

Structural Bioinformatics Tools at PDBj

Daron M. Standley

Today's topics

- Searching PDBj
- Making multiple sequence alignments
- Predicting protein function from sequence

Searching PDBj

- Sequence Navigator
- Structure Navigator

Making multiple sequence alignments

- MAFFTash

Predicting protein function from sequence

- SFAS
- Spanner
- PDBj Quat and PDBj Het
- SeSAW

Sequence Navigator

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To Enter Navigator, Input a PDB ID and Chain ID

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Clustering Options

No Clustering Cluster by E-value 10^{\wedge}

[+](#) (more clusters) [-](#) (fewer clusters)

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type a PDB ID here

Clustering Options

No Clustering Cluster by E-value 10^{\wedge}

(more clusters) (fewer clusters)

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To Enter Navigator, Input a PDB ID **2qfb** **and Chain ID** **B**

OR Input an AA Sequence

Clustering Options
 No Clustering Cluster by E-value 10^{\wedge}

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(fewer clusters)

Find All Homologs
Clear Form

type a chain ID here (red text)
type a PDB ID here (red text)

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OR Input an AA Sequence

type a chain ID here 
type a PDB ID here 
paste a sequence here 

Clustering Options
 No Clustering Cluster by E-value 10^{\wedge}

 (more clusters)
 (fewer clusters)

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Results (1-15) / 15

Sequence Navigator results

2QFDB Exact Matches: 2QFDJ 2QFBF 2QFDF 2QFDD 2QFBB 2QFBH 2QFBJ 2QFDH 2QFBG 2QFBD 2QFDC 2QFDA 2QFDG 2

Seq. Identity: 30% Seq. Positives: 50% E-value: 2e-11 Score: 63 Compound: INTERFERON-INDUCED HELICASE CDOMAIN-CONTAINING

New Search [2RQBA] Structural Superposition

2QFDB 7 101 LCRKCKALACYTADVRVIEECHYTVLGDAFKECFVSRPHPK-PKQFSSFEKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIKIESFVVEDIATGVQTLYSKW
2RQBA 16 101 LCKNCSVLA CGSEDIHVIEKMHVNMTPEFKELYIVRENKALQKKCADYQINGEIIC---KCGQAWGTMMVHKGLDLPCLKIRNFVVVFKNNSTKKQYKKW

Seq. Identity: 30% Seq. Positives: 50% E-value: 2e-11 Score: 63 Compound: INTERFERON-INDUCED HELICASE CDOMAIN-CONTAINING

New Search [3GA3A] Structural Superposition

2QFDB 7 101 LCRKCKALACYTADVRVIEECHYTVLGDAFKECFVSRPHPK-PKQFSSFEKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIKIESFVVEDIATGVQTLYSKW
3GA3A 14 101 LCKNCSVLA CGSEDIHVIEKMHVNMTPEFKELYIVRENKALQKKCADYQINGEIIC---KCGQAWGTMMVHKGLDLPCLKIRNFVVVFKNNSTKKQYKKW

Seq. Identity: 29% Seq. Positives: 48% E-value: 1e-08 Score: 54 Compound: ATP-DEPENDENT RNA HELICASEDHX58 5'-R(*GP*CP*GP*CP*GP*CP*(

New Search [3EQTB] Structural Superposition

2QFDB 2 118 ENKKLLCRKCKALACYTADVRVIEECHYTVLGDAFKECF-VSR-PHPKPKQFSSFEKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIKIESFVVEDIATGVQTLYSK
3EQTB 7 118 EHVOQLLCINCMVAVGHGSDLRKVEGTHHVNVPNSNYYNSRDPVVINKVFKDWKPGGVISC--RNCGEVWGLQMIYKSVKLVLKVRSMLETPQGRIQA--KK
3EQTB Exact Matches: 3EQTA

Seq. Identity: 29% Seq. Positives: 48% E-value: 1e-08 Score: 54 Compound: ATP-DEPENDENT RNA HELICASEDHX58

New Search [2RQAA] Structural Superposition

2QFDB 2 118 ENKKLLCRKCKALACYTADVRVIEECHYTVLGDAFKECF-VSR-PHPKPKQFSSFEKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIKIESFVVEDIATGVQTLYSK
2RQAA 9 118 EHVOQLLCINCMVAVGHGSDLRKVEGTHHVNVPNSNYYNSRDPVVINKVFKDWKPGGVISC--RNCGEVWGLQMIYKSVKLVLKVRSMLETPQGRIQA--KK

Seq. Identity: 29% Seq. Positives: 47% E-value: 1e-08 Score: 54 Compound: PROBABLE ATP-DEPENDENT RNAHELICASE DHX58

New Search [2W4RA] Structural Superposition

2QFDB 2 117 ENKKLLCRKCKALACYTADVRVIEECHYTVLGDAFKECF-VSRPHPKPKQFSSFEKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIKIESFVVEDIATGVQTLYSK
2W4RA 7 117 EHVOQLLCINCMVAVGHGSDLRKVEGTHHVNVPNSNYYNSRDPVVINKVFKDWKPGGVISC--RNCGEVWGLQMIYKSVKLVLKVRSMLETPQGRIQA--KK

Seq. Identity: 28% Seq. Positives: 47% E-value: 5e-08 Score: 52 Compound: PROBABLE ATP-DEPENDENT RNAHELICASE DHX58

New Search [2W4RD] Structural Superposition

2QFDB 2 117 ENKKLLCRKCKALACYTADVRVIEECHYTVLGDAFKECF-VSRPHPKPKQFSSFEKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIKIESFVVEDIATGVQTLYSK
2W4RD 7 117 EHVOQLLCINCMVAVGHGSDLRKVEGTHHVNVPNSNYYNSRDPVVINKVFKDWKPGGVISC--RNCGEVWGLQMIYKSVKLVLKVRSMLETPQGRIQA--KK

Seq. Identity: 28% Seq. Positives: 47% E-value: 9e-08 Score: 51 Compound: PROBABLE ATP-DEPENDENT RNAHELICASE DHX58

New Search [2W4RC] Structural Superposition

2QFDB 2 117 ENKKLLCRKCKALACYTADVRVIEECHYTVLGDAFKECF-VSRPHPKPKQFSSFEKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIKIESFVVEDIATGVQTLYSK
2W4RC 8 117 EHVOQLLCINCMVAVGHGSDLRKVEGTHHVNVPNSNYYNSRDPVVINKVFKDWKPGGVISC--RNCGEVWGLQMIYKSVKLVLKVRSMLETPQGRIQA--KK

Seq. Identity: 27% Seq. Positives: 46% E-value: 6e-07 Score: 48 Compound: PROBABLE ATP-DEPENDENT RNAHELICASE DHX58

New Search [2W4RB] Structural Superposition

2QFDB 2 117 ENKKLLCRKCKALACYTADVRVIEECHYTVLGDAFKECF-VSRPHPKPKQFSSFEKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIKIESFVVEDIATGVQTLYSK
2W4RB 7 117 EHVOQLLCINCMVAVGHGSDLRKVEGTHHVNVPNSNYYNSRDPVVINKVFKDWKPGGVISC--RNCGEVWGLQMIYKSVKLVLKVRSMLETPQGRIQA--KK

Seq. Identity: 26% Seq. Positives: 39% E-value: 0.80 Score: 28 Compound: BETA-2-MICROGLOBULIN

New Search [3CIQH] Structural Superposition

2QFDB 36 71 FKECFVSRPHPKPKQFSSFEKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIKIESFVVEDIATGVQTLYSK
3CIQH 23 71 FLNCYVSGFHPSDIEVDLLKNIKEVHSDLSFSKDWFSYLLYYTEPTPEKDEYACRVNHVTLSQPKIVKW

Seq. Identity: 34% Seq. Positives: 53% E-value: 1.8 Score: 27 Compound: MYOSIN

New Search [2MYSA] Structural Superposition

2QFDB 55 32 EKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIK
2MYSA 724 32 ERRESIFCIQYNVRSFMNVHWPWMLFFIPLLK

Seq. Identity: 34% Seq. Positives: 53% E-value: 1.8 Score: 27 Compound: SKELETAL MUSCLE MYOSIN IISKELETAL MUSCLE MYOSIN II REGULAT

New Search [1O1EG] Structural Superposition

2QFDB 55 32 EKRAKIFCARQNCSDHWGIHVVKYKTFEIPVIK
1O1EG 764 32 ERRESIFCIQYNVRSFMNVHWPWMLFFIPLLK
1O1EG Exact Matches:

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Chain ID: (required)

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PDB ID: or **PDB File:** no file selected

Chain ID: (required)

return e-mail (address:) return web

type a chain ID here (arrow points to the Chain ID input field)

type a PDB ID here (arrow points to the PDB ID input field)

structure-based queries take a lot of time
so please type your email address here!

Structure Navigator

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Templ	NER(4)	%NER(4)	%Seq ID	RMSD	Score	Domain	Details
2qfbB	121	100	100	0.222	147		alignment
2qfdG	118	98	100	0.740	140		alignment
2qfdE	118	98	100	0.696	139		alignment
2qfbG	117	97	100	0.762	139		alignment
2qfbE	117	97	100	0.772	139		alignment
2qfdD	117	97	100	0.797	139		alignment
2qfdJ	117	97	100	0.742	138		alignment
2qfdA	117	97	100	0.897	137		alignment
2qfbD	117	97	100	0.824	137		alignment
2qfdI	116	96	100	0.971	136		alignment
2qfdC	116	96	100	0.916	136		alignment
2qfdF	115	96	98	0.899	136		alignment
2qfbA	116	96	100	0.957	136		alignment
2qfdH	116	96	100	0.994	136		alignment
2qfbJ	117	97	100	0.807	136		alignment
2qfbC	116	96	100	0.924	135		alignment
2qfbF	115	96	98	0.927	134		alignment
2qfbI	116	96	100	0.965	133		alignment
2qfbH	113	93	100	1.158	132		alignment
2w4rA	103	90	24	1.413	111		alignment
2w4rC	101	89	24	1.527	106		alignment
3ga3A	103	87	26	1.609	105		alignment
3eqtB	103	89	23	1.491	101		alignment
2rmjA	89	77	93	2.266	100		alignment
3eqtA	104	89	23	1.580	97		alignment
2rgbA	94	82	27	1.937	95		alignment
2w4rD	100	89	24	1.437	94		alignment
2w4rB	98	90	24	1.420	91		alignment
2rqaA	95	81	24	1.996	90		alignment
3cezA	66	79	10	2.215	49		alignment
3cezB	65	77	10	2.259	48		alignment
3cxkB	65	76	10	2.347	47		alignment
3cxkA	65	76	10	2.415	47		alignment
2fu5B	54	72	18	2.540	47	b.88.1.1	alignment
1l1dB	67	78	7	2.213	42	b.88.1.3	alignment
3e0oB	66	79	8	2.225	41		alignment
3e0oE	65	77	8	2.273	41		alignment
1l1dA	66	77	6	2.291	40	b.88.1.3	alignment

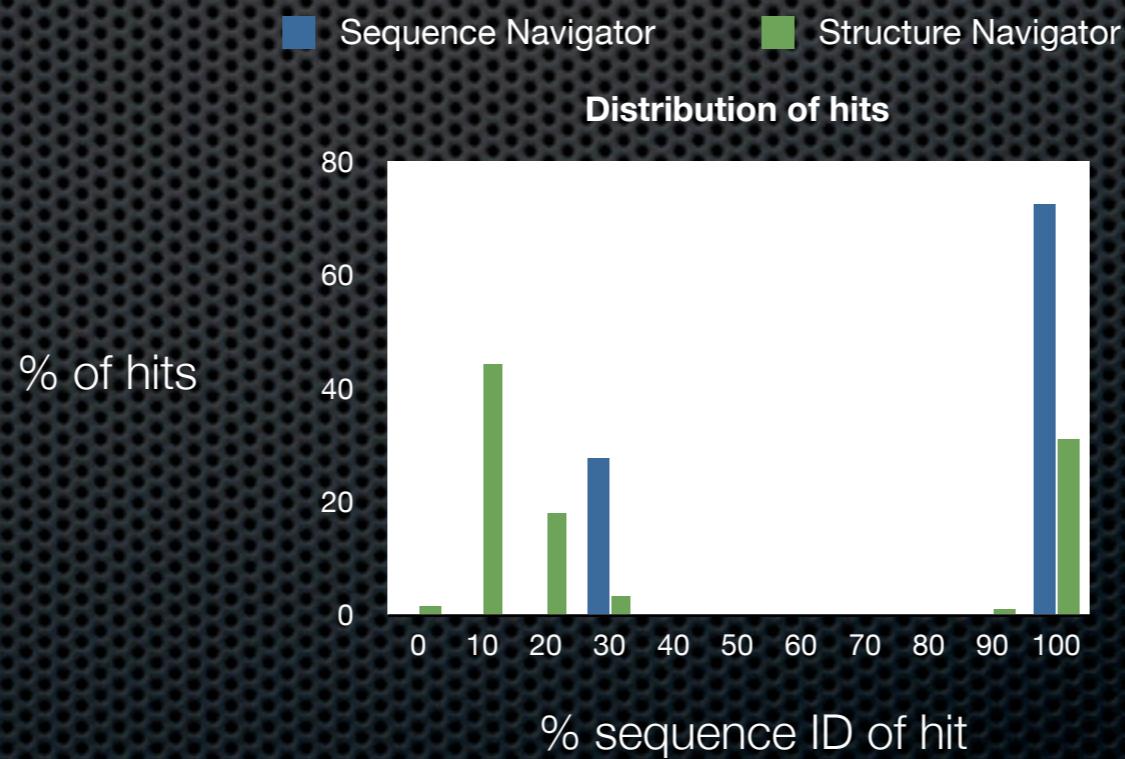
Structure Navigator (cont.)

3e0oD	64	74	8	2.457	39	alignment
3e0oA	64	75	8	2.364	38	alignment
3e0oC	63	74	8	2.422	37	alignment
3e0oF	64	76	8	2.315	37	alignment
3djmB	54	64	5	3.019	34	alignment
2fu5A	48	65	14	2.908	33	b.88.1.1 alignment
1hxra	47	64	18	2.943	32	b.88.1.1 alignment
1fwqA	49	66	17	2.763	32	b.88.1.1 alignment
3djmD	52	65	4	2.885	30	alignment
3djmA	50	60	7	3.142	29	alignment
2kaoA	50	65	12	2.999	27	alignment
1xm0A	55	67	8	2.829	24	b.88.1.3 alignment
3djmC	46	52	8	3.567	24	alignment
3djmE	46	55	7	3.404	22	alignment
2k8dA	49	61	10	3.069	16	alignment
3facE	43	58	9	3.321	11	alignment
3facA	42	62	11	3.128	10	alignment
1hxrb	37	53	15	3.586	9	b.88.1.1 alignment
3facG	41	55	9	3.444	8	alignment
3facC	41	56	9	3.357	8	alignment
3facF	41	59	9	3.292	7	alignment
3facB	40	56	8	3.375	4	alignment
3facH	39	54	7	3.467	3	alignment

Sequence Navigator finds 29 hits
Structure Navigator finds 62 hits

Sequence vs. Structure Alignment

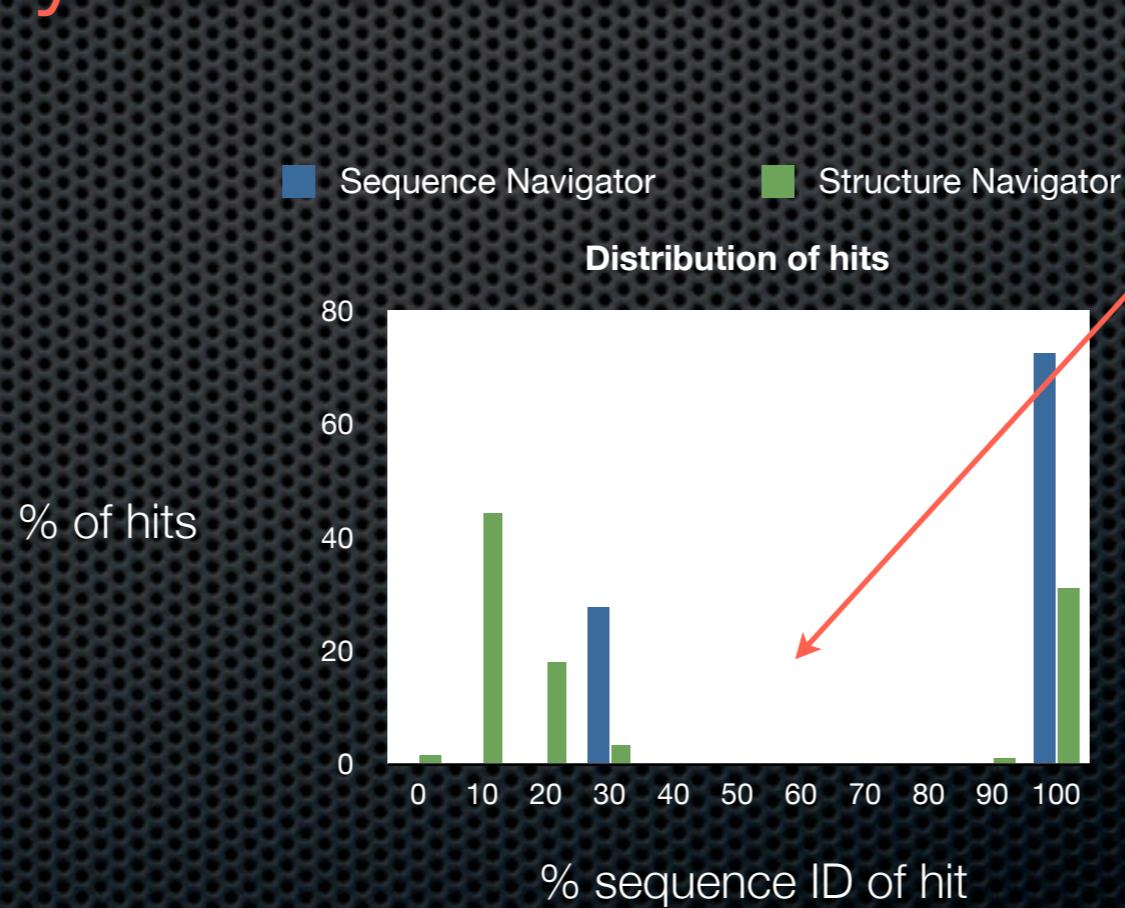
- Sequence alignment is fast, but not very sensitive
- Structure alignment is very sensitive, but slow



Sequence vs. Structure Alignment

- Sequence alignment is fast, but not very sensitive
- Structure alignment is very sensitive, but slow

question: why don't we see hits in the 40-90% range?



