCCCCHHHHHHCCCCCCCCCCCCHHHHHHCCCCCCCC
10       20       30       40       50       60

```

```

10       20       30       40
-----CCCCCHHHHHHHCCCHHHHHHHHHCCCCCCCCCCCCHHHHHH
1k1aA00  -----EDGDTPLHIAVVQGNLPAVHRLVNLFFQGGRELDIYNLRLQTPLHLAVI
| | | | | | | | | | | | | | | |

```

Query RGSEPWKQQLTEDGDSFLHLAI IHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
 CCCCCCCCCCCCCHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHH
 70 80 90 100 110 120

1k1aA00 60 70 80 90 100
 CCCCHHHHHHHCCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHHHCCCCCCCC--CCCC
 TTLPSVVRLLVTAGASPMALDRHGQTA AHLACEHRSPTCLR ALLDSAAPGTL DL--EARN
 | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
 Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVL TQSCTTPHLHSILKATN
 CCCHHHHHHHHCCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHHHCCCCCCCCCCCC
 130 140 150 160 170 180

1k1aA00 110 120 130 140 150 160
 CCCCCHHHHHHHHCCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCHHHHHCC
 YDGLTALHVANTECQETVQLLERGADIDDAVIDKSGRSPLIHAVENNSLSMVQLLQHG
 | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
 Query YNGHTCLHLASI HGYLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSLLKCG
 CCCHHHHHHHHCCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCHHHHHHCC
 190 200 210 220 230 240

1k1aA00 170 180 190 200
 CCCCCCCCCCCC HHHHHHCCHHHHHHCC-----CCCCCCCC-----
 ANVNAQMYSGSSALHSASGRGLLPLVRTLVRSG-----ADSSLKNCH-----
 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
 Query ADVNRVTYQQSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTFTE
 CCCCCCCCCCCC HHHHHHCCHHHHHHCCCCCCCCCCCCCCCCHHCCCC
 250 260 270 280 290 300

1k1aA00 210 220
 -----CCCCCCCCCCC HHHHHHCC-----
 -----NDTPLMVARSRVIDILRG
 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
 Query DELPYDDCVFGGQRLLT-----
 CCCCCCCCCCCCCCCC-----
 310

Percentage Identity = 31.6.

>>> Alignment with lympA00:

lympA00 -----

Query MFQAERPQEWAMEGPRDGLKKERLLDDRHDGLDSMKDEEYEQMVKELQEIRLEPQEV
 CCCCCCCCCC HHHHHCCCCCCCCHHHHHHCCCCCCCCCCCCHHHHHHCCCC
 10 20 30 40 50 60

lympA00 10 20
 -----CCCCCCCCCCCCHHHHHH-----
 -----RATDLDARMHDGTTPLILAAR
 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
 Query RGSEPWKQQLTEDGDSFLHLAI IHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
 CCCCCCCCCCCCHHHHHCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCCHHHHHH
 70 80 90 100 110 120

lympA00 30 40 50 60 70
 HCCCCHHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCC-----C
 LALEGMLLEDLINSHADVNAVDDLGKSALHWAAAVNNVDAAVVLLKGANKDMQ-----N
 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
 Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVL TQSCTTPHLHSILKATN
 CCCHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCC
 130 140 150 160 170 180

lympA00 80 90 100 110 120 130
 CCCCCHHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCHHHHHHHC---
 NKEETPLFLAAREGSYETAKVLLDHFA NR DIT-DHM DRL PRDIAQERMHH DIV RLLD---
 | | | | | | | | | | | | | | | | | | | | | | | | | | | |
 Query YNGHTCLHLASI HGYLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSLLKCG
 CCCHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCCCCCCCCCHHHHHHCCCC
 190 200 210 220 230 240

lympA00 -----

Query ADVNRVTYQQSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTFTE
 CCCCCCCCCCCC HHHHHHCCHHHHHHCCCCCCCCCCCCCCCCCCCCHHCCCC
 250 260 270 280 290 300

```

1lympA00 -----
Query DELPYDDCVFGGQLRTL
CCCCCCCCCC
310

Percentage Identity = 22.9.

>>> Alignment with 1wdyA00:

1wdyA00 -----
Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDGLDSMKDEEYEQMVKELEIRLEPQEVP
CCCCCCCCHHHHHCCCCCCCCHHHHHHHCCCCCCCCCCCCHHHHHHCCCCCCCC
10 20 30 40 50 60

10 20 30 40
1wdyA00 -----CHHHHHHHHHHHHHCCC---HHHHHHHHCCCCCCCCCCCCCHHH
-----AAVEDNHLLIKAVQNED---VDLVQQLLEGGANVNFQEEEGGWTPHL
Query RGSEPWKQQLTED---GDSFLHLAIIHEEKALTMEVIROVKGDLAFLNFO-NNLQQTPLH
CCCCCCCCCCCC---CCCHHHHHHHCCCCHHHHHHHHCCCCCCCC-CCCCCHHH
70 80 90 100 110

50 60 70 80 90
1wdyA00 -----HHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCCC
-----NAVQMSREDIVELLRHGADPVLRKKNATPFLLAAIAGSVKLKLFLSKGADV-----
Query LAVITNQPEIAEALLGAGCDPELDRFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSI
HHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCCCCCCC
120 130 140 150 160 170

110 120 130 140 150
1wdyA00 -----CCCCCCCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCCCCCHHHHHH
-----ECDFYGFATFMEAAYGVKALKFLYKRGANVNRRTKEDQERLRKGGAALMDAAEK
Query KATNYNIGHTCLHLASIHYLGIVELLVSLGADVNAQEP-----C
CCCCCCCCCHHHHHHHCCCCCCCCCCCC-----HHHHHHCCCCCCCCHHHHHH
180 190 200 210

170 180 190 200 210
1wdyA00 -----CCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCCCCCHHHHHHHHCCCC
-----GHVEVLKILDEMGAADVACDNMGRNALIHALLSSDDSDVEAITHLLDHGADVNRGER
Query -----N
-----C

230 240 250 260 270
1wdyA00 -----CCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCC
-----GKTPLILAVEKKHLGLVQRLLQEHEIEINDTDGKTALLAVELKLKIAELLCKRGAS
Query GRTALHLAVDLQNPDLVSLLLKC-GADVNRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLE
CCCCCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCCCHHHHHHCCC
220 230 240 250 260 270

280
1wdyA00 -----CCCCCCC-----
-----TDCGDLV-----
Query NLQMLPESEDEESYDTESEFTEFTEDEL PYDDCVFGGQLRTL
CCCCCCCCCCCCCCCCCHHHCCCCCCCCCCCCCCCCCCCC
280 290 300 310

Percentage Identity = 18.9.

>>> Alignment with 2bkgA00:

2bkgA00 -----
Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDGLDSMKDEEYEQMVKELEIRLEPQEVP
CCCCCCCCHHHHHCCCCCCCCHHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCCCCC
10 20 30 40 50 60

2bkgA00 -----CHHHHHHHH
-----SDLGKKLLE

```

	20	30	40	50	60	
2bkga00	HHHHCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCCCCCC-----	AARAGQDDEVRLMANGADVNAEDTYGDTPLHLAARVGHLIEIVEVLLKNGADVNAL-----				
Query	AVITNQPEIAEALLGAGCDPELIRDFRGNTPLHLACEQGCLASGVGLTQSCTTPHLHSILK	HHHCCCCHHHHHHHHCCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCC				
	120	130	140	150	160	170

	70	80	90	100	110	120
2bkqA00	--CCCCCCC HHHHHHHHCCCCHHHHHHHHCCCCCCCC--	--CCCCCCC HHHHHHHHCCCCHHHHHHHHCCCCHHHHHH				
	--DFSGSTPLHLAKRGHLEIIVEVLLKYGADVNA-DDTIGSTPLHLAA DTGHLIEIVEVLL					
Query	ATNYNGHTCLHLASLTHGYLGIVELLVSLGADVNQAEPNCN GRTALHLA DVLQNPDLVSLLLL	CCCCCCCCHHHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHHHCCCCHHHHHHHHHHHHHH				
	180	190	200	210	220	230

	130	140	150			
2bkgA00	HCCCCCCCCCCCCCCC	HHHHHHHHHHHHHHH	CCCCCCCCHHHHCC	- - -		
	KYGADVNAQDKF	GKTAFDISIDNGN	-DLAEIL			
Query	KCGADVN	RVTYQGSPYQLT	WGRPSTRIQQQLGQLT	LENLQMLPESEDEE		
	WGRPSTRIQQQLGQLT	LENLQMLPESEDEE	SYDTESEFTE			
	HCCCCCCCCCCCCCCC	HHHHHHHHHHHHHHH	CCCCCCCCCCCCCCCC	CCCC		
	240	250	260	270	280	290

2bkgA00 -----
Query FTEDELPLYDDCVFGGQLRTL
CCCCCCCCCCCCCCCCCCCCCC
300 310

Percentage Identity = 35.5.