MAFFTash

- Multiple sequence alignment based on MAFFT program by Katoh, Misawa, Kuma, Miyata 2002 (Nucleic Acids Res. 30:3059-3066)
- Uses structural information from ASH program by Standley, Toh, and Nakamura 2005 (BMC Bioinformatics 6, 221)

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MAFFTash

alignment of multiple sequences and structures

Paste your sequences and PDB IDs (plus chain IDs) here:

Example:

```
>PDBID
3ygsC
>Q6Q899|DDX58_MOUSE| 1-91
MTAAQRQNLQAFRDYIKKILDPTYILSYMSSWLEDEEVQYIQAENKNKGPMEAASLFLQY
LLKLQSEGWFQAFLDALYHAGYCGLCEAIES
>Q6Q899|DDX58_MOUSE| 101-176
EEHRLLLRRLEPEFKATVDPNDILSELSECLINQECEEIRQIRDTKGRMAGAEKMAECLI
RSDKENWPKVQLALE
>PDBID
2p1hA
```

Need help picking PDB IDs? Use [Prep-MAFFTash](#).

OR upload a file no file selected

Structure wt. 0.2

email address (required)

Submit Clear Form

Do you want to upload your own structures?

A new form will be generated

No. structures 0 (max 10)

New form Clear Form

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Paste your sequences and PDB IDs (plus chain IDs) here:

Example:

```
>PDBID
3ygsC
>Q6Q899|DDX58_MOUSE| 1-91
MTAAQRQNLQAFRDYIKKILDPTYILSYMSSWLEDEEVQYIQAENKGPMEAASLFLQY
LLKLQSEGWFQAFLDALHAGYCGLCEAIES
>Q6Q899|DDX58_MOUSE| 101-176
EEHRLRLRRLEPEFKATVLPNDILSELSECLINQECEEIRQIRDTKGRMAGAEKMAECLI
RSDKENWPVKVLQLALE
>PDBID
2p1hA
```

Need help picking PDB IDs? Use [prep-MAFFTash](#).

type sequences like this:

>Q6Q899...
MTAAQRQNL...

OR upload a file no file selected

Structure wt. 0.2

email address (required)

Submit Clear Form

Do you want to upload your own structures?

A new form will be generated

No. structures 0 (max 10)

New form Clear Form

Molecule of the Month

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MAFFTash

alignment of multiple sequences and structures

Paste your sequences and PDB IDs (plus chain IDs) here:

Example:

```
>PDBID
3ygsC
>Q6Q899|DDX58_MOUSE| 1-91
MTAAQRQNLQAFRDYIKKILDPTYILSYMSSWLEDEEVQYIQAENKNKGPMEAASLFLQY
LLKLQSEGWFQAFLDALHAGYCGLCEAIES
>Q6Q899|DDX58_MOUSE| 101-176
EEHRLRLRRLEPEFKATVLPNDILSELSECLINQECEEIRQIRDTKGRMAGAEKMAECLI
RSDKENWPKVQLALE
>PDBID
2plhA
```

Need help picking PDB IDs? Use [Prep-MAFFTash](#).

type sequences like this:

**>Q6Q899...
MTAAQRQNL...**

type a PDB IDs like this:

**>PDBID
2plhA**

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MAFFTash results

From: standley@protein.osaka-u.ac.jp
Subject: MAFFTash Result
Date: July 13, 2009 2:03:55 PM JST
To: Daron Standley

Thank you for using the MAFFTash server.

The results of your query will be stored for 2 weeks at the following URL:

<http://sysimm100.protein.osaka-u.ac.jp/tmp/MS25086/index.html>

We hope these results will be useful for your research.

-MAFFTash

MAFFTash Result

[Jalview Window](#)

[Text File](#)

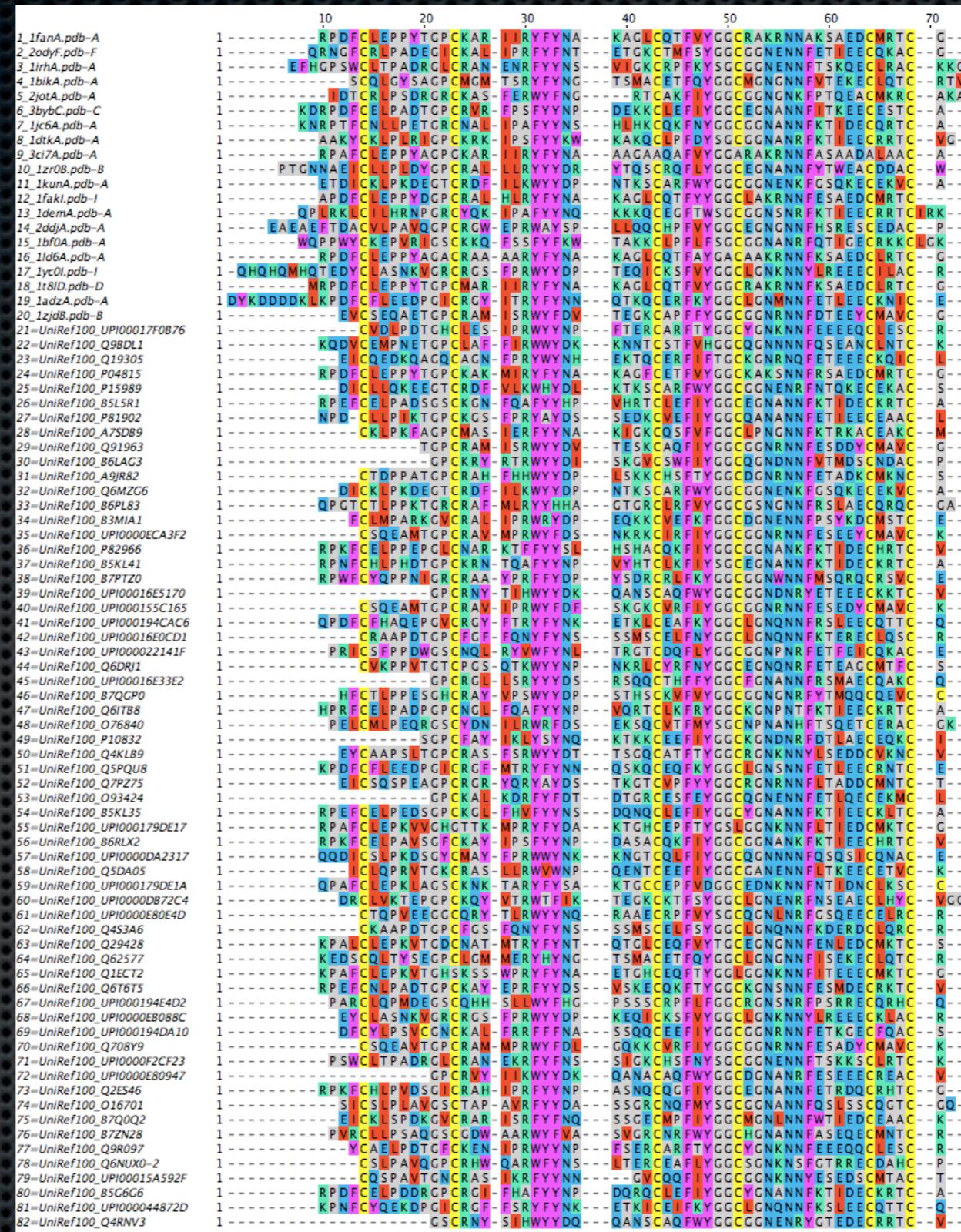
PDBj

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jalview alignment viewer

Waterhouse A.M., Procter J.B., Martin D.M., Clamp M., Barton G.J.
 "Jalview Version 2--a multiple sequence alignment editor and analysis
 workbench." Bioinformatics. (2009) 25(9):1189-91.



MAFFTash

alignment of multiple sequences and structures

Paste your sequences and PDB IDs (plus chain IDs) here:

Example:

```
>PDBID
3ygsC
>Q6Q899|DDX58_MOUSE| 1-91
MTAAQRQNLQAFRDYIKKILDPTYILSYMSSWLEDEEVQYIQAENKNKGPMEAASLFLQY
LLKLQSEGWFQAFLDALYHAGYCGLCEAIES
>Q6Q899|DDX58_MOUSE| 101-176
EEHRLLLRRLEPEFKATVDPNDILSELSECLINQECEEIRQIRDTKGRMAGAEKMAECLI
RSDKENWPKVQLALE
>PDBID
2p1hA
```

Need help picking PDB IDs? Use [Prep-MAFFTash](#).

OR upload a file no file selected

Structure wt.

email address (required)

Do you want to upload your own structures?

A new form will be generated

No. structures (max 10)

If typing input is difficult,
please use
Prep-MAFFTash



Prep-MAFFTash

MAFFTash
alignment of multiple sequences and structures

Paste your sequences below. Missing PDB IDs will be automatically added.

OR upload a file [Browse...](#)

email address (required)

Add structures
 Use Blast to add structures (from PDB)
Max seq ID between added structures
Min seq ID from original input

Add ASH structural neighbors
Max seq ID between added structures
Min seq ID from original input

Add sequences
 Use Blast to add sequences (from UniRef100)
Max seq ID between added sequences
Min seq ID from original input

[Submit](#) [Clear Form](#)

Prep-MAFFTash
automatically finds
PDB IDs and sequences
and formats them for
MAFFTash

Prep-MAFFTash

MAFFTash
alignment of multiple sequences and structures

Paste your sequences below. Missing PDB IDs will be automatically added.

```
>PDBID  
2qfbB
```

OR upload a file [Browse...](#)

email address (required)

Add structures
 Use Blast to add structures (from PDB)
Max seq ID between added structures
Min seq ID from original input

Add ASH structural neighbors
Max seq ID between added structures
Min seq ID from original input

Add sequences
 Use Blast to add sequences (from UniRef100)
Max seq ID between added sequences
Min seq ID from original input

[Submit](#) [Clear Form](#)

Prep-MAFFTash
automatically finds
PDB IDs and sequences
and formats them for
MAFFTash

Prep-MAFFTash

MAFFTash
alignment of multiple sequences and structures

Paste your sequences below. Missing PDB IDs will be automatically added.

```
>PDBID  
2qfbB
```

OR upload a file

email address (required)

Add structures
 Use Blast to add structures (from PDB)
Max seq ID between added structures
Min seq ID from original input

Add ASH structural neighbors
Max seq ID between added structures
Min seq ID from original input

Add sequences
 Use Blast to add sequences (from UniRef100)
Max seq ID between added sequences
Min seq ID from original input

Prep-MAFFTash
automatically finds
PDB IDs and sequences
and formats them for
MAFFTash

Prep-MAFFTash

Thank you for using the prep-MAFFTash server.

The results of your query will be stored for 2 weeks at the following URL:

<http://sysimm100.protein.osaka-u.ac.jp/tmp/Prep9316/index.html>

We hope these results will be useful for your research.

-MAFFTash

Result

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PDBj

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Prep-MAFFTash

Thank you for using the prep-MAFFTash server.

The results of your query will be stored for 2 weeks at the following URL:

<http://sysimm100.protein.osaka-u.ac.jp/tmp/Prep9316/index.html>

We hope these results will be useful for your research.

-MAFFTash

Result

[Text File](#)

PDBj

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Prep-MAFFTash

```
>PDBID  
2rmjA  
>PDBID  
2rqbA  
>PDBID  
3eqtB  
>UniRef100_UPI000184A4B6  
CKKCSQACCGTDIQLVIATAHHVNTTPKFKTLYSKGPNTLQEKFADYQINGDIICKECGKTWTTMVHGIEVPCLQIRNFVVKYDDKKMTKDTYDKWSELP  
>UniRef100_UPI000180C60D  
LCKKCKKVATTSDKFQHINHQHVVVDAGFIERAEIVQYPAIKHKVFGEOTIIGIVKCKSCRSDWGAYMRHRQQPISVLKIVNFVLQH  
>UniRef100_O44165  
KIICKCEAILCTSNDIRSNTQYLVCDPGFWSLVRKTRLTDEQQALIKYNATGSINCRRNCGLKLGQLIEVNTVDPCLSALSIVLLVEGTDKRIIVKKWNILDKYFTPTEIR  
>UniRef100_UPI00015A774A  
QLQCRSCFASVCSGGDIRKIENSHHVNNTFNETMFIMPENKPQFSNDLEVKNADLHPSFSQDWGFEIKFKVAILPCLKIKSFSFNTPKETKPYKKWDVEFQVTEFDF  
>UniRef100_B6NSL9  
LHCKKCNCQKACDAEELRLIEGAHHVHPDPEFLRNVGKADEAEEPLQKFOEWSRIGSVKCRKCEQDWGMLMLHGMNLPCLSVKNFTLRKGIPPRPKWKDSGIAVAEFDY  
>UniRef100_UPI00016E726B  
KFSCRGCSQEVCTGEDIEVIEDIHRVNVTPOFREL FIRKESTKRKDSLLDYETNGYIVCGKCGQRGSMMYFRGIQCP SLHVKNFVVAISGKNMPKCSKWTDVPARFSAFDY  
>UniRef100_UPI000175F4DC  
QLQCRSCFASVCSGGDIRKIENSHHVNNTFKNHYKVGDQVN MERTFEDWE PGRIISCRKCKDWGFEIKFKVAILPCLKIKSFSFNTPKETKPYKKWDVEFQVTEFDF  
>UniRef100_UPI0001796BE9  
QLLCINCMVAVGYGSDLRKVEGTHHVNVNPNSIYYKVSPKAVVIDREFKDWP GGAVSCRNCGESWGMQMIYKSVKLPVIKVRSMLETPRGRVQAKKWSHVPFP  
>UniRef100_Q6Q899  
KENKKLLCGKCKNFACYTADIRVVETSHYTVLGDAFKERFVCKPHPKPKIYDNFEKKAKIFCAKQNCSHDWGIFVRYKTFEIPVIKIESFVVEDIVSGVQNRHSWKDFHFER  
EMS  
>UniRef100_UPI000194DF7F  
KKLYCGKCKAYACSTDIDIRIKGSHHIVLGNAFQERYTTKPHRPVQFDDFVKKSKMHCRNTECQHDWGIIVKYKIFDNLPIKRSFVLEDVESGSQMDFQKWR SINLSLKN  
>UniRef100_UPI000069F51F  
NRKLLCKKCKTYACNTDDIRVIKDHMIIDKTFKDRYITKKHPKPRTFEGYKKMYKIFCKRPECHEDGVSGTYQGFQDLPLIKIEQFVIENPDGTQEYKDKWVDVHFT  
>UniRef100_Q9GLV6  
AFACYTADIRMVEKCHFTVVGDAFRERFVSKLHPKPKSFGNIEKRAKIYCARPDCSHDWGIVYVRYKAFEMPFIKIESFVVEDIATGVQTVHAKWKDFNFEKLSFDAEMA  
>UniRef100_UPI00005BBBB1  
FLCKNCVGPACSGEDIHVIEKMHHVNMTPEFKKLYLVRGNKALQTMCDYQTNGEIIDCNCGQAWGTMVHGLDLPLCLKIKNFVVVFQNNLPKKQYKKWV  
>UniRef100_UPI00015A61DA  
LSCRQCSVFCVCSGEDIEIIKMHVNVTQFSMEFKTFRENASLQERLLDYETNGVIACKCGQOWGSMMLYRSTECPLHIKNFVVTYGSKKTFSKWRELSISFPADY  
>UniRef100_UPI00017B3B5E  
QLLCRNCFRQVASGSDIRLVNDTHYVNINPDFKRFYKTGERVIINRRFEDWE PGRTISCNGSCNKKWGAEI KYKKVALLPNLSIENFALETPEGRMTPRKWDITFT  
>UniRef100_UPI0000EB32D5  
KENKKLLCRKCKAFACYTADIRVVEECHYT VVGDAFTKCFVSKLHPKPKSF GHFEKRAKIFCARRNCGH DWGIVHVKYKTFEIPVIKIESFVVEDIATGAQKLYAKWKDFPFEK  
EIP  
>UniRef100_UPI000194AF36  
EHVQLLCINCMVAVGHGSDLRKVEGTHHVNVNPNSNYYNVS RDPPVINKVFKDWKPGGVISCRNCGEVWGLQMIYKSVKLPVLKVRSMLETPQGRIQAKKWSRVPFSVPDF  
>UniRef100_B3KN51  
KENKKLLCRKCKALACYTADVRVIEECHYT VLGDAFKECFVSRPHPKPKQFSSFEKRAKIFCARQNC SHDWGIVHVKYKTFEIPVIKIESFVVEDIATGVQTLYSWKDFHFEK  
EMS  
>UniRef100_UPI00017978A2  
.  
.  
.
```

Paste the Prep-MAFFTash output into MAFFTash

MAFFTash

alignment of multiple sequences and structures

Paste your sequences and PDB IDs (plus chain IDs) here:

OR upload a file no file selected

Structure wt.

email address (required)

Do you want to upload your own structures?

A new form will be generated

No. structures (max 10)

Prep-MAFFTash → MAFFTash

	10	20	30	40	50	60	70	80	90	100	110	120	130	140	150	
1_2rmjA.pdb-A	DSQEKPKPVPDKENKLLCRCKAKALACYTADVR-VIEECHYTVLGDAFK-ECFVSRPHPK-PK-QFS-SFEKRAKIFCARQNCSDHWGIVHVKYKTFE-IPVIKESFVVVEDIATGVQTL-YSKWKDFHFEKIPFDPAEMSK-----															134
2_2rbA.pdb-A	-GPGLGSYKNNPSLITFLCKNCVLAQSGEDIH-VIEKMHVNMTPEFK-ELYIVRENKA-LQK-KCA-DYQINGEIJC--KGQAWGTMVHKGLD-LPCLKJRNFFVVVFKNNSTKKQ-YKKWELPITFPNLDDYSECCLFSDDED															135
3_3eqtB.pdb-B	RQQFPVEHVQLLCINCMVAVGHSDLR-KVEGTHHVNVPNFS-NYYNVSRDPVVINK-VFK-DWKPGGVISCRNCGEVWLQMIYKSVK-LPVLKVRSMMLLETPQ-GRIQ-AKKWSRVPFSVPDFDFLQHCAENLSLSDLEHHHHHH															142
4_UniRef100_UP1000184A4B6	--CKKCSKQACCGTDIQ-VIATAHHNTTPFK-TLYSKGPNKTL-QE-KFA-DYQINGDIIC-KECGKTWTGTTMVHKGIE-VPCLOJRNFFVVFKNNSTKKQ-YKKWELPITFPNLDDYSECCLFSDDED															103
5_UniRef100_UP1000180C60D	-LCKKCKKVATTSDKFO-HJNHQHHVVVDAGFI-ERAELVQYPAIKHK-VFG-EQTJGIVKC-KCSRSDWGAYMRHRQQP-ISVLUJVNFVLQH															88
6_UniRef100_O44165	KIICKKCEAIALCTSNDI-R-SR-NTQYLVCDPGFW-SLVRKTRLTD-EQQ-ALI-KYNATGSINCRRENCGLKLQGLIEVNTVD-LPCLSALSIVLLVEGTDKRII-VKKWKNILDKYFTPTETR															116
7_UniRef100_UP100015A774A	QLQCRSCFASVCSGGDIR-KIENSHHVNNTFNETMFIMPENKPQFSN-DL-EVLKNAIDLH-PSFSQDWGFEIKFKKVAJLPCLKJKSFSFNTPK-ETKP-YKKWKDVEFQVTEFDF															112
8_UniRef100_B6NSL9	LHCKCNQKACDAAEERL-LIEGAHHVHPDEFL-RNVGKADEAEEPQ-LKFQ-EWSRIGSVK-RKECDWGMMLHKGMN-LPCLSVKFNTRKQCPPRR-PKKWKGDSGAVAEFDYAQD															115
9_UniRef100_UP100016E726B	KFSCRGCSQEVTGEDIE-VIEDIHRVNVNTPEFK-SLL-DYETNGYIVC-GKCGQRWGSMMYFRGIQ-CPSLHVKNFVVAISGKMPK-CSKWTDVPARSAFDY															112
10_UniRef100_UP1000175F4DC	QLQCRSCFASVCSGGDIR-KIENSHHVNNTFNETMFIMPENKPQFSN-DL-EVLKNAIDLH-PSFSQDWGFEIKFKKVAJLPCLKJKSFSFNTPK-ETKP-YKKWKDVEFQVTEFDF															112
11_UniRef100_UP100017968E9	QLLCINCMVAVGYSDSL-R-KVEGTHHVNVPNFS-JYYKVKSPKAVV IDR-EFK-DWKPGGAVC-RNCGEESWGQMIIYKSVK-LPVLKVRSMMLLETPR-GRVQ-AKKWSHVPFP															106
12_UniRef100_Q6Q899	KENKLLLCGCKNFKACYTAIDR-VVETSHYTVLGDAF-ERFVCKPHPK-PK-LYDNFEKKAKIFCAKQNCSDHWGIVFVYKTFE-IPVIKESFVVVEDIVSGQNR-HSKWKDFHFERQFDPAEMS															122
13_UniRef100_UP1000194DF7F	KKLYCGKCKAYACSTDIDR-VVETSHYTVLGDAF-ERFVCKPHPK-PK-LYDNFEKKAKIFCAKQNCSDHWGIVFVYKTFE-IPVIKESFVVVEDIVSGQNR-HSKWKDFHFERQFDPAEMS															116
14_UniRef100_UP1000069F51F	NRKLLCKKCKTYACNTDDR-VIKDSHHMIIDKTFK-DRYITKHKP-PR-TFE-CYKKMYKIFCKRPRECHEDWGVSGBTYQGFQDPLPLIKEQFVIENPD-GTQEY-KDKWVDVHFT															110
15_UniRef100_Q9GLV6	-AFACYTADIR-MVEKCHFTVVGDAFR-ERFVSKLHPK-PK-SFG-NIEKRAKIFCARPDCSHDWGLYVYKAFE-MPFIKIESFVVVEDIATGVQTV-HAKWKDFNFEKLSFDDAAEMA															110
16_UniRef100_UP100005BBB81	FLCKNCVPAACSGEDIH-VIEKMHVNNTPEFK-KLYLVRGNKA-LQT-MCV-DYQTNGEIJC-NKCGQAWGTMVHKGLD-LPCLKJKNFVVTYGS-KKKT-FSKWRELISISFPADY															101
17_UniRef100_UP100015A61DA	LSCRQCSVFCGEDIE-IIEKMHVNNTPEFK-RLL-DYETNGVIA-C-KCQQGWGSMMLYRSTE-CPCLHJKNFVVTYGS-KKKT-FSKWRELISISFPADY															111
18_UniRef100_UP100017B3B5E	QLLCRNCFRQVASGSDIR-LVDNTHYVNINPDFK-RFYKTGER-VIINR-RFE-DWEGRITSCSNGSCNKKWGAEIYKVKALLPNLISENFALETPE-GRMT-PRWKWDITFT															108
19_UniRef100_UP100006832D5	KENKLLCRCKKAFACTYADIR-VVEECHYTVVGDAFT-KCFVSKLHPK-PK-SFG-HFEKRAKIFCARRNCGDHWGIVHVKYKTFE-IPVIKESFVVVEDIATGVQTV-HAKWKDFNFEKLSFDDAAEMA															122
20_UniRef100_UP1000194AF36	-EHVQLLCINCMVAVGHSDLR-KVEGTHHVNVPNFS-NYYNVSRDPVVINK-VFK-DWKPGGVISCRNCGEVWLQMIYKSVK-LPVLKVRSMMLLETPQ-GRIQ-AKKWSRVPFSVPDFDF															115
21_UniRef100_B3KN51	KENKLLCRCKAKALACYTADVR-VIEECHYTVLGDAF-ECFVSRPHPK-PK-QFS-SFEKRAKIFCARQNCSDHWGIVHVKYKTFE-IPVIKESFVVVEDIATGVQTL-YSKWKDFHFEKIPFDPAEMS															122
22_UniRef100_UP100017978A2	KKNKLLCRCKKAFACTYADIR-VVEECHYTVVGNAFR-ECFVCRSHPK-PK-LFG-SFEKKAKIYCAREDCSDHWGICVVKYKTFE-IPVIKESFVVVEDIATRVQTL-YAKWRDFNFEKIPFDAAEMS															122
23_UniRef100_UP100004E46E98	NHSYHCKHCDALVCHSADIR-IVPGHHVVVIRHQIF-SKIRIVASAGVQDGHWSSEVAHKEE-RCADERCDTKLGSILCKCNRNLL-LLAFTSKSLRSKASKTKT-NKSGWGLPFIIFQKVPVTEAS															124
24_UniRef100_UP1000008137	KENPSLINVCKNCVLAACSGEDIH-VIEKMHVNNTPEFK-ELYIVRENKA-LRK-KFI-DYQTNGEIJC-KMCQAWGTMVHKGLD-LPCLKJKNFVVIJKNNTSKKQ-YKKWV-															109
25_UniRef100_UP10001554F4B	KLLCGCKVLACYANDIR-IVEEESHHTVGETFK-NRFVAEPHPK-QK-RYG-NFEKIMKIKYCKERECHHDWGJFVYKIFE-MPIIKIESFVVVEDIFTGAQHV-CSKWKTFNFRIPFDAAEIS															118
26_UniRef100_Q6GN13	EQVRFYCRCCSQAVALGDDFR-TIEGTHYVNNSDFR-JYYEVCSPLLDFGK-KMV-DWTPGGKIRC-LCQGDWGFEIMYKHVN-FPAISVKNFVVTETPE-IKRP-YARWKDVPFP															108
27_UniRef100_UP1000194AF58	-LCKNCVLAACSGEDIH-VIEKMHVNNTPEFK-ELYIVRENKA-LRK-KCA-DYQINGEIJC-KCQAWGTMVHKGLD-LPCLKJRNFVVIJKNNTSKKQ-YKKWVLELPITFPNLDDYSEL															114
28_UniRef100_UP100000ECB7C9	-LCKNCVHLCKLACSGEDIQ-VIENMHHVSVKDFQ-HLYHKRENRT-LQD-KHA-DYQTNEVIE-C-KDCGQVGWNMMVYRGLD-LPCLKJRNFVVAEDFKKTTKE-IFKKWGEELP															104
29_UniRef100_B5X2V9	QLSCRGCVPVMAFGNDIK-VIENAHHVNPDFE-KYYKTGGKPA-LK-TFE-DWEGRVVIS-AACGKQWGMEMVYKEIALLPILAENFALETPE-GRRRL-AKKWKVNVEFT															105
30_UniRef100_UP10000E47298	LHCKNCSEACSLDDIR-CIEDQHVVNTNDLFL-DKIDLCNPTK-KRL-SDD-KFRPLKDIHC-GNCPYKWTMMKYQKQD-FPLIAVKNFRLMDDK-GNKFL-YKKWTDVVPFA															105
31_UniRef100_UP10000586468	LHCKCKFESCKLDDIR-SIRNQHHVVTSDLFL-DKMKLIDLKK-QP-IIIDGFTHQKQHIC-GNCQHKWQGTMVYQQQE-LPLIAJKNFTLKKDK-GKKWF-PKAWKDVPFP															104
32_UniRef100_UP100004C11CD	EQVQLLCVNCVMAVGHSDLR-KVEGTHHVNVPNFS-IYYNVSRGPVVIDR-TFK-DWRPGGTIHC-RNCNGEAWGLQMIYKSVK-LPALKVRSMLETPR-GRVQ-AKKWSRVPFPVPDFDY															115
33_UniRef100_Q99J87	EHVQLLCINCMVAVGYSDSL-R-KVEGTHHVNVPNFS-VYTTSQNPVVINK-VFK-DWRPGGTIHC-SNCGEVWGQMIYKSVT-LPVLKJGSMLETPR-GKIQ-AKKWSRVPFSIPVFDI															115
34_UniRef100_UP10000F2BCC7	RLLCTNCAEPVGYSDSL-R-KVEGTHHVNVPDFK-JYYKTSLRPVAILDR-TFK-DWYPGGTIS-CRKCEAWGLEMIYKSVN-LPVLNIRSLVLETPQ-GRRK-VSQWSKVPFQVADLD															111
35_UniRef100_UP1000048574	KLLCKHCRQFTCTEDIR-SINGQHHIVFDKGFQ-DRVITERLLE-EDY-LYS-DAKASETRK-CRKCKQLGFMMIITEHE-LPLLVIRYLVIELAN-GVVKY-KKKWSET															103
36_UniRef100_UP100000ECA07D	-CVNCVNAVCRGSDIR-TVEAMHHVNPNFR-FYYTVSSGKIHFER-TFR-DWEGRCIYC-SECQREWGMEMIYRNVT-LPILSJKNFFVVTPTD-EKKK-YKKWSTVTFP															103
37_UniRef100_UP100016E90B3	QLLCRNCFKQVASGSDIR-LLDKAHYVNINPDFK-KHYKTGGQ-VFLNRT-TFE-DWEGRCTISCNNGSCNKAWSIEIYKVKALLPNLIESFALETPE-GRTT-PRRWRDITFT															108
38_UniRef100_UP100015A61D7	LSCRQCSVFCGEDIE-IIEKMHVNVTQKFS-ITCLCRPVVNDVNE-RLL-DYETNGVIA-C-KKCGQGWGSMMLYRSTE-CPCLHJKNFVVTYGS-KKKT-FSKWRELISISFPADY															112
39_UniRef100_UP100017B3E85	NVKFQKCSQSCQEVCTGRD-IMANHRVNLKENTK-LSL-DYETNGVIA-C-GKCGQGWGSMMHFRGQ-I-CPCLHJKNFVVTYGS-KKKT-CQQWMDDLPVRLSEFDYAEH															117
40_UniRef100_UP1000155FAED	-LCKNCMЛАCTGEDIY-VIENMHHVNNTPEFK-ELYIVRENKA-LKK-KFA-DYQTNGEIJC-QNCQGAWGTMVHKGLD-LPCLKJKNFVVFKSNSPKKQ-YKKWV-															100
41_UniRef100_UP10000E21E05	KENKLLCRCKAKALACYTADVR-VIE-															32
42_UniRef100_A7LCX1	KDNPSLISFLCKNCVLAACSGEDIH-IIEKMHVNNTPEFK-NLYIVRGNKA-LQT-KFA-DYQTNGEIJC-KCQGAWGTMVHKGLD-LPCLKJKNFVVFKNLFFKKQ-YKKWV-															109
43_UniRef100_UP1000180C762	-LLCKGCKTETVSKSDQFR-HIEKQHHVVTSDLFL-DKASCREVPIEQGK-PVGFQVIIGKVC-KCQGAWGTMVHKGLD-LPCLKJRNFFVVFKNLFFKKQ-YKKWV-															106
44_UniRef100_UP100004E4160	-CKCKFEACSLDDIR-CIKNMHHVVIISDLFL-DKTRL-VD-EFKHRQKIHG-CNCQYKWKGMVYRRRD-LPLIDVKNFELMDDQ-GKKWF-PKAWKDVPFP															94
45_UniRef100_UP10000E48578	KLLCKHCRQFACYTTDIR-SINGQHHIVGEGL-DRVITERLQE-EKN-LYG-DTVSKVQ-CRCKKPLGFMIIIEHE-LPLLAIKHLVIELPN-KAKVH-KKKWSET															103
46_UniRef100_B6P4P6	-															57
47_UniRef100_UP10000F2CFD1	-CKKCNVQACSGEDIQ-VIENMHHVIMTQEFK-SFYIVRENKA-LQK-KFA-DYQTNGEIJC-SQCGQSWGTMVNVKGGLD-LPCLKJRNFFVVFKNLFFKKQ-YKKWV-															113
48_UniRef100_UP100005BD20D	KKNKLLCGCKTFACTEACDFR-CVSGSHYVVISPEKRDKIELKPHKK-PK-LIT-GITMDTKVHC-KKCGQDWGRATAIHGAE-WPLLKJNSFVYQIEG-GPRKL-YRKWT-															122
49_UniRef100_A7RW42	RFYCRKNCNTFACEACDFR-CVSGSHYVVISPEKRDKIELKPHKK-PK-LIT-GITMDTKVHC-KKCGQDWGRATAIHGAE-WPLLKJNSFVYQIEG-GPRKL-YRKWT-															101
50_UniRef100_UP100016E90B4	QLLCRNCFKQVASGSDIR-LLDKAHYVNINPDFK-YVELLR															

What can we do with multiple sequence alignments?

- Easily locate conserved (i.e., important) residues
- We can also use them for predicting the structure of a protein from its sequence

Protein structure prediction

Protein structure prediction

query sequence

Protein structure prediction

query sequence

template structure 1

Protein structure prediction

query sequence

template structure 1

template structure 2

Protein structure prediction

query sequence

template structure 1

template structure 2

template structure 3

Protein structure prediction

query sequence

```
CRKCKAKALACYTADVR-VIEECHYTQL  
CKNCVVLACSGEDIH-VIEKMHHVNM  
CINCMVAVGHGSDLR-KVEGTHHVNV  
CKKCSKQACCGTDIQT-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAAILCTSVDIIR-SR-NTQYLVC  
CRSCFASVCSGGDIR-KIENSHHVNV  
CKKCQNQKACDAAELR-LIEGAHHVHP  
CRGCSQEVTGEDIE-VIEDTHRNVN  
CRSCFASVCSGGDIR-KIENSHHVNV  
CINCMVAVGYGSDLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSHYTQL  
CGKCKAYACSTDDIR-IIKGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHHMII  
---AFACYTADIR-MVEKCHFTVV  
CKNGCPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDIIE-IIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAFACYTADIR-VVVEECHYTVV  
CINCMVAVGHGSDLR-KVEGTHHVNV  
CRKCKAKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHVVV  
CKNCVVLACSGEDIH-VIEKMHHVNM  
CGKCKVVLACYANDIR-JVEESHTV  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVVLACSGEDIH-VIEKMHHVNM  
CKNCVKLLICSGEDIQ-VIENMHHVSV  
CRGCFPVVAFGNDIK-VIENAHHVNI
```

query MSA

template structure 1

template structure 2

template structure 3

Protein structure prediction

query sequence

template structure 1

what program?