```
>>> Alignment with luohA00:
```

```

          10          20
-----CCCCCHHHHHHCCHHHHHHHH
1luohA00 -----CVSNLVCNLAYSGKLEELKESILA

          10          20          30          40          50
MFQAERPQEWAEGPRDGLKKERLLEDRHSGLDSMKD-----EEYEQMVKEILQE
Query   CCCCCCCCCHHHHCCCCCCHHHHHHHHHCCCCCCCCC-----CCHHHHHHHHHH
          10          20          30          40          50

```

	30	40	50	60	70	
1luhA00	CHHHHHHC-----CCCCCCCCHHHHHHHHCC-----HHHHHHHHHHCCCCCCCCCCCC					
	DKSLATR-----TDQDSRTALHWACSAGH-----TEIVEFLQLGVPVNKDAG					
Query	IRLEPQEVPGRGSEPWKQQLTEDGDSFLHLAI1HEEKALTMDEVIRQVKGDLAFLNFQNNLQ					
	CCCCCCCCCCCCCCCCCCCCCCCCCCCCHHHHHHCCCHHHHHHHHHHHHHCCCCCCCCCCCC					
	60	70	80	90	100	110

	80	90	100	110	120	130
1luhA00	CCHHHHHHHHCCHHHHHHHCCCCCCCCCCCCCCCCHHHHHHHHCCCHHHHHHHCCCC	WSPLHIAASAGRDEIVKALLGKGAQVNQNGCTPLHYAASKRNHEIAVMLLEGANPD				
Query		QTPLHLAVITNQPEIIEALLGAGCDPELRDFRGNTPHLACEQGCLASVGVLQTSCSTTPH				
	CHHHHHHHHCCCCHHHHHHCCCCCCCCCCCCHHHHHHHHCCCHHHHHHHCCCC	CHHHHHHHHHCCCCHHHHHHCCCCCCCCCCCCHHHHHHHHCCCHHHHHHHCCCC				
	120	130	140	150	160	170

	140	150	160	170	180	
1luhA00	-----CCCCCCCCHHHHHHCCHHHHHHHHCCCCCCC-----	CCCCCCCCHHHHHHHHCCCCCCC-----	CCCCCCCCHHHHHHHHCCCCCCC-----	CCCCCCCCHHHHHHHHCCCCCCC-----	CCCCCCCCHHHHHHHHCCCCCCC-----	
	-----AKDHYEATAMHRAAKGNLKMIIILLYKASTNIQ-----	DTEGNTPLHLACDEERVE				
Query	LHSILKATNYNGHTCLHLASIHCYGLGIVELLVSLGADVNAQEPCNCRGRTALHLAVLDLNQPND					
	CCCCCCCCCCCCCCCCHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCHH					
	180	190	200	210	220	230

	190	200	210	220		
1uoHA00	HHHHHHHHCCCCCCCCCCCCCCCCHHHHCCCCHHHHHHHHHC-----					
	EAKLLLVSQGASIYIENKEEKTPLQVAKGGGLLILKRMVEG-----					
Query						
	LVSSLKKCAGDVNRVTYQGYSPYQLTWRPSTRIQQQLGQTLLENLQMLPESEDEESYDT					
	HHHHHHHHCCCCCCCCCCCCCCCCHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCCCCC					
	240	250	260	270	280	290

luohA00 -----

Query ESEFTEFTEDELPYDDCVFGGQRLL
HHCCCCCCCCCCCCCCCCCCCCCCCC
300 310

Percentage Identity = 22.4.

>>> Alignment with 2f8yB00:

2f8yB00 -----C--CCC
-----A--VIS

Query MFQAAERPQEWAEGPRDGKKEERLLDDRHDGLDSMKDEEYEQMVKELEQIRLEPQEVP
CCCCCCCCCHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
10 20 30 40 50 60

10 20 30 40 50
HHHHCCCC-CCCCCCCCCCCCCHHHHHHCCCC---HHHHHHHHCCCCCCCCCCCCHHH
2f8yB00 DFIYQGAS-LHNQTDRTGETALHLAARYSR---SDAAKRLLEASADANIQDNMGRTPHL
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query ---RGSEPWKQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLH
---CCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHH
70 80 90 100 110

70 80 90 100 110
HHHHHHCCCHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCHHHHHHHHCCCC
2f8yB00 AAVSADAQGVFQILIRNRATDLDARMHDGTTPLILAARLAVERGMLEDLINSHADVN
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query LAVITNQPEIAEALLGAGC-DPELRDFRGNTPHLACEEQGCLASVGVLTQSCTTPHLHSI
HHHHCCCCHHHHHHHHCCCC---CCCCCCCCCCCCHHHHHHHHCCCCHHHHHHCCCC
120 130 140 150 160 170

120 130 140 150 160 170
--CCCCCCCCHHHHHHCCCCHHHHHHCCCC---CCCCCHHHHHHHCCCCHHHH
2f8yB00 --AVDDLGKSALHWAAAANVDAAVVLLKNGANKDMQ-NNREETPLFLAAREGSYETAKV
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query LKATNYNGHTCLHLASIHYGLGIVELLVSLGADVNAQEPNCNGRTALHLAVDLQNPDLVSL
CCCCCCCCCCCCHHHHHHHHCCCCHHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHH
180 190 200 210 220 230

180 190 200
HHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCC
2f8yB00 LLDHFANRDITDHMDRLFRDIAQERMHDIVRLLDEY
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query LLKGCGADVNRVTVQGYSPQLTWGRPSTRIQQQQLGQLTLENLQMLPESEDEESEYDTESEF
HHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCCCCCCHHCC
240 250 260 270 280 290

2f8yB00 -----

Query TEFTEDELPYDDCVFGGQRLL
CCCCCCCCCCCCCCCCCCCC
300 310

Percentage Identity = 23.0.

>>> Alignment with 2dznA00:

2dznA00 -----CHHHHHHCCCCHHHHHHHH
-----NYPLHQACMENEFFKVQELLHSK

Query MFQAAERPQEWAEGPRDGKKEERLLDDRHDGLDSMKDEEYEQMVKELEQIRLE
CCCCCCCCCHHHHCCCCCCCCHHHHHHHHCCCC
10 20 30 40 50

30 40 50 60 70
-----CCCCCCCCCCCCHHHHHHCCCC---HHHHHHHHCCCCCCCCCCCC
2dznA00 -----PSLLLQKDQDGRIPHLWSVSFQA---HEITSFLLSKMENVNLDDYPDDSGW
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query PQEVPRGSEPWKQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNF---QNNLQQ
CCCCCCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCC
60 70 80 90 100 110

80 90 100 110 120 130
CHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCC

2dznA00 TPFHIACSVGNLEVVKSLYDRPLKPDLNKITNQGVTCILHLAGVKKWFESQFLIENGASV
 Query | | | | |
 | TPLHLAVITNQPEIAEALLGA--GCDPELRDFRGNTPLHLACEQGCLASVGVLTQSCTTP
 HHHHHHHHHCCCHHHHHHHHC--CCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCC
 120 130 140 150 160 170 180

2dznA00 140 150 160 170 180
 C-----CCCCCCCCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCC
 R-----IKDKFNQIPLHRAASVGSKLIELLCGLGKSAVNWQDKQGWTPFLHALAEGHG
 Query | | | | |
 | HLHSILKATNYNGHTCLHLASIHYGLGIVELLVSLGADVNQAQEPNCNRGRTALHLAVDLQNP
 CCCCCCCCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCHHHHHHHCCCC
 180 190 200 210 220 230

2dznA00 190 200 210 220
 HHHHHHHHHCCCCCCCCCCCHHHCCCCC---HHHHHHCCC-----
 DAAVLLVEKYGAEYDLVDNKGAKAEDVALNEQ---VKKFFLNNV-----
 Query | | | | |
 | DLVSSLKK-CGADVNRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESY
 HHHHHHHH-CCCCCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCCCC
 240 250 260 270 280

2dznA00 -----
 Query DTESEFTEFTEDELPYDDCVFGGQRRTL
 CCCCCCCCCCCCCCCCCCCCCCCCC
 300 310

Percentage Identity = 19.5.

>>> Alignment with 1bd8A00:

1bd8A00 -----
 Query MFQAAERPQEWAAMEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEQIRLEPQEVP
 CCCCCCCCCHHHHHHCCCCCCHHHHHHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCCCCC
 10 20 30 40 50 60
 ----- CHHHHHHHHHHHCC---HHHHHHHHCCCCCCCCCCCCCCCCHHHH
 1bd8A00 -----RAGDRLSGAAARGD---VQEVRRLHRELVHPDALNRFGKTALQVM-
 Query | | | | |
 | RGSEPWKQQLTEDGDSFLHLAIIEEKALTMEVIRQVKGD-LAFLNFQNNLQQTPLHLAV
 CCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHHHHHCCCCCCCCHHHHHH
 70 80 90 100 110

1bd8A00 50 60 70 80 90
 CCCCCHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCCCCCCC
 MFGSTAIALELLKQGASPQVQDTSGTSPVHDARTGFIDTLKVLVEHGADVNP-----
 Query | | | | |
 | ITNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSILKAT
 HCCCCHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCC
 130 140 150 160 170

1bd8A00 100 110 120 130 140 150
 CCCCCCHHHHHHHCCCCHHHHHHHC--CCCCCCC-CCCCCCCCHHHHHHCCCCHHHHHH
 DGTGALPIHLAVQEGHTAVVSFLAA-ESDLHRR-DARGLTPLEALQRGADQDLVDILQGH
 Query | | | | |
 | NYNGHTCLHLASIHYGLGIVELLVSLGADVNQAQEPNCNRGRTALHLAVDLQNPDLVSLLLKC
 CCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCHHHHHH
 190 200 210 220 230

1bd8A00 C-----
 M-----
 Query GADVNRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFT
 CCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCCCCHHCCCC
 250 260 270 280 290

1bd8A00 -----
 Query EDEL PYDDCVFGGQRRTL
 CCCCCCCCCCCCCCCCC
 310

Percentage Identity = 25.0.

>>> Alignment with 1s70B01:

1s70B01 -----
Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEIRLEPQEVP
CCCCCCCCHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
10 20 30 40 50 60

1s70B01 -----
Query RGSEPWKQQLTEDGDSFLHLAIIH--EEKALTMEVIRQVKGDLAFL-----NFQNN
CCCCCCCCCCCCCCCCHHHHHH--CCHHHHHHHHHHHCCCC-----CCCC
70 80 90 100

1s70B01 -----
Query CHHHHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCHHHHHHCCCC
DDGAVFLAACSSGDTEEVRLLRLERGADINYANVDGLTALHQACIDNDVDMVKFLVENGAN
120 130 140 150 160

1s70B01 -----
Query LQQTPLHLAVITNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTSQCTT
CCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCC
180 190 200 210 220

1s70B01 -----
Query PHLHSILKATNYNGHTCLHLASIHYGLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQN
CCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCCHHHHHHCCCC
240 250 260 270 280

1s70B01 -----
Query YDTESEFTEFTEDELPYDDCVFGGQRLTL
CCCCHHCCCCCCCCCCCCCCCCCCCCCCCC
300 310

Percentage Identity = 24.1.

>>> Alignment with 3c5rA00:

3c5rA00 -----
Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEIRLEPQEVP
CCCCCCCCHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
10 20 30 40 50 60

3c5rA00 -----
Query RGSEPWKQQLTEDGDSFLHLAIIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
CCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHH
70 80 90 100 110 120

3c5rA00 -----
Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTSQCTTPHLHSILKATN
CCCCHHHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCC
130 140 150 160 170 180

40 50 60 70 80 90

Supplementary Material