CRKCKALACYTADVR-VIEECHYTQL
CKNCVLAACSGEDIH-VIEKMHHVNM
CINCMVAVGHGSDLR-KVEGTHHVNV
CKKCSKQACCGTDIQ-VIATAHHHVNT
CKKCKKVATTSDKFQ-HINHQHHVVV
CKKCEAAILCTSVDLR-SR-NTQYLV
CRSCFASVCSGGDIR-KIENSHHVNV
CKKCQNQKACDAAELR-LIEGAHHVHP
CRGCSQEVTGEDIE-VIEDTHRNV
CRSCFASVCSGGDIR-KIENSHHVNV
CINCMVAVGYGSDLR-KVEGTHHVNV
CGKCKNFACYTADIR-VVETSHYTQL
CGKCKAYACSTDDIR-IIGKSHHIVL
CKKCKTYACNTDDIR-VIKDSHHMII
---AFACYTADIR-MVEVKCHFTVV
CKNGCPACSGEDIH-VIEKMHHVNM
CRQCSVFCSGEDI-E-IIEKMHHVNV
CRNCFRQVASGSDIR-LVDNTHYVNI
CRKCKAFACYTADIR-VVVEECHYTVV
CINCMVAVGHGSDLR-KVEGTHHVNV
CRKCKALACYTADVR-VIEECHYTQL
CRKCKAFACYTADIR-VVVEECHYTVV
CKHCDALVCHSADIR-IVPGGHVVV
CKNCVLAACSGEDIH-VIEKMHHVNM
CGKCKVLACYANDIR-JVEESHHTVI
CRCCSQAVALHGDDFR-TIEGTHYVNI
CKNCVLAACSGEDIH-VIEKMHHVNM
CKNCHKLLICSGEDIQ-VIENMHHVSV
CRGCFPVAFGNDIK-VIENAHHVNI

template structure 2

query MSA

template structure 3

Protein structure prediction

query sequence

```
CRKCKAKALACYTADVR-VIEECHYTQL  
CKNCVVLACSGEDIH-VIEKMHHVNM  
CINCMVAVGHGSDLR-KVEGTHHVNV  
CKKCSKQACCGTDIQT-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAAILCTSVDIIR-SR-NTQYLVC  
CRSCFASVCSGGDIR-KIENSHHVNV  
CKKCQNQKACDAAELR-LIEGAHHVHP  
CRGCSQEVTGEDIE-VIEDTHRNVN  
CRSCFASVCSGGDIR-KIENSHHVNV  
CINCMVAVGYGSDLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSHYTQL  
CGKCKAYACSTDDIR-IIKGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHHMII  
---AFACYTADIR-MVEKCHFTVV  
CKNGCPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDIIE-IIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAFACYTADIR-VVVEECHYTVV  
CINCMVAVGHGSDLR-KVEGTHHVNV  
CRKCKAKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHVVV  
CKNCVVLACSGEDIH-VIEKMHHVNM  
CGKCKVVLACYANDIR-JVEESHTV  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVVLACSGEDIH-VIEKMHHVNM  
CKNCVKLLICSGEDIQ-VIENMHHVSV  
CRGCFPVVAFGNDIK-VIENAHHVNI
```

query MSA

template structure 1

template structure 2

template structure 3

Protein structure prediction

query sequence

MAFFT

Sequence logo of the query MSA, showing conservation of amino acids across positions. The logo uses a color scheme where each column represents a position in the sequence and each row represents an amino acid (A, C, D, E, F, G, H, I, K, L, M, N, P, Q, R, S, T, V, W, Y). The height of each bar indicates the frequency of that amino acid at that position.

```
CRKCKALACYTADVR-VIEECHYTQL  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CINCMVAVGHGSDLR-KVEGTHHVNV  
CKKCSKQACCGTDIQ-VIATAHHHVNT  
CKKKKKVATTSDFQ-HINHQHHVVV  
CKKCEAAILCTSVDIIR-SR-NTQYLV  
CRSCFASVCSGGDIR-KIENSHHVNV  
CKKCQNKACDAAEILR-LIEGAHHVHP  
CRGCSQEVTGEDIE-VIEDTHRNVN  
CRSCFASVCSGGDIR-KIENSHHVNV  
CINCMVAVGYGSDLR-KVEGTHHVNV  
CGKCKNFACYTAIDIIR-VVETSHYT  
CGKCKAYACSTDDIR-IIKGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHHMII  
---AFACYTAIDIIR-MVEVKCHFTVV  
CKNGCPACSGEDIH-VIEKMHHVNM  
CRQCSVFCGSDIE-IIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAFACYTAIDIIR-VVEECHYT  
CINCMVAVGHGSDLR-KVEGTHHVNV  
CRKCKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTAIDIIR-VVEECHYT  
CKHCDALVCHSADIIR-IVPGGHVV  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CGKCKVLACYANDIR-JVEESHTV  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CKNCALKLICSGEDIQ-VIENMHHVSV  
CRGCFPVVAFGNDIK-VIENAHHVNI
```

query MSA

template structure 1

template structure 2

template structure 3

Protein structure prediction

query sequence

MAFFT

```
CRKCKALACYTADVR-VIEECHYTQL  
CKNCVLAGSGEDIH-VIEKMHHVNM  
CINCMVAVGHSIDLK-KVEGTHHVNV  
CKKCNSQACCGTDIQ-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAAILCTSVDLR-SR-NTQYLV  
CRSCFASVCSGGDIR-KIENSHHVNV  
CKKCNSQEVCTGEDIE-VIEDTHRNV  
CRSCFASVCSGGDIR-KIENSHHVNV  
CINCMVAVGYSGLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSHYT  
CGKCKAYACSTDDIR-IIGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHMII  
---AFACYTADIR-MVEVKCHFTVV  
CKNGCPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDI-E-IIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHHVNI  
CRKCKAFACYTADIR-VVEECHYT  
CINCMVAVGHSIDLK-KVEGTHHVNV  
CRKCKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVEECHYT  
CKHCDALVCHSADIR-IVPGGHVV  
CKNCVLAGSGEDIH-VIEKMHHVNM  
CGKCKVLACYANDIR-JVEESHTVI  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVLAGSGEDIH-VIEKMHHVNM  
CKNCNLICSGEDIQ-VIENMHHVSV  
CRGCFPVAFGNDIK-VIENAHHVNI
```

query MSA

template structure 1

template structure 2

template structure 3

Also: psiblast, clustalw, Muscle, etc.

Protein structure prediction

query sequence

MAFFT

```
CRKCKALACYTADVR-VIEECHYTQL  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CINCMVAVGHGSDLR-KVEGTHHVNV  
CKKCNSQACCGTDIQL-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAAILCTSVDLR-SR-NTQYLVC  
CRSCFAASVCSGGDIR-KIENSHHVNP  
CRGCSQEVTGEDIE-VIEDTHRNVN  
CRSCFAASVCSGGDIR-KIENSHHVNV  
CINCMVAVGYGSDLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSHYTQL  
CGKCKAYACSTDDIR-IIKGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHHMII  
---AFACYTADIR-MVEVKCHFTVV  
CKNGCPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDIIE-JIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVN  
CRKCKAFACYTADIR-VVVEECHYTVV  
CINCMVAVGHGSDLR-KVEGTHHVNV  
CRKCKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHVV  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CGKCKVLAACYANDIR-JVEESHHTVI  
CRCCSQAVALHGDDFR-TIEGTHYVN  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CKNCALKLICSGEDIQ-VIENMHHVSV  
CRGCFPVVAFGNDIK-VIENAHHVNI
```

query MSA

template structure 1

template structure 2

template structure 3

Protein structure prediction

query sequence

MAFFT

```
CRKCKAKALACYTADVR-VIEECHYTQL  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CINCMVAVGHGSDLR-KVEGTHHVNV  
CKKCCKQACCGTDIQ-VIATAHHVNT  
CKKCCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAAILCTSVDIIR-SR-NTQYLVC  
CRSCFAAVCSGGDIR-KIENSHHVNP  
CRGCSQEVTGEDIE-VIEDITHRVNV  
CRSCFAAVCSGGDIR-KIENSHHVNV  
CINCMVAVGYGSDLR-KVEGTHHVNV  
CGKCKNFACYTADDIR-VVETSYTQL  
CGKCKAYACSTDDIR-IIGSHHVNL  
CKKCKTYACNTDDIR-VIKDSHMII  
---AFACYTADDIR-MVEVKCHFTVV  
CKNCGVPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDI-E-IIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAKAFACYTADDIR-VVEECHYTVV  
CINCMVAVGHGSDLR-KVEGTHHVNV  
CRKCKAKALACYTADVR-VIEECHYTQL  
CRKCKAKAFACYTADDIR-VVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHVVV  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CGKCKVLAACYANDIR-JVEESHTV  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CKNCCKLICSGEDIQ-VIENMHHVSV  
CRGCFPVVAFGNDIK-VIENAHHVNI
```

query MSA

```
EECHYTQLGDAFK-ECFVSRPHPK--PK  
EKMHHVNVMTPEFK-ELYIVRENKA-LQK  
EGTHHVNVNPNS-NYYNVSRDPPVINK  
ATAHHVNTTPKF-TLYSKGPNKT-LQE  
NHQHHVVVDAGFI-ERAELVQYPAIKHK  
-NTQYLVCDPGFW-SLVRKTRLTD-EQQ  
ENSHHVNVNTEFNETMFIMPENKPQFSN  
EGAHHVHPDPEFL-RNVGKADEAEELQ  
EDIHRVNVTPOFR-ELFIRKESTK-RKD  
ENSHHVNVNTEFK-NHYKVGDQ-VNMER  
EGTHHVNVNPNS-IYYKVSPKAVVIDR  
ETSHYTQLGDAFK-ERFVCKPHPK--PK  
KGSHHIVLGNAFQ-ERYTTKPHRK--PV  
KDSHHMIIIDKTFK-DRYITKKHPK--PR
```

template structure 1

template structure 2

template structure 3

Protein structure prediction

query sequence

MAFFT

```
CRKCKALACYTADVR-VIEECHYTQL  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CINCMVAVGHSGLR-KVEGTHHVNV  
CKKCCKQACCGTDIQ-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAAILCTSKDIR-SR-NTQYLVC  
CRSCFAAVCSGGDIR-KIENSHHVNV  
CKKCNQKACDAAEILR-LIEGAHHVHP  
CRGCSQEVTGEDIE-VIEDITHRVNV  
CRSCFAAVCSGGDIR-KIENSHHVNV  
CINCMVAVGYSGLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSYTQL  
CGKCKAYACSTDDIR-IIGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHHMII  
---AFACYTADIR-MVEKCHFTVV  
CKNCGVPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDIH-JIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAFACYTADIR-VVEECHYTVV  
CINCMVAVGHSGLR-KVEGTHHVNV  
CRKCKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHHVVI  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CGKCKVLAACYANDIR-JVEESHHTVI  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CKNCCKLICSGEDIQ-VIENMHHVSV  
CRGCFPVAFGNDIK-VIENAHHVNI
```

query MSA

```
E E C H Y T V L G D A F K - E C F V S R P H P K - - P K  
E K M H H V N M T P E F K - E L Y I V R E N K A - L Q K  
E G T H H V N V N P N F S - N Y Y N V S R D P V V I N K  
A T A H H V N T T P K F K - T L Y S K G P N K T - L Q E  
N H Q H H V V V D A G F I - E R A E I V Q Y P A I K H K  
- N T Q Y L V C D P G F W - S L V R K T R L T D - E Q Q  
E N S H H V N V N T E F N E T M F I M P E N K P Q F S N  
E G A H H V H P D P E F L - R N V G K A D E A E E P L Q  
E D I H R V N V T P Q F R - E L F I R K E S T K - R K D  
E N S H H V N V N T E F K - N H Y K V G D Q - V N M E R  
E G T H H V N V N P N F S - J Y Y K V S P K A V V I D R  
E T S H Y T V L G D A F K - E R F V C K P H P K - - P K  
K G S H H I V L G N A F Q - E R Y T T K P H R K - - P V  
K D S H H M I I D K T F K - D R Y I T K K H P K - - P R
```

```
C V N C N V A V C R G S D I R - T V E A M  
C R N C F K Q V A S G S D I R - L L D K A  
C R Q C S V F V C S G E D I E - I I E K M  
C R S C S Q E V C T G R D I E - I M A N I  
C K N C S M I A L C T G E D I Y - V I E N M  
C R K C K A L A C Y T A D V R - V I E --  
C K N C S V L A C S G E D I H - I I E K M  
C K G C K T E V T K S D Q F R - H I E K Q  
C I K C F K E A C S L D D I R - C I K N M  
C K H C R Q F A C Y T D D I R - S I N G Q  
---  
C K K C N V Q A C S G E D I Q - V I E N M  
C G K C K T F A C Y T A D I R - V V E E C  
C R K C N T F A C E A C D F R - C V S G S  
C R N C F K Q V A S G S D I R - L L D K A  
C R K C D G I L L C T S Q D I S - S R Q D N  
C R K C H V F I C Q A H E I K - R V R D S  
C K N C S K S I C S G E D I Q V V I E D M  
C I N C M V S V G Y C S D L R - K V E G T  
C V K C K E F A C N V S D F R - K V K E N  
C R N C F K Q V A S G S D I R - L L D K A
```

template structure 1

template structure 2

template structure 3

Protein structure prediction

query sequence

MAFFT

```
CRKCKALACYTADVR-VIEECHYTQL  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CINCMVAVGHSGLR-KVEGTHHVNV  
CKKCCKQACCGTDIQ-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAIICTSKDIR-SR-NTQYLVC  
CRSCFAASVCSGGDIR-KIENSHHVNV  
CKKCNQKACDAAEILR-LIEGAHHVHP  
CRGCSQEVTGEDIE-VIEDITHRVNV  
CRSCFAASVCSGGDIR-KIENSHHVNV  
CINCMVAVGYSGLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSYTQL  
CGKCKAYACSTDDIR-IIGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHHMII  
---AFACYTADIR-MVEKCHFTVV  
CKNGVPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDIH-JIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAFACYTADIR-VVEECHYTVV  
CINCMVAVGHSGLR-KVEGTHHVNV  
CRKCKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHVVV  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CGKCKVLVLAICYANDIR-JVEESHHTVI  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CKNCCKLICSGEDIQ-VIENMHHVSV  
CRGCFPVAFGNDIK-VIENAHHVNI
```

query MSA

template MSAs

```
E E C H Y T V L G D A F K - E C F V S R P H P K - - P K  
E K M H H V N M T P E F K - E L Y I V R E N K A - L Q K  
E G T H H V N V N P N F S - N Y Y N V S R D P V V I N K  
A T A H H V N T T P K F K - T L Y S K G P N K T - L Q E  
N H Q H H V V V D A G F I - E R A E I V Q Y P A I K H K  
- N T Q Y L V C D P G F W - S L V R K T R L T D - E Q Q  
E N S H H V N V N T E F N E T M F I M P E N K P Q F S N  
E G A H H V H P D P E F L - R N V G K A D E A E E P L Q  
E D I H R V N V T P Q F R - E L F I R K E S T K - R K D  
E N S H H V N V N T E F K - N H Y K V G D Q - V N M E R  
E G T H H V N V N P N F S - J Y Y K V S P K A V V I D R  
E T S H Y T V L G D A F K - E R F V C K P H P K - - P K  
K G S H H I V L G N A F Q - E R Y T T K P H R K - - P V  
K D S H H M I I D K T F K - D R Y I T K K H P K - - P R
```

```
C V N C N V A V C R G S D I R - T V E A M  
C R N C F K Q V A S G S D I R - L L D K A  
C R Q C S V F V C S G E D I E - I I E K M  
C R S C S Q E V C T G R D I E - I M A N I  
C K N C S M I A L C T G E D I Y - V I E N M  
C R K C K A L A C Y T A D V R - V I E --  
C K N C S V L A C S C E D I H - I I E K M  
C K G C K T E V T K S D Q F R - H I E K Q  
C I K C F K E A C S L D D I R - C I K N M  
C K H C R Q F A C Y T D D I R - S I N G Q  
---  
C K K C N V Q A C S G E D I Q - V I E N M  
C G K C K T F A C Y T A D I R - V V E E C  
C R K C N T F A C E A C D F R - C V S G S  
C R N C F K Q V A S G S D I R - L L D K A  
C R K C D G I L L C T S Q D I S - S R Q D N  
C R K C H V F I C Q A H E I K - R V R D S  
C K N C S K S I C S G E D I Q V V I E D M  
C I N C M V S V G Y C S D L R - K V E G T  
C V K C K E F A C N V S D F R - K V K E N  
C R N C F K Q V A S G S D I R - L L D K A
```

template structure 1

template structure 2

template structure 3

```
-- D M P L D S D V F Q V P P C Y N A P Q Q V H I T Q G D - H D G K A V J V S W T - E - D E - T T E - S I V E Y G - I G  
-- D M P L D S D V F R V P P C Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - V - D E - P G S - S N V L Y W - S -  
-- E E M P L E T F P P P A C Y N A P E Q V H I T Q G D - H A G R G M I I S W T - P L N E - S V P - S V V D Y G - T -  
-- D M P L D S D V F R V P P C Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - V - D E - D G S - N V V T Y W I A N -  
-- P E Q V H L A F G E S T A - S E I V V T W S T R E L - I V V T W N T R N N - P P S - A E S I V E Y G - I T -  
-- D L P M D H P R L - R R N V T S F F P E Q I S L A T S S - P T - S M W V S W T - G - D S Q I G S N V T P L D P S T V A - S I C E Y G - I D -  
-- D M P L D S D V F K V P P G P N T P Q Q V H I T Q G N - H E G N G V I I S W T - P - S A - P C S - N T V R Y W - S -  
-- P E A V H I A Y G E - D I - H D I V V T W S T R Q D - T Q E - S I V E Y G - I N -  
-- I S W I T - G - D F Q I C Y S I T P L D P A R V A - S I V R Y G - T -
```

Protein structure prediction

query sequence

MAFFT

```
CRKCKALACYTADVR-VIEECHYTQL  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CINCMVAVGHSGLR-KVEGTHHVNV  
CKKCCKQACCGTDIQ-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAIICTSKDIR-SR-NTQYLVC  
CRSCFAASVCSGGDIR-KIENSHHVNV  
CKKCNQKACDAAEILR-LIEGAHHVHP  
CRGCSQEVTGEDIE-VIEDITHRVNV  
CRSCFAASVCSGGDIR-KIENSHHVNV  
CINCMVAVGYSGLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSYTQL  
CGKCKAYACSTDDIR-IIGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHHMII  
---AFACYTADIR-MVEKCHFTVV  
CKNGVPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDIH-JIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAFACYTADIR-VVEECHYTVV  
CINCMVAVGHSGLR-KVEGTHHVNV  
CRKCKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHVVV  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CGKCKVLACAYANDIR-JVEESHHTVI  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CKNCHKLICSGEDIQ-VIENMHHVSV  
CRGCFVPVAFGNDIK-VIENAHHVNI
```

query MSA

template MSAs

what program?

template structure 1

template structure 2

template structure 3

```
E E C H Y T V L G D A F K - E C F V S R P H P K - - P K  
E K M H H V N M T P E F K - E L Y I V R E N K A - L Q K  
E G T H H V N V N P N F S - N Y Y N V S R D P V V I N K  
A T A H H V N T T P K F K - T L Y S K G P N K T - L Q E  
N H Q H H V V V D A G F I - E R A E I V Q Y P A I K H K  
- N T Q Y L V C D P G F W - S L V R K T R L T D - E Q Q  
E N S H H V N V N T E F N E T M F I M P E N K P Q F S N  
E G A H H V H P D P E F L - R N V G K A D E A E E P L Q  
E D I H R V N V T P Q F R - E L F I R K E S T K - R K D  
E N S H H V N V N T E F K - N H Y K V G D Q - V N M E R  
E G T H H V N V N P N F S - J Y Y K V S P K A V V I D R  
E T S H Y T V L G D A F K - E R F V C K P H P K - - P K  
K G S H H I V L G N A F Q - E R Y T T K P H R K - - P V  
K D S H H M I I D K T F K - D R Y I T K K H P K - - P R
```

```
C V N C N V A V C R G S D I R - T V E A M  
C R N C F K Q V A S G S D I R - L L D K A  
C R Q C S V F V C S G E D I E - I I E K M  
C R S C S Q E V C T G R D I E - I M A N I  
C K N C S M I A L C T G E D I Y - V I E N M  
C R K C K A L A C Y T A D V R - V I E --  
C K N C S V L A C S G E D I H - I I E K M  
C K G C K T E V T K S D Q F R - H I E K Q  
C I K C F K E A C S L D D I R - C I K N M  
C K H C R Q F A C Y T D D I R - S I N G Q  
---  
C K K C N V Q A C S G E D I Q - V I E N M  
C G K C K T F A C Y T A D I R - V V E E C  
C R K C N T F A C E A C D F R - C V S G S  
C R N C F K Q V A S G S D I R - L L D K A  
C R K C D G I L L C T S Q D I S - S R Q D N  
C R K C H V F I C Q A H E I K - R V R D S  
C K N C S K S I C S G E D I Q V V I E D M  
C I N C M V S V G Y C S D L R - K V E G T  
C V K C K E F A C N V S D F R - K V K E N  
C R N C F K Q V A S G S D I R - L L D K A
```

```
-- D M P L D S D V F Q V P P G Y N A P Q Q V H I T Q G D - H D G K A V J V S W T - E - D E - T T E - S I V E Y G - I G  
-- D M P L D S D V F R V P P G Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - V - D E - P G S - S N V L Y W - S -  
-- E E M P L E T F P P P A C Y N A P E Q V H I T Q G D - H A G R G M I I S W T - P L N E - S V P - S V V D Y G - T -  
-- D M P L D S D V F R V P P G Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - V - D E - D G S - N V V T Y W I A N -  
-- P E Q V H L A F G E S T A - S E I V V T W S T R E L - I V V T W N T R N N - P P S - A E S I V E Y G - I T -  
-- D L P M D H P R I L R R N V T S F F P E Q I S L A T S S - P T - S M W V S W T - G - D S Q I G S N V T P L D P S T V A - S I C E Y G - I D -  
-- D M P L D S D V F K V P P G P N T P Q Q V H I T Q G N - H E G N G V I I S W T - P - S A - P C S - N T V R Y W - S -  
-- P E A V H I A Y G E D I - H D I V V T W S T R Q D - T Q E - S I V E Y G - I N -  
-- I S W I T - G - D F Q I G Y S I T P L D P A R V A - S I V R Y G - T -
```

Protein structure prediction

query sequence

MAFFT

```
CRKCKALACYTADVR-VIEECHYTQL  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CINCMVAVGHSGLR-KVEGTHHVNV  
CKKCCKQACCGTDIQ-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAIICTSKDIR-SR-NTQYLVC  
CRSCFAASVCSGGDIR-KIENSHHVNV  
CKKCNQKACDAAEILR-LIEGAHHVHP  
CRGCSQEVTGEDIE-VIEDITHRVNV  
CRSCFAASVCSGGDIR-KIENSHHVNV  
CINCMVAVGYSGLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSYTQL  
CGKCKAYACSTDDIR-IIGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHHMII  
---AFACYTADIR-MVEKCHFTVV  
CKNGVPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDIH-JIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAFACYTADIR-VVEECHYTVV  
CINCMVAVGHSGLR-KVEGTHHVNV  
CRKCKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHVVV  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CGKCKVLVLAICYANDIR-JVEESHHTVI  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CKNCCKLICSGEDIQ-VIENMHHVSV  
CRGCFPVAFGNDIK-VIENAHHVNI
```

query MSA

template MSAs

```
E E C H Y T V L G D A F K - E C F V S R P H P K - - P K  
E K M H H V N M T P E F K - E L Y I V R E N K A - L Q K  
E G T H H V N V N P N F S - N Y Y N V S R D P V V I N K  
A T A H H V N T T P K F K - T L Y S K G P N K T - L Q E  
N H Q H H V V V D A G F I - E R A E I V Q Y P A I K H K  
- N T Q Y L V C D P G F W - S L V R K T R L T D - E Q Q  
E N S H H V N V N T E F N E T M F I M P E N K P Q F S N  
E G A H H V H P D P E F L - R N V G K A D E A E E P L Q  
E D I H R V N V T P Q F R - E L F I R K E S T K - R K D  
E N S H H V N V N T E F K - N H Y K V G D Q - V N M E R  
E G T H H V N V N P N F S - J Y Y K V S P K A V V I D R  
E T S H Y T V L G D A F K - E R F V C K P H P K - - P K  
K G S H H I V L G N A F Q - E R Y T T K P H R K - - P V  
K D S H H M I I D K T F K - D R Y I T K K H P K - - P R
```

```
C V N C N V A V C R G S D I R - T V E A M  
C R N C F K Q V A S G S D I R - L L D K A  
C R Q C S V F V C S G E D I E - I I E K M  
C R S C S Q E V C T G R D I E - I M A N I  
C K N C S M I A L C T G E D I Y - V I E N M  
C R K C K A L A C Y T A D V R - V I E --  
C K N C S V L A C S C E D I H - I I E K M  
C K G C K T E V T K S D Q F R - H I E K Q  
C I K C F K E A C S L D D I R - C I K N M  
C K H C R Q F A C Y T D D I R - S I N G Q  
---  
C K K C N V Q A C S G E D I Q - V I E N M  
C G K C K T F A C Y T A D I R - V V E E C  
C R K C N T F A C E A C D F R - C V S G S  
C R N C F K Q V A S G S D I R - L L D K A  
C R K C D G I L L C T S Q D I S - S R Q D N  
C R K C H V F I C Q A H E I K - R V R D S  
C K N C S K S I C S G E D I Q V V I E D M  
C I N C M V S V G Y C S D L R - K V E G T  
C V K C K E F A C N V S D F R - K V K E N  
C R N C F K Q V A S G S D I R - L L D K A
```

template structure 1

template structure 2

template structure 3

```
-- D M P L D S D V F Q V P P C Y N A P Q Q V H I T Q G D - H D G K A V J V S W T - E - D E - T T E - S I V E Y G - I G  
-- D M P L D S D V F R V P P C Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - V - D E - P G S - S N V L Y W - S -  
-- E E M P L E T F P P P A C Y N A P E Q V H I T Q G D - H A G R G M I I S W T - P L N E - S V P - S V V D Y G - T -  
-- D M P L D S D V F R V P P C Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - V - D E - D G S - N V V T Y W I A N -  
-- P E Q V H L A F G E S T A - S E I V V T W S T R E L - I V V T W N T R N N - P P S - A E S I V E Y G - I T -  
-- D L P M D H P R L - R R N V T S F F P E Q I S L A T S S - P T - S M W V S W T - G - D S Q I G S N V T P L D P S T V A - S I C E Y G - I D -  
-- D M P L D S D V F K V P P G P N T P Q Q V H I T Q G N - H E G N G V I I S W T - P - S A - P C S - N T V R Y W - S -  
-- P E A V H I A Y G E - D I - H D I V V T W S T R Q D - T Q E - S I V E Y G - I N -  
-- I S W I T - G - D F Q I C Y S I T P L D P A R V A - S I V R Y G - T -
```

Protein structure prediction

query sequence

MAFFT

```
CRKCKALACYTADVR-VIEECHYTQL  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CINCMVAVGHSGLR-KVEGTHHVNV  
CKKCCKQACCGTDIQ-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAIICTSKDIR-SR-NTQYLVC  
CRSCFAASVCSGGDIR-KIENSHHVNV  
CKKCNQKACDAAEILR-LIEGAHHVHP  
CRGCSQEVTGEDIE-VIEDITHRVNV  
CRSCFAASVCSGGDIR-KIENSHHVNV  
CINCMVAVGYSGLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSYTQL  
CGKCKAYACSTDDIR-IIGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHHMII  
---AFACYTADIR-MVEKCHFTVV  
CKNCGVPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDIH-JIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAFACYTADIR-VVEECHYTVV  
CINCMVAVGHSGLR-KVEGTHHVNV  
CRKCKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHVVV  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CGKCKVLACYANDIR-JVEESHHTVI  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CKNCCKLICSGEDIQ-VIENMHHVSV  
CRGCFPVAFGNDIK-VIENAHHVNI
```

query MSA

template MSAs

```
E E C H Y T V L G D A F K - E C F V S R P H P K - - P K  
E K M H H V N M T P E F K - E L Y I V R E N K A - L Q K  
E G T H H V N V N P N F S - N Y Y N V S R D P V V I N K  
A T A H H V N T T P K F K - T L Y S K G P N K T - L Q E  
N H Q H H V V V D A G F I - E R A E I V Q Y P A I K H K  
- N T Q Y L V C D P G F W - S L V R K T R L T D - E Q Q  
E N S H H V N V N T E F N E T M F I M P E N K P Q F S N  
E G A H H V H P D P E F L - R N V G K A D E A E E P L Q  
E D I H R V N V T P Q F R - E L F I R K E S T K - R K D  
E N S H H V N V N T E F K - N H Y K V G D Q - V N M E R  
E G T H H V N V N P N F S - J Y Y K V S P K A V V I D R  
E T S H Y T V L G D A F K - E R F V C K P H P K - - P K  
K G S H H I V L G N A F Q - E R Y T T K P H R K - - P V  
K D S H H M I I D K T F K - D R Y I T K K H P K - - P R
```

```
C V N C N V A V C R G S D I R - T V E A M  
C R N C F K Q V A S G S D I R - L L D K A  
C R Q C S V F V C S G E D I E - I I E K M  
C R S C S Q E V C T G R D I E - I M A N I  
C K N C S M I A L C T G E D I Y - V I E N M  
C R K C K A L A C Y T A D V R - V I E --  
C K N C S V L A C S C E D I H - I I E K M  
C K G C K T E V T K S D Q F R - H I E K Q  
C I K C F K E A C S L D D I R - C I K N M  
C K H C R Q F A C Y T D D I R - S I N G Q  
---  
C K K C N V Q A C S G E D I Q - V I E N M  
C G K C K T F A C Y T A D I R - V V E E C  
C R K C N T F A C E A C D F R - C V S G S  
C R N C F K Q V A S G S D I R - L L D K A  
C R K C D G I L L C T S Q D I S - S R Q D N  
C R K C H V F I C Q A H E I K - R V R D S  
C K N C S K S I C S G E D I Q V V I E D M  
C I N C M V S V G Y C S D L R - K V E G T  
C V K C K E F A C N V S D F R - K V K E N  
C R N C F K Q V A S G S D I R - L L D K A
```

```
-- D M P L D S D V F Q V P P G Y N A P Q Q V H I T Q G D - H D G K A V J V S W T - E - D E - T T E - S I V E Y G - I G  
-- D M P L D S D V F R V P P G Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - V - D E - P G S - S N V L Y W - S -  
-- E E M P L E T F P P P A C Y N A P E Q V H I T Q G D - H A G R G M I I S W T - P L N E - S V P - S V V D Y G - T -  
-- D M P L D S D V F R V P P G Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - V - D E - D G S - N V V T Y W I A N -  
-- P E Q V H L A F G E S T A - S E I V V T W S T R E L - I V V T W N T R N N - P P S - A E S I V E Y G - I T -  
-- D M P M D H P R L - R R N V T S F F P E Q I S L A T S S - P T - S M W V S W T - G - D S Q I G S N V T P L D P S T V A - S I C E Y G - I D -  
-- D M P L D S D V F K V P P G P N T P Q Q V H I T Q G N - H E G N G V I I S W T - P - S A - P C S - N T V R Y W - S -  
-- P E A V H I A Y G E - D I - H D I V V T W S T R Q D - T Q E - S I V E Y G - I N -  
-- I S W I T - G - D F Q I C Y S I T P L D P A R V A - S I V R Y G - T -
```

MAFFTash

template structure 1

template structure 2

template structure 3

Protein structure prediction

query sequence

MAFFT

```
CRKCKALACYTADVR-VIEECHYTQL  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CINCMVAVGHSGLR-KVEGTHHVNV  
CKKCCKQACCGTDIQ-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAIICTSKDIR-SR-NTQYLVC  
CRSCFASVCSGGDIR-KIENSHHVNP  
CKKCCKQACDAAELR-LIEGAHHVHP  
CRGCSQEVTGEDIE-VIEDITHRVNV  
CRSCFASVCSGGDIR-KIENSHHVNV  
CINCMVAVGYSGLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSYTQL  
CGKCKAYACSTDDIR-IIGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHMII  
---AFACYTADIR-MVEKCHFTVV  
CKNGVPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDIH-JIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAFACYTADIR-VVEECHYTVV  
CINCMVAVGHSGLR-KVEGTHHVNV  
CRKCKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHVVV  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CGKCKVLACYANDIR-JVEESHHTVI  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CKNCCKLICSGEDIQ-VIENMHHVSV  
CRGCFPVAFGNDIK-VIENAHHVNI
```

query MSA

template MSAs

```
E E C H Y T V L G D A F K - E C F V S R P H P K - - P K  
E K M H H V N M T P E F K - E L Y I V R E N K A - L Q K  
E G T H H V N V N P N F S - N Y Y N V S R D P V V I N K  
A T A H H V N T T P K F K - T L Y S K G P N K T - L Q E  
N H Q H H V V V D A G F I - E R A E I V Q Y P A I K H K  
- N T Q Y L V C D P G F W - S L V R K T R L T D - E Q Q  
E N S H H V N V N T E F N E T M F I M P E N K P Q F S N  
E G A H H V H P D P E F L - R N V G K A D E A E E P L Q  
E D I H R V N V T P Q F R - E L F I R K E S T K - R K D  
E N S H H V N V N T E F K - N H Y K V G D Q - V N M E R  
E G T H H V N V N P N F S - J Y Y K V S P K A V V I D R  
E T S H Y T V L G D A F K - E R F V C K P H P K - - P K  
K G S H H I V L G N A F Q - E R Y T T K P H R K - - P V  
K D S H H M I I D K T F K - D R Y I T K K H P K - - P R
```

```
C V N C N V A V C R G S D I R - T V E A M  
C R N C F K Q V A S G S D I R - L L D K A  
C R Q C S V F V C S G E D I E - I I E K M  
C R S C S Q E V C T G R D I E - I M A N I  
C K N C S M I A L C T G E D I Y - V I E N M  
C R K C K A L A C Y T A D V R - V I E - -  
C K N C S V L A C S G E D I H - I I E K M  
C K G C K T E V T K S D Q F R - H I E K Q  
C I K C F K E A C S L D D I R - C I K N M  
C K H C R Q F A C Y T D D I R - S I N G Q  
---  
C K K C N V Q A C S G E D I Q - V I E N M  
C G K C K T F A C Y T A D I R - V V E E C  
C R K C N T F A C E A C D F R - C V S G S  
C R N C F K Q V A S G S D I R - L L D K A  
C R K C D G I L L C T S Q D I S - S R Q D N  
C R K C H V F I C Q A H E I K - R V R D S  
C K N C S K S I C S G E D I Q V V V I E D M  
C I N C M V S V G Y C S D L R - K V E G T  
C V K C K E F A C N V S D F R - K V K E N  
C R N C F K Q V A S G S D I R - L L D K A
```

```
-- D M P L D S D V F Q V P P G Y N A P Q Q V H I T Q G D - H D G K A V J V S W T - - E - D E - T T E - S I V E Y G - I G  
-- D M P L D S D V F R V P P G Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - - V - D E - P G S - S N V L Y W - S -  
-- E E M P L E T F P P P A C Y N A P E Q V H I T Q G D - H A G R G M I I S W T - - P L N E - S V P - S V V D Y G - T -  
-- D M P L D S D V F R V P P G Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - - V - D E - D G S - N V V T Y W I A N -  
-- P E Q V H L A F G E S T A - S E I V V T W S T R E L - I V V T W N T R N N - P P S - A E S I V E Y G - I T -  
-- D M P M D H P R L - R R N V T S F F P E Q I S L A T S S - P T - S M W V S W T - - G - D S Q I G S N V T P L D P S T V A - S I C E Y G - I D -  
-- D M P L D S D V F K V P P G P N T P Q Q V H I T Q G N - H E G N G V I I S W T - - P - S A - P C S - N T V R Y W - S -  
-- P E A V H I A Y G E - D I - H D I V V T W S T R Q D - T Q E - S I V E Y G - I N -  
-- I S W I T - - G - D F Q I G Y S I T P L D P A R V A - - - S I V R Y G - - T -
```