```

3c5rA00   CCCCCCHHHHHHHCCCHHHHHHHCCCCC-CCCCCCCCCHHHHHHHCCCHHHHHHHCC
          HAGWTPLHEACNHGHLKVVELLQHKALVN-TTGYQNDSPLHDAAKNGHVDIVKLLLSYG
          | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query    YNGHTCLHLASIHGYLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSLLKCG
          CCCCHHHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCC
          190      200      210      220      230      240

```

```

          100      110      120
3c5rA00   CCCCCCCCCCCCCHHHHCCCHHHHHHHCCC-----ASRNAVNIFGGLRPVDYTDDESMKSLLLLP-----
          | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query    ADVNRVTYQQGSPYQLT--WGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTEF
          CCCCHHHHHHHHHCCCHHHHH--HHCCCHHHHHHHCCCCCCCCCCCCCCCCCCCCHHCCCCC
          250      260      270      280      290

```

```

3c5rA00   -----
Query    TEDELPYDDCVFGGQRRLTL
          CCCCCCCCCCCCCCCCCCCC
          310

```

Percentage Identity = 33.9.

>>> Alignment with 1ycsB01:

```

1ycsB01  -----
Query   MFQAAERPQEWAEGPRDGALKERLLDDRHDSGLDSMKDEEYEQMVKELEIRLEPQEVP
          CCCCCCCCHHHHHCCCCCCCCHHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCCC
          10       20       30       40       50       60

```

```

1ycsB01  -----CHHHHHH
          -----PLALLLD
Query   RGSEPWKQQLTEDGDSFLHLATIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTP--LHL
          CCCCCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHH---HHH
          70       80       90       100      110

```

```

          10      20      30      40      50      60
1ycsB01  HHHHCCCHHHHHCCCCCCCCCCCCCHHHHHHHHHCCCCHHHHHHHHCCCCCCCCC
          SSLEGEFDLVQRRIYEVDDPSLPNDEGITALTHNAVCAGHTEIVKFLVQFGGVNVN-----
          | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query   AVITNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTSQSCTTPHLHSILK
          HHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCC
          120     130     140     150     160     170

```

```

          70      80      90      100      110      120
1ycsB01  CCCCCCCCCHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCCCCCCCCCHHHH
          AADSDGWTPLHCAASCNNVQCKFLVESGAAVFAMTYSDMQTAADKCEEMEEGYTQCSQF
          | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query   ATNYNGHTCLHLASIHGYLGIVELLVSLGADVNAQEPCNGRTALHLAVDL--QNPDLVSL
          CCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHC--CCHHHHHH
          180     190     200     210     220     230

```

```

          HHHHHHC-----
1ycsB01  LYGVQEK-----
          | |
Query   LLKGCGADNRVTYQQGSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEF
          HHHCCCCCCCCCCCCCCHHHHHHHCCCCCCCCCCCCCCCCCCCCHHCC
          240     250     260     270     280     290

```