MAFFTash

template structure 1

MAFFTash

template structure 2

template structure 3

Protein structure prediction

query sequence

MAFFT

```
CRKCKALACYTADVR-VIEECHYTQL  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CINCMVAVGHSGLR-KVEGTHHVNV  
CKKCCKQACCGTDIQ-VIATAHHVNT  
CKKCKKVATTSDKFQ-HINHQHHVVV  
CKKCEAAILCTSKDIR-SR-NTQYLVC  
CRSCFAAVCSGGDIR-KIENSHHVNV  
CKKCNQKACDAAEILR-LIEGAHHVHP  
CRGCSQEVTGEDIE-VIEDITHRVNV  
CRSCFAAVCSGGDIR-KIENSHHVNV  
CINCMVAVGYSGLR-KVEGTHHVNV  
CGKCKNFACYTADIR-VVETSYTQL  
CGKCKAYACSTDDIR-IIGSHHIVL  
CKKCKTYACNTDDIR-VIKDSHHMII  
-AFACYTADIR-MVEKCHFTVV  
CKNGVPACSGEDIH-VIEKMHHVNM  
CRQCSVFCSGEDIH-JIEKMHHVNV  
CRNCFRQVASGSDIR-LVDNTHYVNI  
CRKCKAFACYTADIR-VVEECHYTVV  
CINCMVAVGHSGLR-KVEGTHHVNV  
CRKCKALACYTADVR-VIEECHYTQL  
CRKCKAFACYTADIR-VVEECHYTVV  
CKHCDALVCHSADIR-IVPGGHVVV  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CGKCKVLAACYANDIR-JVEESHHTVI  
CRCCSQAVALHGDDFR-TIEGTHYVNI  
CKNCVLAACSGEDIH-VIEKMHHVNM  
CKNCCKLICSGEDIQ-VIENMHHVSV  
CRGCFPVAFGNDIK-VIENAHHVNI
```

query MSA

template MSAs

```
E E C H Y T V L G D A F K - E C F V S R P H P K - - P K  
E K M H H V N M T P E F K - E L Y I V R E N K A - L Q K  
E G T H H V N V N P N F S - N Y Y N V S R D P V V I N K  
A T A H H V N T T P K F K - T L Y S K G P N K T - L Q E  
N H Q H H V V V D A G F I - E R A E I V Q Y P A I K H K  
- N T Q Y L V C D P G F W - S L V R K T R L T D - E Q Q  
E N S H H V N V N T E F N E T M F I M P E N K P Q F S N  
E G A H H V H P D P E F L - R N V G K A D E A E E P L Q  
E D I H R V N V T P Q F R - E L F I R K E S T K - R K D  
E N S H H V N V N T E F K - N H Y K V G D Q - V N M E R  
E G T H H V N V N P N F S - J Y Y K V S P K A V V I D R  
E T S H Y T V L G D A F K - E R F V C K P H P K - - P K  
K G S H H I V L G N A F Q - E R Y T T K P H R K - - P V  
K D S H H M I I D K T F K - D R Y I T K K H P K - - P R
```

```
C V N C N V A V C R G S D I R - T V E A M  
C R N C F K Q V A S G S D I R - L L D K A  
C R Q C S V F V C S G E D I E - I I E K M  
C R S C S Q E V C T G R D I E - I M A N I  
C K N C S M I A L C T G E D I Y - V I E N M  
C R K C K A L A C Y T A D V R - V I E - -  
C K N C S V L A C S G E D I H - I I E K M  
C K G C K T E V T K S D Q F R - H I E K Q  
C I K C F K E A C S L D D I R - C I K N M  
C K H C R Q F A C Y T D D I R - S I N G Q  
- - - - -  
C K K C N V Q A C S G E D I Q - V I E N M  
C G K C K T F A C Y T A D I R - V V E E C  
C R K C N T F A C E A C D F R - C V S G S  
C R N C F K Q V A S G S D I R - L L D K A  
C R K C D G I L L C T S Q D I S - S R Q D N  
C R K C H V F I C Q A H E I K - R V R D S  
C K N C S K S I C S G E D I Q V V I E D M  
C I N C M V S V G Y C S D L R - K V E G T  
C V K C K E F A C N V S D F R - K V K E N  
C R N C F K Q V A S G S D I R - L L D K A
```

```
- D M P L D S D V F Q V P P C Y N A P Q Q V H I T Q G D - H D G K A V J V S W T - E - D E - T T E - S I V E Y G - I G  
- P Q Q V H I S L A G - E K - H M R V T F V T - D - D N - P G S - S N V L Y W - S -  
- E E M P L E T F P P P A C Y N A P E Q V H I T Q G D - H A G R G M I I S W T - P L N E - S V P - S V V D Y G - T -  
- D M P L D S D V F R V P P P C Y N A P Q Q V H I T Q G D - H V G K A M I V S W T - V - D E - D G S - N V V T Y W I A N -  
- P E Q V H L A F G E S T A - S E I V V T W S T R E L - I V V T W N T R N N - P P S - A E S I V E Y G - I T -  
- D P M D H P R L - R R N V T S F F P E Q I S L A T S S - P T - S M W V S W T - G - D S Q I G S N V T P L D P S T V A - S I C E Y G - I D -  
- D M P L D S D V F K V P P G P N T P Q Q V H I T Q G N - H E G N G V I I S W T - P - S A - P C S - N T V R Y W - S -  
- P E A V H I A Y G E - D I - H D I V V T W S T R Q D - T Q E - S E V W Y G - K -  
- I S W I T - G - D F Q I C Y S I T P L D P A R V A - S I V R Y G - T -
```

MAFFTash

template structure 1

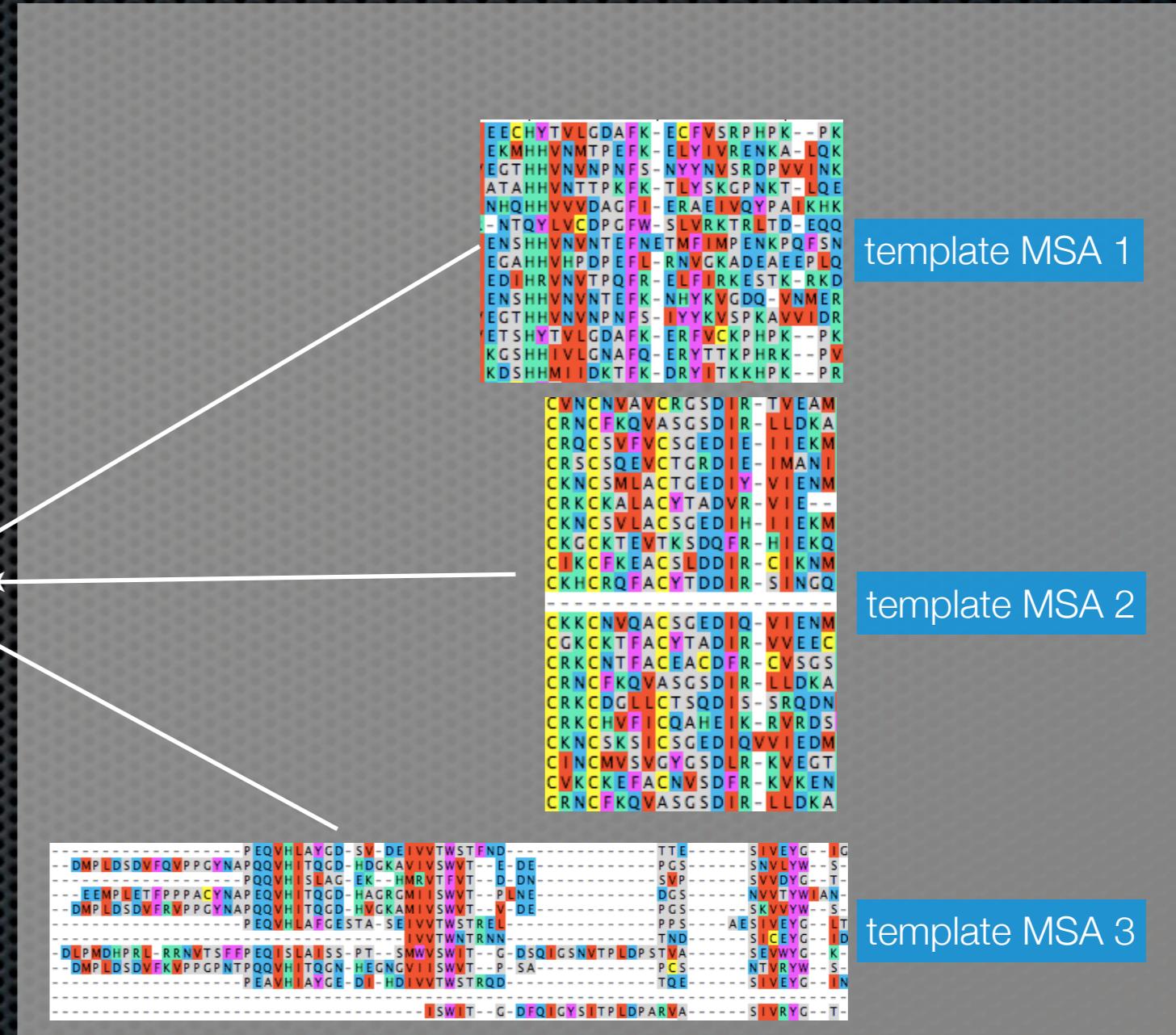
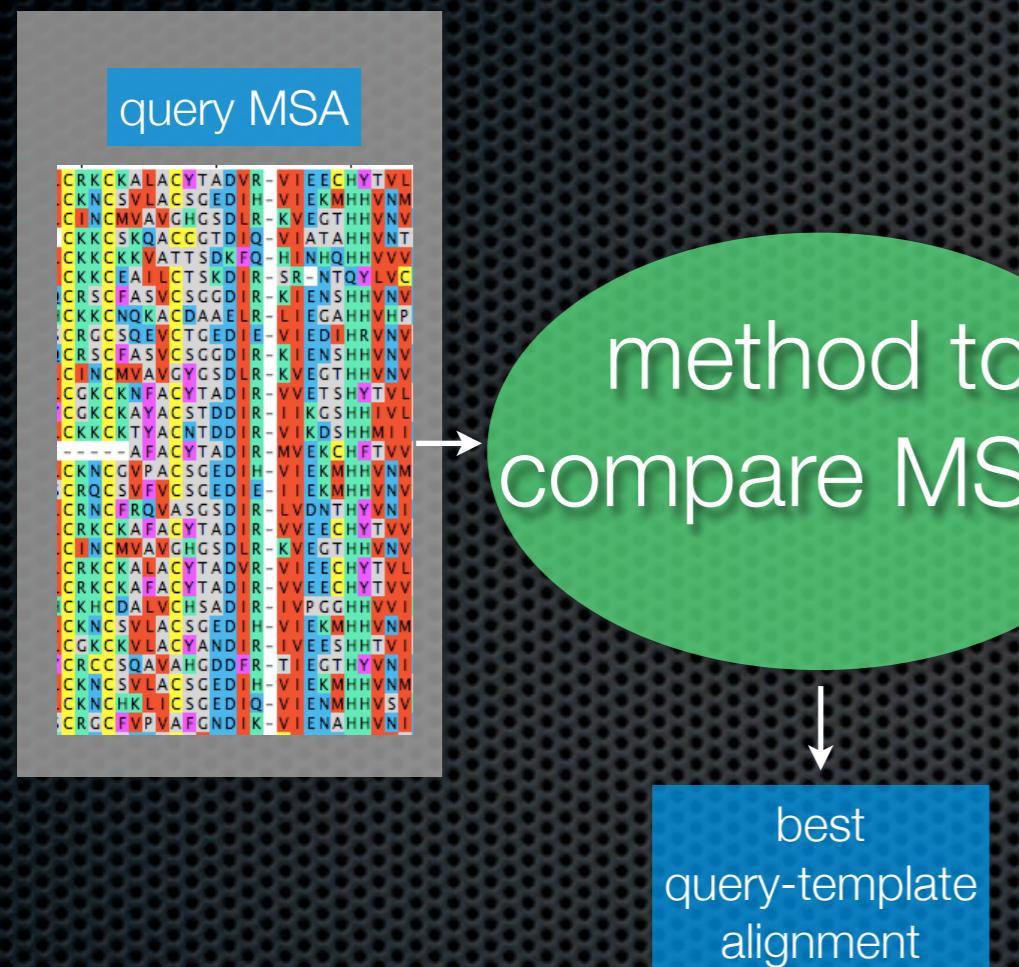
MAFFTash

template structure 2

MAFFTash

template structure 3

Protein structure prediction



PDBj 

Sequence to Function Annotation Server

Please enter your query

Name:

Sequence:

Or

Upload a FASTA-formatted sequence file: no file selected

Select Alignment methods

<input checked="" type="checkbox"/> Blast	<input type="radio"/> Whole PDB	<input type="radio"/> Rep. Domains
<input checked="" type="checkbox"/> PsiBlast	<input type="radio"/> Whole PDB	<input checked="" type="radio"/> Rep. Domains
<input checked="" type="checkbox"/> HHpred	<input checked="" type="radio"/> PDB + SCOP	

Send results to this email address

[Send feedback](#) [About SFAS](#)

PDBj 

Sequence to Function Annotation Server

Please enter your query

Name: Sequence:

```
AVLFLLMCTFALIAHWLACIWIYAIQNMEQPHMDSRIGWLHNLGDQIGKP  
YNSSGLGGPSIKDKYVTALYFTSSLTSVFGNVSPNTNSEKIFSICVMLI  
GSLMYASIFGNVSATIQRLYSGTARY
```

Or

Upload a FASTA-formatted sequence file: no file selected

Select Alignment methods

<input checked="" type="checkbox"/> Blast	<input type="radio"/> Whole PDB	<input checked="" type="radio"/> Rep. Domains
<input checked="" type="checkbox"/> PsiBlast	<input type="radio"/> Whole PDB	<input checked="" type="radio"/> Rep. Domains
<input checked="" type="checkbox"/> HHpred	<input checked="" type="radio"/> PDB + SCOP	

Send results to this email address

[Send feedback](#) [About SFAS](#)

Example: hERG potassium channel protein

hERG Results

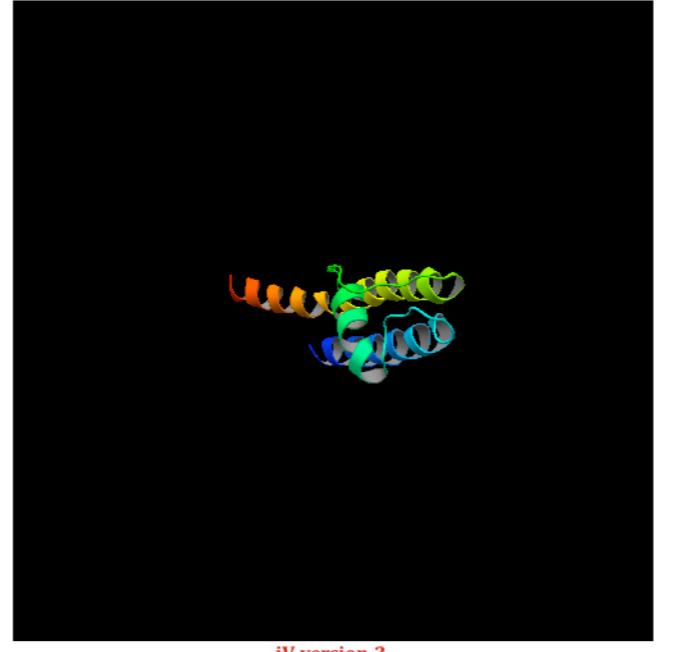
Method	Template	E-value	Coverage	Alignment	Model
HHpred	2r9rB	jV 1.10e-19	75	Text Jalview	Spanner
HHpred	1orqC	jV 9.70e-20	46	Text Jalview	Spanner
HHpred	3behA	jV 2.20e-19	75	Text Jalview	Spanner
HHpred	1xl4A	jV 8.20e-17	47	Text Jalview	Spanner
HHpred	2a9hA	jV 3.70e-17	49	Text Jalview	Spanner
HHpred	2ih3C	jV 4.10e-16	48	Text Jalview	Spanner
HHpred	2q67A	jV 2.40e-16	67	Text Jalview	Spanner
HHpred	2qksA	jV 5.60e-13	45	Text Jalview	Spanner
Psiblast	1lnqG	jV 1.74e-08	40	Text Jalview	Spanner
Psiblast	1lnqH	jV 1.74e-08	40	Text Jalview	Spanner
Psiblast	1lnqB	jV 1.74e-08	40	Text Jalview	Spanner
Psiblast	1lnqA	jV 1.74e-08	40	Text Jalview	Spanner
Psiblast	1lnqF	jV 1.74e-08	40	Text Jalview	Spanner
Psiblast	1lnqE	jV 1.74e-08	40	Text Jalview	Spanner
Psiblast	1lnqC	jV 1.74e-08	40	Text Jalview	Spanner
Psiblast	1lnqD	jV 1.74e-08	40	Text Jalview	Spanner
Psiblast	1orqC	jV 1.67e-07	42	Text Jalview	Spanner
Psiblast	2a0lB	jV 4.19e-07	41	Text Jalview	Spanner
Blast	1ujlA	jV 8.03e-20	33	Text Jalview	Spanner
Blast	2q6aB	jV 7.93e-04	29	Text Jalview	Spanner
Blast	2q67B	jV 7.48e-04	29	Text Jalview	Spanner
Blast	2q67A	jV 7.24e-04	29	Text Jalview	Spanner
Blast	2ahzB	jV 8.62e-04	29	Text Jalview	Spanner
Blast	3e89B	jV 1.03e-03	31	Text Jalview	Spanner
Blast	3e8hB	jV 1.03e-03	31	Text Jalview	Spanner
Blast	2q6aA	jV 8.13e-04	29	Text Jalview	Spanner
Blast	2ahyA	jV 8.84e-04	29	Text Jalview	Spanner
Blast	3e83B	jV 1.03e-03	31	Text Jalview	Spanner

Method	Template	E-value	Coverage	Alignment	Model
HHpred	2r9rB	jV 1.10e-19	75	Text Jalview	Spanner

SFAS results for HHpred alignment

J. Söding, A. Biegert, A. N. Lupas (2005) “The HHpred interactive server for protein homology detection and structure prediction.” Nucleic Acids Res, 33:W244-248.

2r9rB_hhpred



jV version 3

Method	Template	E-value	Coverage	Alignment	Model
HHpred	2r9rB	jV 1.10e-19	75	Text Jalview	Spanner

SFAS results for HHpred alignment

J. Söding, A. Biegert, A. N. Lupas (2005) "The HHpred interactive server for protein homology detection and structure prediction." Nucleic Acids Res, 33:W244-248.