```

1ycsB01  -----
Query   TEFTEDELPYDDCVFGGQRRLTL
          CCCCCCCCCCCCCCCCCCCC
          300      310

```

Percentage Identity = 22.7.

>>> Alignment with 1bi7B00:

```

1bi7B00  -----

```

```

Query      MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELQEIRLEPQEVP
          CCCCCCCCCHHHHHCCCCCCCCHHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCCCCC
          10       20       30       40       50       60

          10
1bi7B00  -----C-----CCCCCHHHHHH
          -----EPSADWLATAAA
          | |
          | |
Query   RGSEPWKQQLTEDGDSFLHLAIIEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
          CCCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHHHHHCCCCCCCCCCCCCHHHHHHH
          70       80       90       100      110      120

          20       30       40       50       60
1bi7B00  HCCCCHHHHHHCCCCCCCCCCCCCCCC-C-----CCCCCHHHHHHHCCCCCCCC
          RGRVEEVRAILLEAGANPNAPNSYGRRPPIQV-MMMGSARVAELLLLHGAEPNCAD---P
          | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query   TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSILKATN
          CCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCC
          130      140      150      160      170      180

          70       80       90       100      110      120
1bi7B00  ATLTRPVHDAREGFLDTLVVLHRAGARDV-DAWGRLPVDLAEELGHRDVARYLRAA-
          | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query   YNGHTCLHLASIHYGLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSLLLKCG
          CCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCC
          190      200      210      220      230      240

          C-----
1bi7B00  A-----
          | |
Query   ADVNRVTYQGYSPYQLTWGRPSTRIQQOLGOLTLENLQMLPESEDEESYDTESEFTEFTE
          CCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCCCCCHHHCCCC
          250      260      270      280      290      300

          -----
1bi7B00  -----
Query   DELPYDDCVFGGQRRTL
          CCCCCCCCCCCCCCCC
          310

```

Percentage Identity = 23.2.

>>> Alignment with 1n0qB00:

```

          10       20
1n0qB00  -----CCCCHHHHHHCCCCHHHHH
          -----NGRTPLHLAARNNGHLEVVKLL
          || |
Query   MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELQEIRLEPQEVP
          CCCCCCCCCHHHHHCCCCCCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCCCCC
          10       20       30       40       50       60

          30       40       50       60       70
1n0qB00  HHCCCCCCCCCCCCCHHHHHHCCC---HHHHHHHHCCCCCCCCCCCCCHHHHHH
          LEAGADVNAKDKNRTPLHLAARNNGH---LEVVKLLLEAGADVNAKDKNRTPLHLAAR
          | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
Query   RGSEPWKQQLTEDGDSFLHLAIIEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
          CCCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHHHHHCCCCCCCCCCCCCHHHHHHH
          70       80       90       100      110      120

          80       90
1n0qB00  CCCHHHHHHHHCCCC----NGHLEVVKLLLEAGAY-----
          | | | |
Query   TNQPEIAEALLGAGCDPELRD
          CCCHHHHHHHHCCCCCCCC
          130      140

```

Percentage Identity = 23.7.

>>> Alignment with 1s70B02:

```

          -----
1s70B02  -----
Query   MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELQEIRLEPQEVP

```

CCCCCCCCHHHHCCCCCCCCHHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
 10 20 30 40 50 60

1s70B02 -----CCCHHHHHH
 |
 Query RGSEPWKQQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
 CCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCCCCCCCCCCCCHHHHHHHH
 70 80 90 100 110 120

20 30 40 50 60
 HHHHHHHHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCCCCCCCC----
 1s70B02 EERIRMLRDARQWLNSGHINDVRHAKSGGTALHVAAAKGYTEVLKLLIQARYDVN----
 | | | | | |
 Query TNQPEIAEALLGAGCDPEL---RDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSIL
 CCCCHHHHHHHHHCCCCCCC---CCCCCCCCHHHHHHCCCHHHHHHHHHCCCCCCCC
 130 140 150 160 170

70 80 90 100 110 120
 -CCCCCCCCHHHHHHCCCHHHHHHHCCCCCCCC-CCCCCCCCCCCCCHHHHHHHHH
 1s70B02 -IKDYDGWTPLHAAAHWGKEEACRILVENLCDMEAV-NKVQTAFDVADEDILGYLEELQ
 | | | | | |
 Query KATNYNGHTCLHLASIHYGLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSLL
 CCCCHHHHHHHHHCCCCCCCCHHHHHHCCCHHHHHHHCCCCCCCCCCCCHHHHHHCCCCHHHHHH
 180 190 200 210 220 230

HHCCCCC-----
 1s70B02 KKQNLLH-----
 |
 Query LKCGADVNRTYQGYSPYQLTWGRPSTRIQQQQLGQLTLENLQMLPESEDEESYDTESEFT
 HHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCCHHCCC
 240 250 260 270 280 290

1s70B02 -----
 Query EFTEDELPYDDCVFGGQRITL
 CCCCCCCCCCCCCCCCCCCCC
 300 310

Percentage Identity = 20.9.

>>> Alignment with 1sw6A00:

10 20
 -----CCEEECCC-----CCCCCCCCCCC-----CCCE
 1sw6A00 -----GPIITFT-----HDLTSDFLSSP-----LKIM
 | | | | | |
 Query MFQAAERPQEWAEGP---RDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEIRLEPQ
 CCCCHHHHHHHCCC---CCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCC
 10 20 30 40 50

30 40 50 60 70 80
 ECCCCCCCCCHHHHHHHHHHHHHHCC---HHHHHHHHCCCCCCCCCCCCCCCCHH
 1sw6A00 KALPSPVVNDNEQKMKLEAFLQRLLFS---FDSLQEVNDAFPNTQLNLNIPVDEHGNTPL
 | | | | | |
 Query EVPRGSEPWKQQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDL-AFLNFQ-NNLQQTPL
 CCCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCCCC-CCCC-CCCCHHH
 60 70 80 90 100 110

90 100 110 120 130 140
 HHHHHCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCHHHHHH
 1sw6A00 HWLTSIANLELVKHLVKHGSNRLYGDNMGESCLVKAVKSVNNYDSGTFEALLDYLYPCLI
 | | | | | |
 Query HLAVITNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSI
 HHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCHHHHHHCCCHHHHHHHCCCCCCCC
 120 130 140 150 160 170

150 160 170 180 190
 EECCCCCCCCHHHHHHCCCCCCCCHHHHHHHHHHHHHHCCCCEEECC---HHHHHCC
 1sw6A00 LEDSMNRTILHHIIITSGMTGCSAAKYLDILMGWIVKKQNRPIQSGD---SILENLD
 | | | | | |
 Query LKATNYNGHTCLHLASIH-----GYLGIVELLVSLG
 CCCCCCCCCCHHHHHHHCC---CCCCCCCCCCCCCCCCCCCCCCCCHHHHHCC
 180 190 200

200 210 220 230 240 250
 HHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCHHHCC--

```

1sw6A00  LKWIIANMLNAQDSNGDTCLNIAARLGNISIVDALLDYADPFIAKSGLRPVDFGAG--
| | | | | | | | | | | | | | | |
Query   ----ADVNAQEPCNGRTALHLAVDLQNPDLVSLLKGADVNRTVYQGYSPYQLTWGRP
-----CCCCCCCCCCCHHHHHHHHHCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCC
210      220      230      240      250      260

```

```

1sw6A00 -----
Query  STRIQQQLGQLTLENLQMLPES EDESYDTESEFTEFTEDPYDDCVFGGQR LTL
CHHHHHHHHHCCCCCCCCCCCCCHHCCCCCCCCCCCCCCCCCCCCCCCC
270      280      290      300      310

```

Percentage Identity = 17.3.

>>> Alignment with 3c5rA00:

```

10          20
-----CCCCCCCCCHHHHHHHHHCCHHHHHHHH
3c5rA00 -----PFTNHRGETLLHIASIKGDIPSVEYL
Query   MFQAAERPQEWAEGPRDGLKKERLLDDRHDGSDSMKDEEYEQMVKELQEIRLE-PQEVE
CCCCCCCCCHHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHCCCC
10          20      30      40      50

```

```

30          40          50          60          70          80
HHCCCCCC---CCCCCCCCHHHHHHHCC---HHHHHHHHCCCCCCCCCCCCCHHHHHH
3c5rA00 LQNGDPNVK---DHAGWTPLHEACNHGH---LKVVELLQHKALVNTGYQNDSP LHDA
Query   PRGSEPWKQLTEDGDSFLHLAIIEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAV
CCCCCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCCHHHHHH
70          80          90          100         110

```

```

90          100         110         120
HCCCCHHHHHHHHCCCCCCCCCCCCCHHHHHCCCCHHHHHHCC
3c5rA00 KNGHV DIVKLLL SYGASR NAVNIFGLRPVDY TDDESMKS LLLP
Query   ITNQPEIAEALLGAGCD-----
HCCCCHHHHHHHHCCCCHHHHHHCC
130

```

Percentage Identity = 13.7.

>>> Alignment with 1n0rA00:

```

10          20          30          40          50
---CCCCHHHHHHHC---HHHHHHHHC---CCCCCCCCCCCCHHHHHHCCHHHHHH
1n0rA00 ---NG RTPPLA ARNGH---LEV VKL LEAG---ADVNAKDKN GRTP LHL AAR NGH LEV VKL
Query   MFQAAERPQEWAEGPRDGLKKERLLDDRHDGSDSMKDEEYEQMVKELQEIRLE PQEVEP
CCCCCCCCCHHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHCCCCCCCC
10          20      30      40      50      60

```

```

60          70          80          90          100         110
HHCCCCCCCCCCCCCCCHHHHHHHCC---HHHHHHHHCCCCCCCCCCCCCHHHHHH
1n0rA00 LEAGADVN AKDKN GRTP LHL AAR NGH---LEV VKL LEAG ADVN AKDKN GRTP LHL AAR
Query   RG SEP WK QQL TED GDS F LHL AI IEEK ALT MEV IRQ VK GDL AFL NF QN-----
CCCCCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCC-----CC
70          80          90          100

```

```

120
CCCCHHHHHHHHHHCC
1n0rA00 NGH LEV VKL LEAGAY
Query   -----

```

Percentage Identity = 12.7.

>>> Alignment with 2bkgA00:

```

10          20          30          40          50
CHHHHHHHHHHHCCHHHHHHHHCCCCCCCCCCCCHHHHHHCC---HHHHHHHH
2bkgA00 SDLGKKL LEA ARAG QD DE VRIL MANG ADVN AE DT YGD TPL HL AAR VGH---LEIVE VL LK
Query   -----MFQAAERPQEWAEGPRDGLKKERLLDDR
-----CCCCCCCCCHHHHHCCCCCCCCHHHHHHHH
10          20

```

	120	130	140	150
2bkgA00	-HHHHHHHHHC-----CCCCCCCCCCCCHHHHHHCCCCCHHHHCC	-LEIVEVLLKYGADVNAQDKFGKTAFDISIDNGN-DLAEIL-		
Query	TMEVIRQVKGDLAFLNFQPNNLQQ-----	HHHHHHHHHHHCCCCCCCCCCCC		
	100	110		

Percentage Identity = 9.7.

```
>>> Alignment with 1s70B02:
```

	60	70	80	90	100	110
1s70B02	HHCCCCCCCCCCCCCCC	HHHHHHHHHHHCCCC	HHHHHHHHHHHCCCC	CCCCCCCCCCCCCCCC	CCCCCCCCCCCCCCCC	CCCCCCCCCCCCCCCC
	LIQARYDVNIKYDGVTP	PLHAAAHWGK	EEACRILVENLC	CDMEA	VNKVGQTAFDVAD	
Query	PRGSEPWKQLTDEGDSFLHLAI	IHEEKALTMEVIRQVKGDGLAFLN	FQNNLQQ	-----	-----	-----
	CCCCCCCCCCCCCCCCCCC	HHHHHHHHHHHCCCC	HHHHHHHHHHHCCCC	CCCCCCCCCCCCCCCC	CCCCCCCCCCCCCCCC	-----
	70	80	90	100	110	

1s70B02	120
Query	CHHHHHHHHHHHCCCC EDILGYLEELQKKQNLH ----- -----

Percentage Identity = 13.2.

```
>>> Alignment with lycsB01:
```

	60	70	80	90	100	
lycsb01	HHHHHHHHCCCCCCCCCCCCHHHHHHHHCCC-----HHHHHHHHCCCCCCCCCCCCCCCCHH					
	VKFLVQFGVNVAASDGTWPLHCAASCNN-----QVQCKFLVESGAVFAMTYSDMQTAA					
Query	QEVPGRGSEPWKQQLTEDGDSFLHLAIIHEEKALTMEVIRQVKQGDLAFLNQFQNN-LQQTPT-					
	CCCCCCCCCCCCCCCCCCCCHHHHHHHHHHHHHHCCCCHHHHHHHHHHHHCCCCCCCCCCCC-CCCHH-					
	60	70	80	90	100	110

	110	120
lycsB01	HHCCCCCCCCCCCCHHHHHHHHHC DKCEEMEEGYTQCSQFLYGVQEK	
Query	----- -----	

Percentage Identity = 13.3.

```
>>> Alignment with lawcB00:
```

	10	20	30	40	50
lawcB00	CHHHHHHHHHHHCHHHHHHHHHCCCCCCCC--	CCHHHHHHHHHC--	-HHHHHHHH		
	DLGKKLLEAARAGQDDEVRILMANGAPFTTDWL--	GTSPHLAAQYGH--	FSTTEVLL		
Query	<pre> -----MFQAAERPQEWA -----CCCCCCCCHHHHCCCCCCCCHHHHHHHH 10 20 </pre>				

```

      60       70       80       90       100      110
CCCCCCCCCCCHHHHHHHCCHHHHHHCCCCCCCCCCCCCHHHHHHCC --
lawcB00 RAGVSARDARTKVDRTPHLMAASEGHANIVEVLLKGADVNAKDMLKMTALHWATEHNH --
| | | | |
Query  RHDSGLDSMKDEEYEQMVKELEIRLEPQEVPGRGSEPWKQQLTEDGDSFLHLAIIHEEKAH
HCCCCCCCCCCCCCHHHHHHHCCCCCCCCCCCCCCCCCCCCCCCCHHHHHHCCCHH
        40       50       60       70       80

```

```

      120      130      140      150
--HHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHCC --
lawcB00 --QEVVELLIKYGAADVHTQSFKCTAFDISIDNGNEDLAEILQ
| | | |
Query  LTMEVIRQVKGDLAFLNFQN-----
HHHHHHHHHHCCCCCCCCC-----
        100

```

Percentage Identity = 9.8.

>>> Alignment with lympA00:

```

      10       20       30       40       50
CCCCCCCCCCCCCHHHHHHHCCCCHHHHCCCCCCCCCCCCCHHHHHHCC --
lympA00 RATLDARMHDGTTPLILAARLALEGMLEDLINSHADVNAVDDLGSALHWAAVNN --
| |
Query  -----MFQAAERPQEWAEGPRDGL
-----CCCCCCCCHHHHCCCCCCC
        10       20

```

```

      60       70       80       90       100      110
HHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHCCCCCCCCCCCCCHHHH
lympA00 VDAAVVLLNGANKDMQNNKEETPLFLAAREGSYETAKVLLDHFANRDITDHMDRLPRDI
| |
Query  KKERLDDDRHDSGLDSMKDEEYEQMVKELOEIRLEPQEVPGRGSEPWKQQLTEDGDSFLHL
HHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCCCCCCCCCCCCCCCCCCHHHH
        30       40       50       60       70       80

```