2r9rB_hhpred

jV version 3

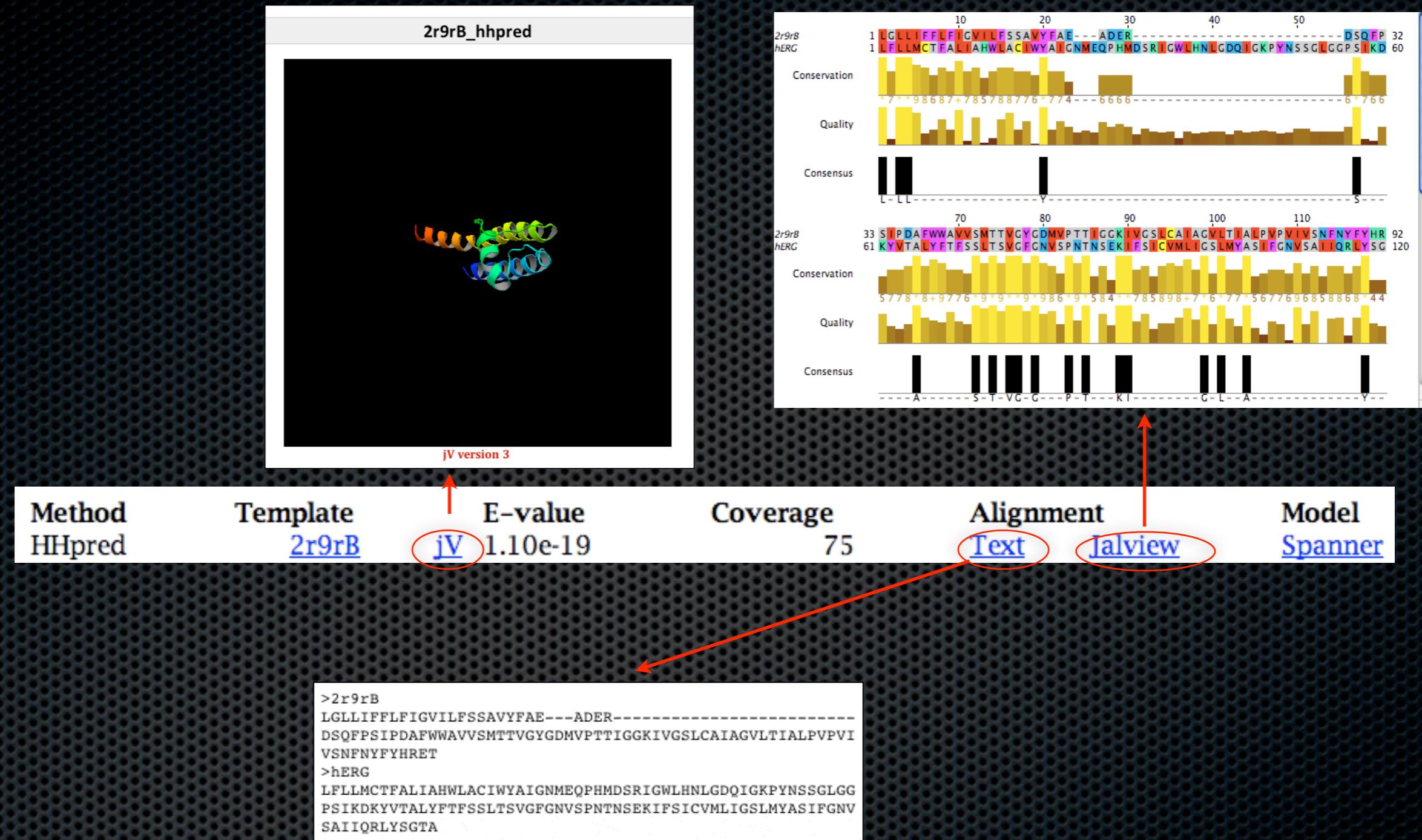
Method	Template	E-value	Coverage	Alignment	Model
HHpred	2r9rB	jV 1.10e-19	75	Text	Jalview

[Text](#)

```
>2r9rB
LGLLIFFLFIGVILFSSAVYFAE---ADER-----
DSQFPSIPDAFWAWVSMTTVGYGDMVPTTIGGKIVGSLCAIAGVLTIALPVPVI
VSNFNYFYHRET
>hERG
LFLLMCTFALIAHWLACIWAIGNMEQPHMDSRIGWLHNLDQIGKPYNSSGLGG
PSIKDKYVTALYFTFSSLTSVGFGNVSPNTNSEKIFSICVMLIGSLMYASIFGNV
SAIIQRLYSGTA
```

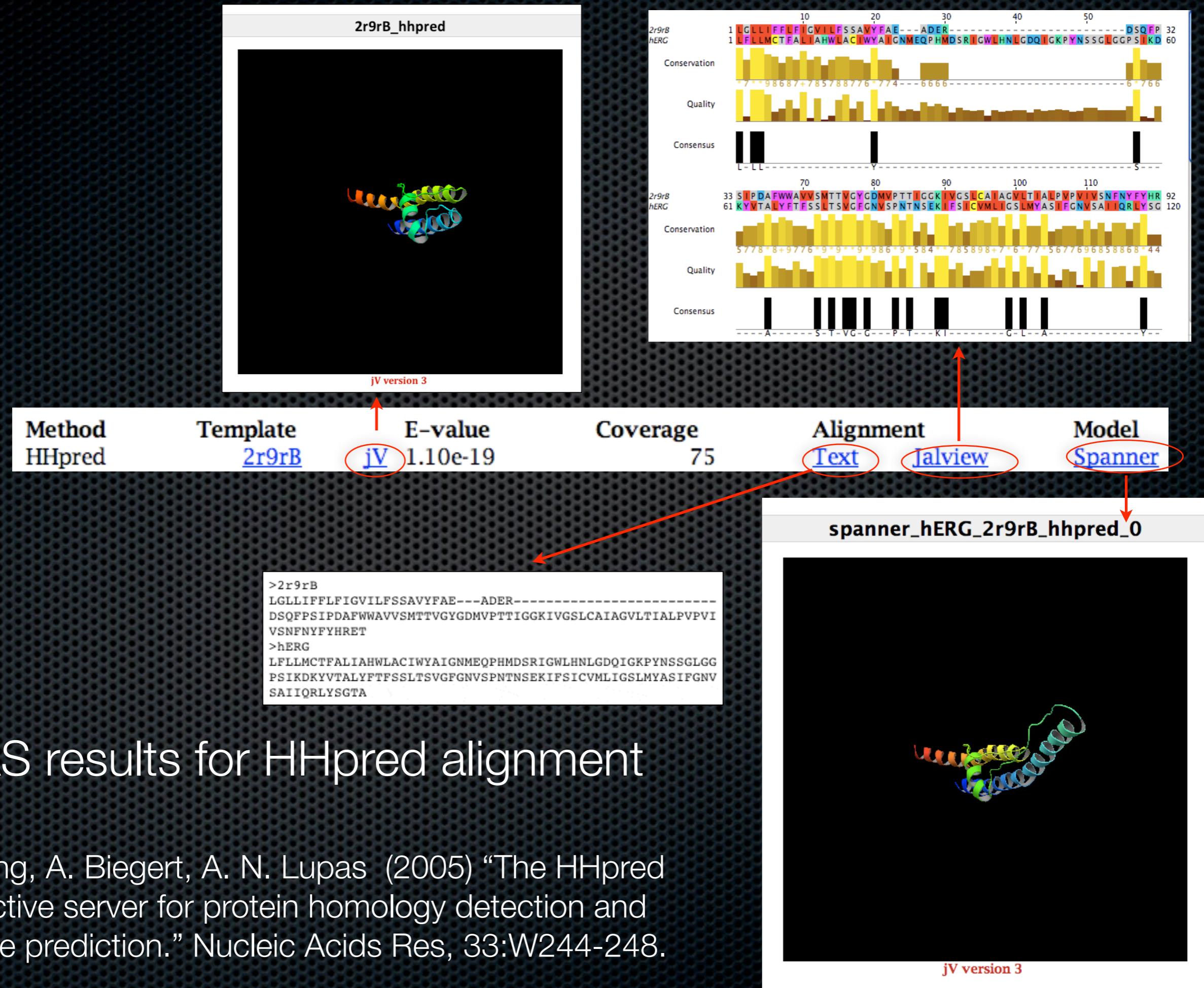
SFAS results for HHpred alignment

J. Söding, A. Biegert, A. N. Lupas (2005) "The HHpred interactive server for protein homology detection and structure prediction." Nucleic Acids Res, 33:W244-248.



SFAS results for HHpred alignment

J. Söding, A. Biegert, A. N. Lupas (2005) "The HHpred interactive server for protein homology detection and structure prediction." Nucleic Acids Res, 33:W244-248.



SFAS results for HHpred alignment

J. Söding, A. Biegert, A. N. Lupas (2005) "The HHpred interactive server for protein homology detection and structure prediction." Nucleic Acids Res, 33:W244-248.

Spanner

Spanner is a structural homology modeling program—that is, it threads a specific amino-acid sequence onto a specific PDB structure, patching up the gaps as best it can.

To create a model, you must provide a template structure, as well as an alignment of the sequence you wish to model onto the template sequence. Spanner will replace matching residues, fill any gaps caused by inserted or deleted residues, and thermodynamically optimize the resulting structure.

The resulting PDB, as well as a log file, will be emailed to you when the modeling task finishes. If an error prevented a homology model from being generated (for example, when the alignment you provided does not match the template structure), the log file will explain which part of the modeling sequence failed.

Template PDB structure (PDB format):

[Browse...](#)

Sequence alignment (FASTA format; first sequence is the template, second sequence is the query):

[Browse...](#)

Model: (not necessary if PDB file contains only one model)

Chain: (not necessary if PDB file contains only one chain)

Email address for results:

[START!](#)

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The homo-tetramer can be generated by extracting the symmetry info from the template

PDBj 

Quaternary Structure Service

Please enter your query

Upload a PDB-formatted file: Choose File no file selected

Please enter your template ID

PDB ID: (template PDB file must contain the crystallographic symmetry info.)

[Send feedback](#) [About PDB Quat](#)

The homo-tetramer can be generated by extracting the symmetry info from the template

Monomeric model



PDBj WPI Osaka University **iFReC**

Quaternary Structure Service

Please enter your query

Upload a PDB-formatted file: Choose File no file selected

Red arrow pointing to the "Choose File" button.

Please enter your template ID

PDB ID: (template PDB file must contain the crystallographic symmetry info.)

[Send feedback](#) [About PDB Quat](#)

The homo-tetramer can be generated by extracting the symmetry info from the template

Template: 2r9rA Monomeric model



The screenshot shows the "Quaternary Structure Service" page. At the top left is the PDBj logo, and at the top right is the iFReC logo. Below the logos are two images of the protein structure: a monomeric model on the left and a homo-tetramer on the right. A red arrow points from the "Please enter your query" text to the "Choose File" button in the form below. Another red arrow points from the "Upload a PDB-formatted file:" label to the same "Choose File" button.

PDBj

iFReC

Quaternary Structure Service

Please enter your query

Upload a PDB-formatted file: Choose File no file selected

Please enter your template ID

PDB ID: (template PDB file must contain the crystallographic symmetry info.)

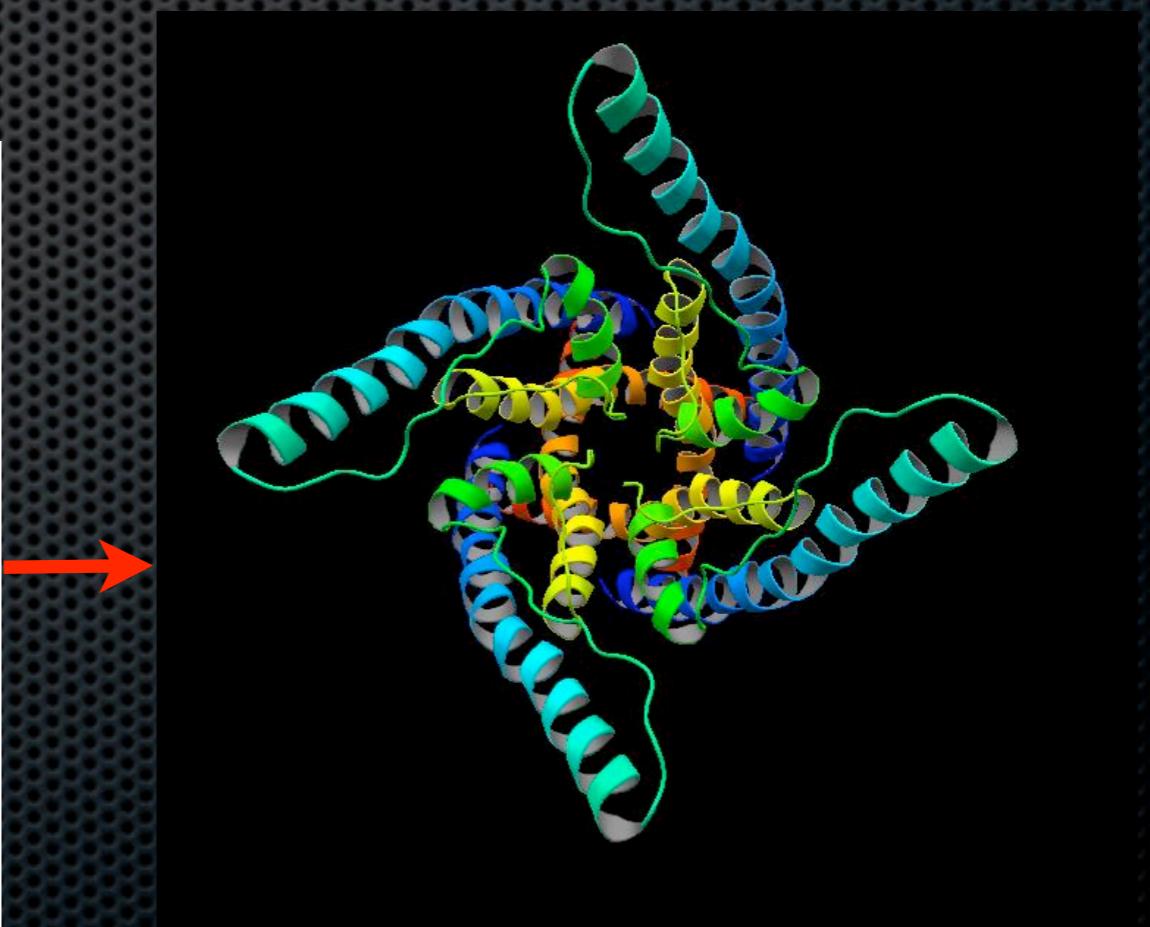
[Send feedback](#) [About PDB Quat](#)

The homo-tetramer can be generated by extracting the symmetry info from the template

Template: 2r9rA Monomeric model

The screenshot shows the "Quaternary Structure Service" interface. At the top left is the PDBj logo, and at the top right is the iFReC logo. Below the header, there is a text input field labeled "Please enter your query" and a file upload input field labeled "Upload a PDB-formatted file:" with a "Choose File" button. A red arrow points from the "Choose File" button to the monomeric model image above. Below these fields, there is a text input field labeled "Please enter your template ID" with a value of "2r9r". At the bottom of the form are "Submit" and "Clear Form" buttons, and links for "Send feedback" and "About PDB Quat".

Tetrameric model





Sequence to Function Annotation Server

Please enter your query

Name:

Sequence:

Or

Upload a FASTA-formatted sequence file: no file selected

Select Alignment methods

Blast

PsiBlast

HHpred

Whole PDB

Whole PDB

PDB + SCOP

Rep. Domains

Rep. Domains

Send results to this email address

[Send feedback](#)

[About SFAS](#)

Example 2: JUN transcription factor

PDBj 

Sequence to Function Annotation Server

Please enter your query

Name: JUN_MOUSE
Seqeunce:

```
MTAKMETTFYDDALNASFLQSESGAYGYSNPKILKQSMTLNADPGSLKPHLRAKNSDLTS  
PDVGLLKLASPELERLIIQSSNGHITTTPTPTQFLCPKVNVTDEQEGFAEGFVRALAEHLHSQNT  
LPSVTSAAPVSGAGMVAPAVASVAGAGGGGYSASLHSEPPVYANLSNPNPGALSSGGAPS  
YGAAGLAFPSQPQQQQPQPQPHLPQQIPVQHPRLQALKEEPQTPEMPGETPPLSPIDMES  
QERIKAERKRMNRNRIAASKCRKRKLERIARLEEKVKTLKAQNSELASTANMLREQVAQLKQKV  
MNHVNNSGCQLMLTQQLQTF
```

Or

Upload a FASTA-formatted sequence file: no file selected

Select Alignment methods

Blast Whole PDB Rep. Domains
 PsiBlast Whole PDB Rep. Domains
 HHpred PDB + SCOP

Send results to this email address

[Send feedback](#) [About SFAS](#)

JUN_Mouse Results

Method	Template	E-value	Coverage	Alignment	Model
HHpred	1jnma	jV 3.80e-12	19	Text	Jalview
HHpred	1fosE	jV 1.40e-11	19	Text	Jalview
HHpred	1hjba	jV 7.20e-11	19	Text	Jalview
HHpred	1ci6A	jV 8.60e-11	19	Text	Jalview
HHpred	1t2kD	jV 5.80e-11	18	Text	Jalview
HHpred	1a02F	jV 1.40e-10	17	Text	Jalview
HHpred	1gu4A	jV 1.30e-10	19	Text	Jalview
HHpred	1gd2E	jV 7.80e-10	18	Text	Jalview
HHpred	2dgca	jV 8.70e-10	17	Text	Jalview
HHpred	d1a02f	jV 2.40e-09	15	Text	Jalview
Psiblast	1t2kD	jV 9.53e-19	18	Text	Jalview
Psiblast	1t2kC	jV 4.81e-17	19	Text	Jalview
Psiblast	1fosH	jV 1.92e-16	17	Text	Jalview
Psiblast	2h7hB	jV 2.68e-16	17	Text	Jalview
Psiblast	2h7hA	jV 2.68e-16	17	Text	Jalview
Psiblast	1jnma	jV 3.09e-16	17	Text	Jalview
Psiblast	1fosE	jV 3.50e-16	18	Text	Jalview
Psiblast	1fosF	jV 5.14e-16	17	Text	Jalview
Psiblast	1jnmB	jV 4.85e-16	17	Text	Jalview
Psiblast	1s9kE	jV 4.85e-16	16	Text	Jalview
Blast	1t2kC	jV 6.52e-27	19	Text	Jalview
Blast	1fosH	jV 6.05e-25	17	Text	Jalview
Blast	2h7hA	jV 1.54e-24	17	Text	Jalview
Blast	2h7hB	jV 1.54e-24	17	Text	Jalview
Blast	1fosF	jV 2.54e-24	17	Text	Jalview
Blast	1jnmB	jV 4.87e-24	17	Text	Jalview
Blast	1jnma	jV 1.84e-23	17	Text	Jalview
Blast	1s9kE	jV 1.45e-22	16	Text	Jalview
Blast	1a02I	jV 2.34e-21	16	Text	Jalview
Blast	1junA	jV 5.01e-15	12	Text	Jalview