```

      120      130
HHHCCC---HHHHHHHC--
lympA00 AQERMH---HDIVRLLD--
| |
Query  AIIHEEKALTMEVIRQVKGD
HHHCCCCHHHHHHHHHHHHH
        90       100

```

Percentage Identity = 6.9.

>>> Alignment with 1s70B01:

```

      10       20       30       40       50
CCCCHHHHHHHHHHHHHHCCCCCCCCCCCCCCCCCHHHHHHHHHHHHCC --HHHHHH
1s70B01 MKMADAKQRNEQLKRWIGSETDLEPPVVKRKTKVFKFDGAVFLAACSSGD --TEEVL
| |
Query  -----MFQAAER-----PQEWAEGPRDGLKKERL
-----CCCCCCC-----CHHHHHCCCCCCCCHHHHH
        10       20

```

```

      70       80       90       100      110
HHHHC-CCCCCCCCCCCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCHHHHHHCC
1s70B01 LLERG-ADINYANVDGLTALHQACIDDNVDMVKFLVENGANINQPDNEGWIPLHAAASCG
| |
Query  LDDDRHDSGLDSMKDEEYEQMVKELEIRLEPQEVPGRGSEPWKQQLTEDGDSFLHLAII --
HHHHCCCCCCCCCCCCCHHHHHHHCCCCCCCCCCCCCCCCCCCCCCCCCHHHHHH --
        30       40       50       60       70       80

```

```

      120      130      140      150      160
CHHHHHHHHCCCCCCCCCCCCCHHHHHCCCHHHHHHHHHHHHCC --
1s70B01 YLDIAEYLISQGAHVGVAVNSEGDTPLDIAEEFAMEELLQNEVNRQ
| |
Query  -----

```

Percentage Identity = 4.9.

>>> Alignment with 2pw8I00:

```

-----2pw8I00 -----
| |
Query  MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKELEIRLEPQEVP

```

CCCCCCCCHHHHCCCCCCCCHHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
 10 20 30 40 50 60

2pw8I00 -----
Query RGSEPWKQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
 CCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCCCCCCCCCCCCHHHHHHHH
 70 80 90 100 110 120

2pw8I00 -----
Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSILKATN
 CCCCHHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCCCCCCCCCCCC
 130 140 150 160 170 180

2pw8I00 -----
Query YNGHTCLHLASIHYGLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSLLKCG
 CCCCHHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHHHCCCCHHHHHHHH
 190 200 210 220 230 240

2pw8I00 -----
Query ADVNRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTEFTE
 CCCCCCCCCCCCCHHHHHHHCCCHHHHHHHCCCCCCCCCCCCCCCCCCCCCHHHCCCC
 250 260 270 280 290 300

10 20 30 40 50
 --CCCCCCCCCCEEECCCCCCCCCCCCCEECCCCCCCCCEECCCCCCCCCCCC
 2pw8I00 --LTYTDCTESQNLCLCEGSN-CGQGNKCILG-DGEKNQCVTGEGTKPKPQSGDFEEIP-
 | | | | | | | |
Query DELPYDDCVFGQRQLTL-----
 CCCCCCCCCCCCCCCC-----
 310

2pw8I00 CCC
 ELQ
Query ---

Percentage Identity = 13.1.

>>> Alignment with 1bi7B00:

1bi7B00 -----
Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDGSDMSMKDEEYEQMVKEQIRLEPQEVP
 CCCCCCCCCCHHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
 10 20 30 40 50 60

10 20 30 40
 -----CCCCCHHHHHHHCC---HHHHHHHHCCCCCCCCCCCCCCCCCCCC
1bi7B00 -----EPSADWLATAAARGR---VEEVRALLEAGANPNAPNSYGRRIPIQVMM
Query RGSEPWKQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNFQNN-----
 CCCCCCCCCCCCCCCCCHHHHHHHCCCHHHHHHHHHCCCCCCCCCCCC
 70 80 90 100

50 60 70 80 90 100
 CCCCCCCCCCCCCCCCCCCCCHHHHHHCCCHHHHHHHHHCCCCCCCCCCCC
1bi7B00 GSARVAELLLLHGAEPNCADPATLTRPVHDAAREGFLDTLVVLHRAGARLDVRDAWGRLP
Query -----

110 120
 HHHHHHHCCHHHHHHCCCC

1bi7B00 VDLAEELGHRDVARYLRAAA

Query -----

Percentage Identity = 6.4.

>>> Alignment with 1gupA02:

1gupA02 -----

Query MFQAAERPQEWAEGPRDGLKKERLLDRHDSGLDSMKDEEYEQMVKELQEIRLEPQEVP
CCCCCCCCHHHHHCCCCCHHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCC
10 20 30 40 50 60

1gupA02 -----

Query RGSEPWKQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
CCCCCCCCCCCCCCCCHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHH
70 80 90 100 110 120

1gupA02 -----

Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASVGVLTQSCTTPHLHSILKATN
CCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCC
130 140 150 160 170 180

1gupA02 -----

Query YNGHTCLHLASIHYGLGIVELLVSLGADVNAQEPCNGRTALHLAVDLQNPDLVSLLKCG
CCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCC
190 200 210 220 230 240

1gupA02 -----

Query ADVNRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTEFTE
CCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCCCCCCHHCCCC
250 260 270 280 290 300

1gupA02 10 20 30 40 50
-CCCCCCCCCCCCCCCCCCCCCCCCCEEECCCCCCCCCCCCCCCCCCCC
-VLPFAHDPCFLCAGNVRVTGDKNPDYTGTVFTNDFAALMSDTPDAPESHDPLMRCQSA
| | | | |
Query DELP-YD-DCVF--GGQRRTL-----
CCCC-CC-CCCC--CCCCCCC-----
310

1gupA02 70 80 90 100 110
CEEEEEEECCCCCCCCCCCCHHHHHHHHHHHHHHHHHHCCCCCEECCCCCCCC
1gupA02 RGTSRVICFSPDHSKTLPELSVAALTEIVKTWQEQTAELGKTYPWVQFENKGAAAGCSN

Query -----

1gupA02 130
CCCEEEEEEECCC
1gupA02 PHPGGQIWANSFL

Query -----

Percentage Identity = 6.1.

>>> Alignment with 1wdyA00:

1wdyA00 10 20 30 40 50 60
CHHHHHHHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHCCCCHHHHHH
1wdyA00 AAVEDNHLLIKAVQNEDVDLVQQLEGGANVNPFQEEGGWTPLHNAVQMSREDIVELLRL

Query -----

1wdyA00 70 80 90 100 110
 CCCCCCCCCCCCCCHHHHHHHCCC--HHHHHHHHHHC-CCCCCCCCCCCCCCHHHHHHHHCC
 HGADPVLRKNGATPFLLAAIAGS--VKLLKLFLSK-GADVNECDFYGFTAFMEAAYGK
 | | |
 Query -----MFQA--AERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKEIQLQEIR
 -----CCCC--CCCCHHHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCHHHHHHHHHHHCC
 10 20 30 40 50

1wdyA00 120 130 140 150 160 170
 HHHHHHHHHHHCCCCCCCCCCCCCHHHHHCCCCCCCCHHHHHHHHHCCCCCCCCCCCC
 VKALKFLYKRGANVNLRKTKEDQERLRKGATALMDAEKGHVEVLKILLDEMGADVNA
 Query -----LEPQEVPGRGSEPWKQQLTED-----
 CCCCCCCCCCCCCCCCCCCCC
 60 70

1wdyA00 180 190 200 210 220 230
 CCCCCCHHHHHHHCCCCCCCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHH
 CDNMGRNALIHALLSSDDSDVEAITHLLDHGADVNRGERGKTPLILAVEKKHLGLVQR
 Query -----

1wdyA00 240 250 260 270 280
 HHHCCCCCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCC
 LLEQEHEIEINDTSDGKTALLLAVELKLKKIAELLCKRGASTDCGDLV
 Query -----

Percentage Identity = 1.4.

>>> Alignment with 1ubdC04:

1ubdC04 -----

Query MFQAAERPQEWAEGPRDGLKKERLLDDRHDSGLDSMKDEEYEQMVKEIQLQERLEPQEVP
 CCCCCCCCCCCCCCCCCCHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCCCCCCCCC
 10 20 30 40 50 60

1ubdC04 -----

Query RGSEPWKQQLTEDGDSFLHLAIHEEKALTMEVIRQVKGDLAFLNFQNNLQQTPLHLAVI
 CCCCCCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCCHHHHHH
 70 80 90 100 110 120

1ubdC04 -----

Query TNQPEIAEALLGAGCDPELRDFRGNTPLHLACEQGCLASGVVLTQSCTTPHLHSILKATN
 CCCHHHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCCCCCCCCCCCC
 130 140 150 160 170 180

1ubdC04 -----

Query YNGHTCLHLASIHYGLGIVELLVSLGADVNAQEPNGRTALHLAVDLQNPDLVSLLLKCG
 CCCCHHHHHHHCCCCHHHHHHCCCCCCCCCCCCCHHHHHHHCCCCHHHHHHHHCC
 190 200 210 220 230 240

1ubdC04 -----

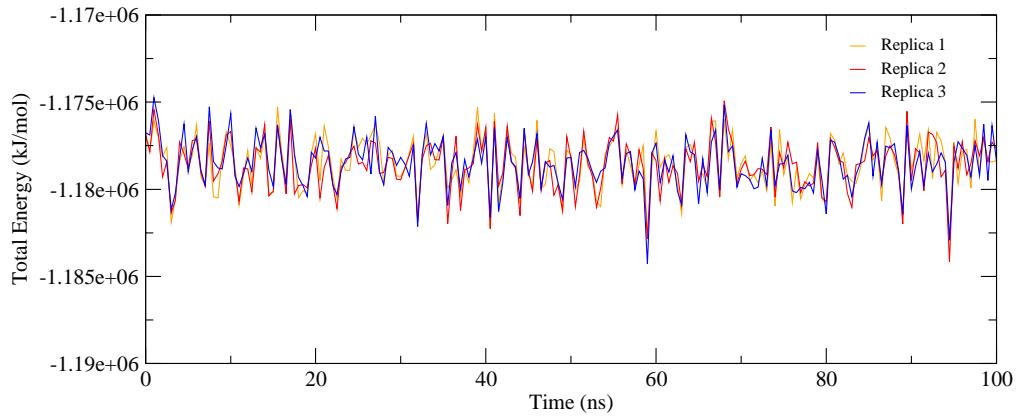
Query ADVNRVTYQGYSPYQLTWGRPSTRIQQQLGQLTLENLQMLPESEDEESYDTESEFTEFTE
 CCCCCCCCCCCCCHHHHHHCCCCHHHHHHCCCCCCCCCCCCCCCCCCCCHHCCCC
 250 260 270 280 290 300

```
1ubdC04 -CCCCC-CCCCCCCCCCCCCCCCHHHHHHHC  
          | | | | |  
          DRPYV-CPFDGCNKFAQSTNLKSHILTHA  
Query  DELPYDDCVFGG-----QRLTL-----  
          CCCCCCCCCCCC-----CCCCC-----  
          310
```

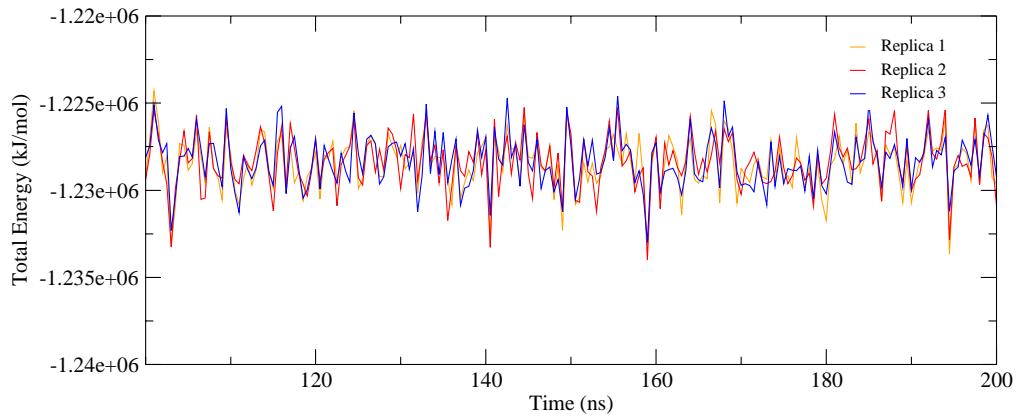
Percentage Identity = 24.1.

Supplementary Figure 3. pDomThreader prediction results identifying 46 possible structural templates with reliable secondary structural similarity.

A

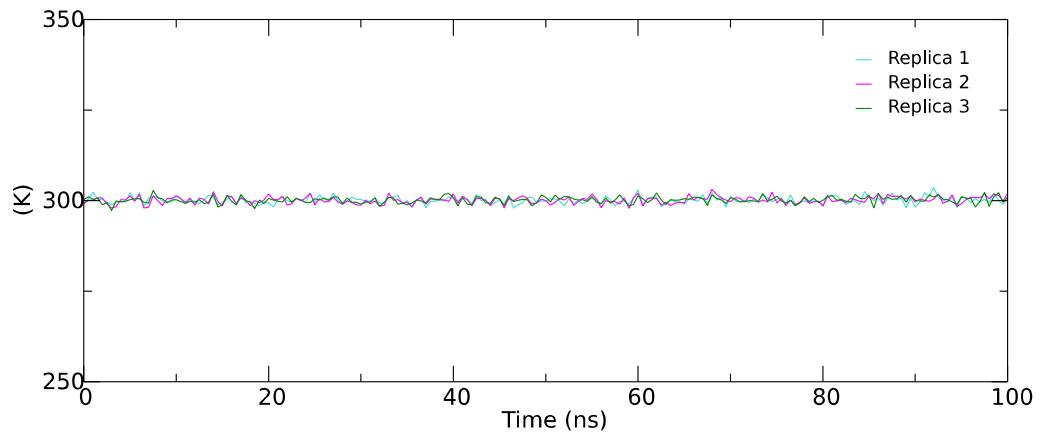


B

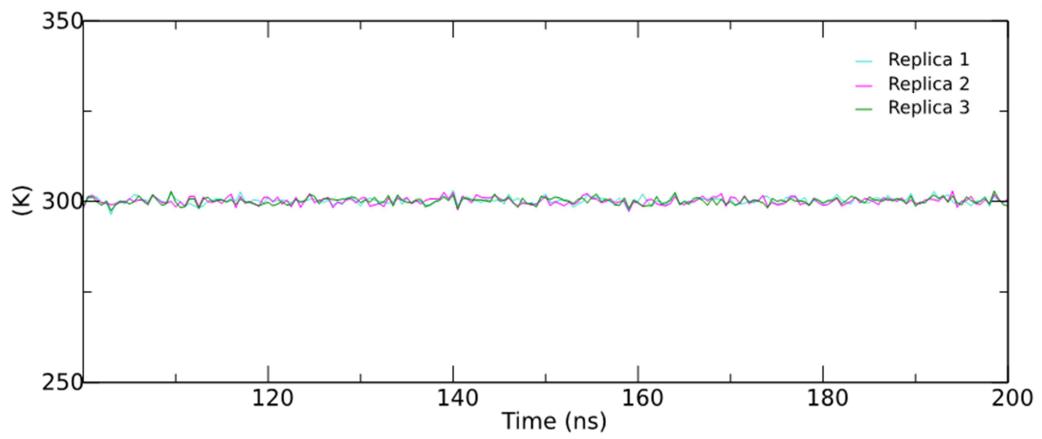


Supplementary Figure 4. The total energy variation of the three system replicas for the initial (A) and final (B) 100ns simulation.

A

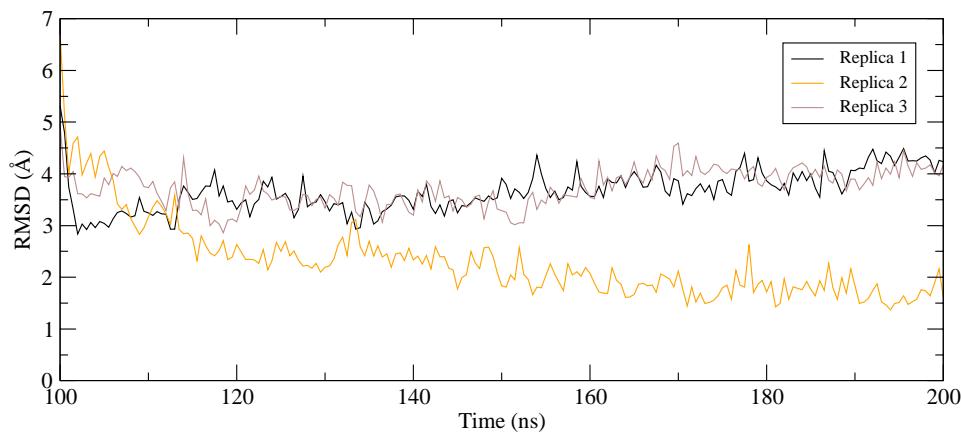


B

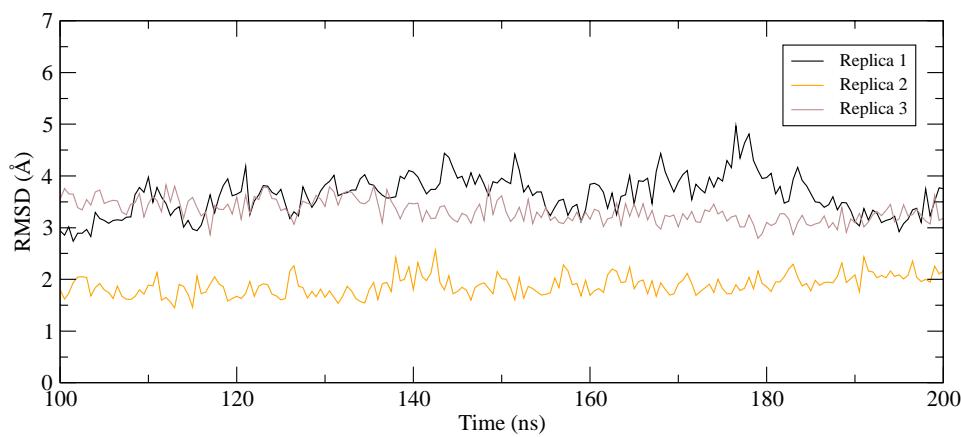


Supplementary Figure 5. Temperature of the three system replicas for the initial 100 ns (A) and the final 100ns (B).

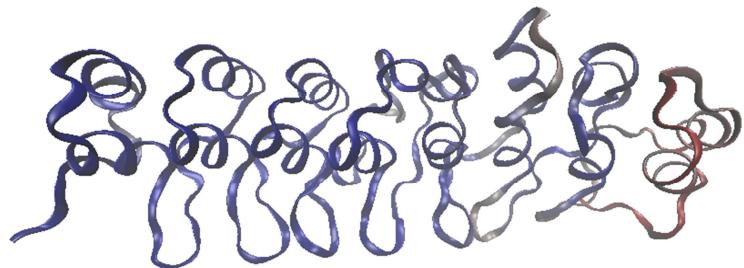
A



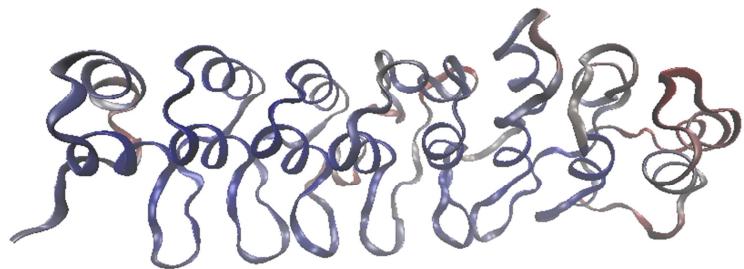
B



Supplementary Figure 6. RMSD of the complexed I κ B α /NF- κ B protein backbone against the average structure of the three system replicas for the initial 100 ns (A) and the final 100 ns (B).



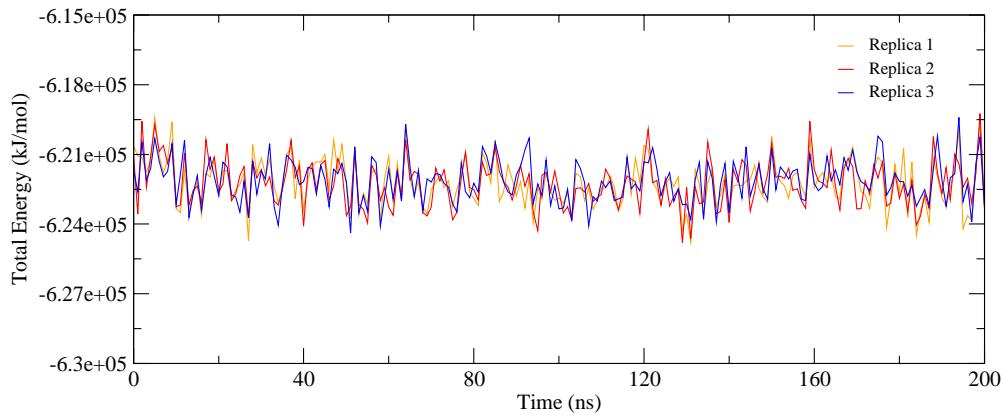
(RMSF after 100ns)



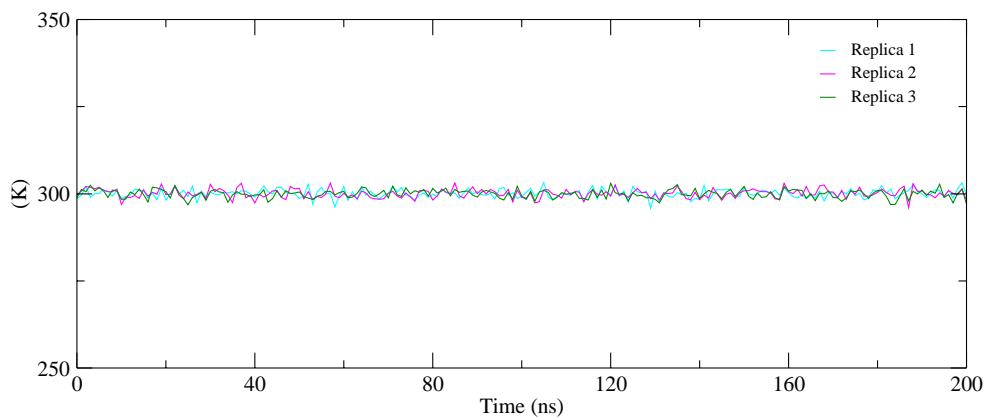
(RMSF after 200ns)

Supplementary Figure 7. Root mean square fluctuations of amino acid residues mapped onto C α -backbone atoms of I κ B α (from blue to red) after 100 ns (top) and 200 ns (bottom).

A



B



Supplementary Figure 8. (A) The total energy variation of the three system replicas for the free IkB α simulations. (B) Temperature of the three system replicas for the free IkB α simulations.