JUN_Mouse Results

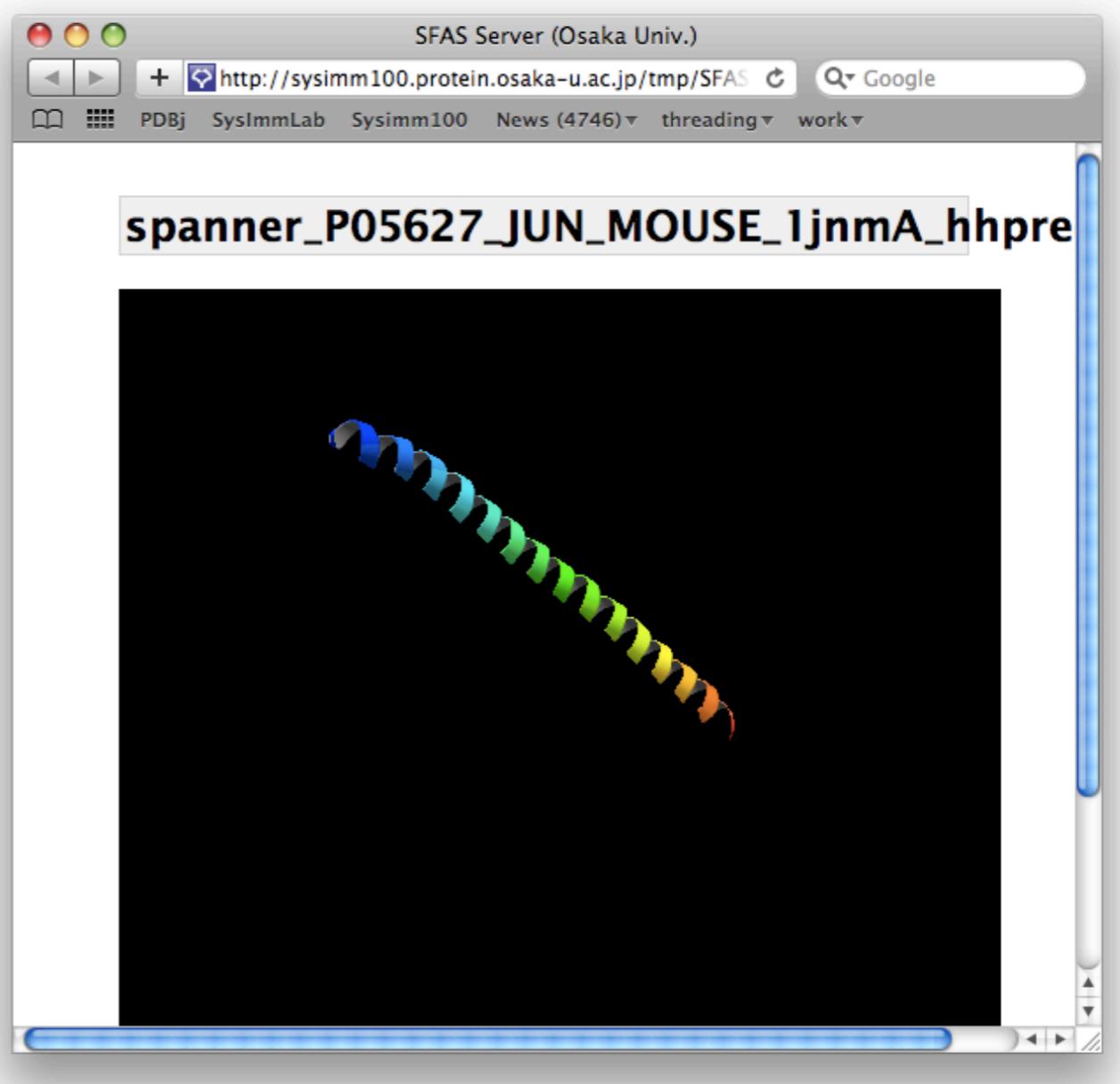
Method	Template	E-value	Coverage	Alignment	Model
HHpred	1jnma	jV 3.80e-12	19	Text Jalview	Spanner
HHpred	1fosE	jV 1.40e-11	19	Text Jalview	Spanner
HHpred	1hjba	jV 7.20e-11	19	Text Jalview	Spanner
HHpred	1ci6A	jV 8.60e-11	19	Text Jalview	Spanner
HHpred	1t2kD	jV 5.80e-11	18	Text Jalview	Spanner
HHpred	1a02F	jV 1.40e-10	17	Text Jalview	Spanner
HHpred	1gu4A	jV 1.30e-10	19	Text Jalview	Spanner
HHpred	1gd2E	jV 7.80e-10	18	Text Jalview	Spanner
HHpred	2dgca	jV 8.70e-10	17	Text Jalview	Spanner
HHpred	d1a02f	jV 2.40e-09	15	Text Jalview	Spanner
Psiblast	1t2kD	jV 9.53e-19	18	Text Jalview	Spanner
Psiblast	1t2kC	jV 4.81e-17	19	Text Jalview	Spanner
Psiblast	1fosH	jV 1.92e-16	17	Text Jalview	Spanner
Psiblast	2h7hB	jV 2.68e-16	17	Text Jalview	Spanner
Psiblast	2h7hA	jV 2.68e-16	17	Text Jalview	Spanner
Psiblast	1jnma	jV 3.09e-16	17	Text Jalview	Spanner
Psiblast	1fosE	jV 3.50e-16	18	Text Jalview	Spanner
Psiblast	1fosF	jV 5.14e-16	17	Text Jalview	Spanner
Psiblast	1jnmB	jV 4.85e-16	17	Text Jalview	Spanner
Psiblast	1s9kE	jV 4.85e-16	16	Text Jalview	Spanner
Blast	1t2kC	jV 6.52e-27	19	Text Jalview	Spanner
Blast	1fosH	jV 6.05e-25	17	Text Jalview	Spanner
Blast	2h7hA	jV 1.54e-24	17	Text Jalview	Spanner
Blast	2h7hB	jV 1.54e-24	17	Text Jalview	Spanner
Blast	1fosF	jV 2.54e-24	17	Text Jalview	Spanner
Blast	1jnmB	jV 4.87e-24	17	Text Jalview	Spanner
Blast	1jnma	jV 1.84e-23	17	Text Jalview	Spanner
Blast	1s9kE	jV 1.45e-22	16	Text Jalview	Spanner
Blast	1a02I	jV 2.34e-21	16	Text Jalview	Spanner
Blast	1junA	jV 5.01e-15	12	Text Jalview	Spanner

JUN_Mouse Results

Method	Template	E-value	Coverage	Alignment	Model
HHpred	1jnmA	jV 3.80e-12	19	Text Jalview	Spanner
HHpred	1fosE	jV 1.40e-11	19	Text Jalview	Spanner
HHpred	1hjbA	jV 7.20e-11	19	Text Jalview	Spanner
HHpred	1ci6A	jV 8.60e-11	19	Text Jalview	Spanner
HHpred	1t2kD	jV 5.80e-11	18	Text Jalview	Spanner

The Spanner model can be downloaded [here](#)
The model can be viewed in your browser [here](#)

Return to [SFAS Results](#)



PDBj



Heter-oligomer Modeling Service

Please enter your structural model

Upload a PDB-formatted file: [Browse...](#)

Please enter your template ID

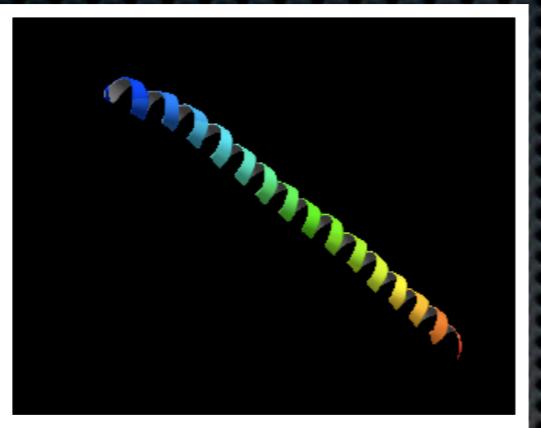
PDB ID: 5 characters: (PDB ID + chain ID) required!

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Heter-oligomer Modeling Service

Please enter your structural model

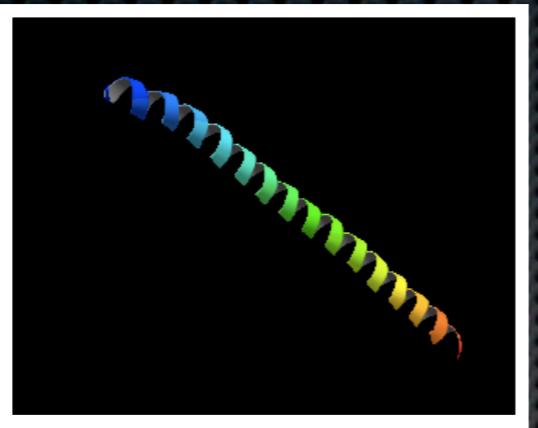
Upload a PDB-formatted file: Browse...

Please enter your template ID

PDB ID: 5 characters: (PDB ID + chain ID) required!

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Heter-oligomer Modeling Service

Please enter your structural model

Upload a PDB-formatted file: Browse...

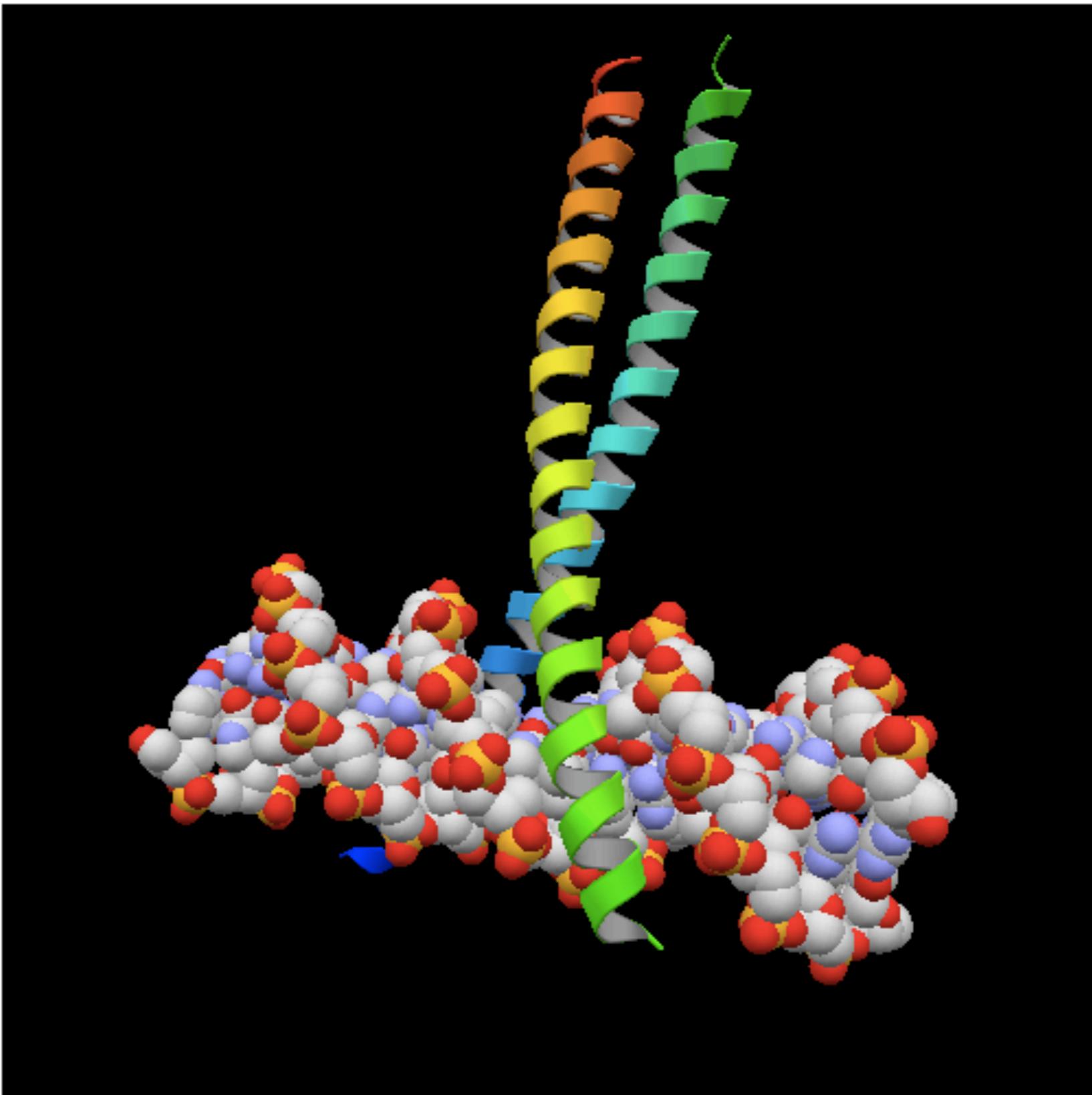
Please enter your template ID

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spanner_P05627_JUN_MOUSE_1jnmA_hhpred_0_0_1jnm_all



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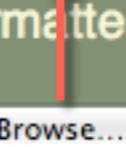
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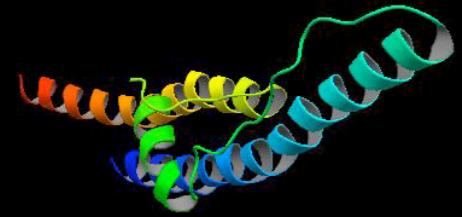
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If your query is a structural model, the following information is requested

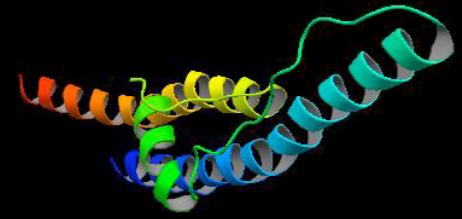
Template PDB ID Template Chain ID A

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standley@ifrec.osaka-u.ac.jp

If your query is a structural model, the following information is requested

Template PDB ID Template Chain ID

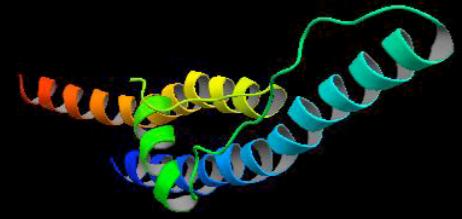
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If your query is a structural model, the following information is requested

Template PDB ID **2rqr** Template Chain ID A

type template PDB ID here

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Template	Score	Identity	Coverage	Domain	Annot	Alignment	Superposition
2q68A	163.1	26	65		GO	Alignment	<i>f</i> View Sup
2q67A	163.1	27	63		GO	Alignment	<i>f</i> View Sup
2q69B	162.7	27	65		GO	Alignment	<i>f</i> View Sup
2q69A	162.2	27	61		GO	Alignment	<i>f</i> View Sup
2a79B	161.3	20	76		GO	Alignment	View Sup
2ahyA	159.3	27	65		GO	Alignment	<i>f</i> View Sup
2q6aB	158.8	27	65		GO	Alignment	<i>f</i> View Sup
2ahyB	158.2	27	65		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2ahzA	154.4	27	66		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q6aA	153.9	27	60		GO	Alignment	<i>f</i> View Sup
2q68A	153.8	27	65		GO	All	<i>f</i> View Sup

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Template	Score	Identity	Coverage	Domain	Annot	Alignment	Superposition
2q68A	163.1	26	65		GO	Alignment	<i>f</i> View Sup
2q67A	163.1	27	63		GO	Alignment	<i>f</i> View Sup
2q69B	162.7	27	65		GO	Alignment	<i>f</i> View Sup
2q69A	162.2	27	61		GO	Alignment	<i>f</i> View Sup
2a79B	161.3	20	76		GO	Alignment	View Sup
2ahyA	159.3	27	65		GO	Alignment	<i>f</i> View Sup
2q6aB	158.8	27	65		GO	Alignment	<i>f</i> View Sup
2ahyB	158.2	27	65		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2ahzA	154.4	27	66		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q6aA	153.9	27	60		GO	Alignment	<i>f</i> View Sup
2q68A	153.8	27	65		GO	All	<i>f</i> View Sup

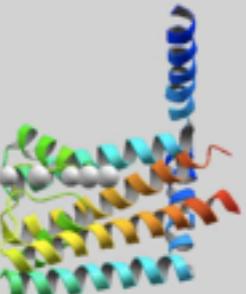
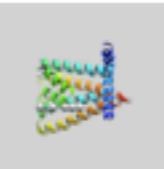
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 Structure Viewers jV3 / Jmol jV and Jmol require Java(TM)Plug-in 1.5 or later.  rotated about x by 90° 250X250 500X500	PDB ID	2q68 sequence information (FASTA format) download PDB format file
	RELATED PDB ID	2ahy , 2ahz , 2q67 , 2q69 , 2q6a
	Descriptor	Potassium channel protein
	Title	Crystal Structure of Nak channel D66A, S70E double mutants
	Functional Keywords	INVERTED TEEPEE, HELIX BUNDLE, TETRAMER, CENTRAL CAVITY, ION BINDING, METAL TRANSPORT, MEMBRANE PROTEIN
	Biological source	Bacillus cereus
	Total number of polymer chains	2
	Total molecular weight	25804 (the details in Structural Details Page)
	Authors	Alam, A. , Shi, N. , Jiang, Y. (deposition date : 2007-06-04, release date : 2007-10-02)
	Primary citation	Alam, A. , Shi, N. , Jiang, Y. Structural insight into Ca ²⁺ specificity in tetrameric cation channels. <i>Proc.Natl.Acad.Sci.U.S.A.</i> , 104:15334 - 15339, 2007. (PubMed : 17878296) (DOI: 10.1073/pnas.0707324104)
	Experimental method	X-RAY DIFFRACTION (2.500[Å])
	Other Database Information	CATH , CE , FSSP , SCOP , VAST , UniProt (UNP - Q81HW2) , eF-site

2ahzA	154.4	27	66	GO	Alignment	<i>f</i>	View	Sup
2q69A	154.2	27	61	GO	Alignment	<i>f</i>	View	Sup
2q69A	154.2	27	61	GO	Alignment	<i>f</i>	View	Sup
2q6aA	153.9	27	60	GO	Alignment	<i>f</i>	View	Sup

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Template	Score	Identity	Coverage	Domain	Annot	Alignment	Superposition
2q68A	163.1	26	65		GO	Alignment	<i>f</i> View Sup
2q67A	163.1	27	63		GO	Alignment	<i>f</i> View Sup
2q69B	162.7	27	65		GO	Alignment	<i>f</i> View Sup
2q69A	162.2	27	61		GO	Alignment	<i>f</i> View Sup
2a79B	161.3	20	76		GO	Alignment	View Sup
2ahyA	159.3	27	65		GO	Alignment	<i>f</i> View Sup
2q6aB	158.8	27	65		GO	Alignment	<i>f</i> View Sup
2ahyB	158.2	27	65		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2ahzA	154.4	27	66		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q6aA	153.9	27	60		GO	Alignment	<i>f</i> View Sup
2q68A	153.8	27	65		GO	All	<i>f</i> View Sup

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Template	Score	Identity	Coverage	Domain	Annot	Alignment	Superposition
2q68A	163.1	26	65		GO	Alignment	<i>f</i> View Sup
2q67A	163.1	27	63		GO	Alignment	<i>f</i> View Sup
2q69B	162.7	27	65		GO	Alignment	<i>f</i> View Sup
2q69A	162.2	27	61		GO	Alignment	<i>f</i> View Sup
2a79B	161.3	20	76		GO	Alignment	View Sup
2ahyA	159.3	27	65		GO	Alignment	<i>f</i> View Sup
2q6aB	158.8	27	65		GO	Alignment	<i>f</i> View Sup
2ahyB	158.2	27	65		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2ahzA	154.4	27	66		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q6aA	153.9	27	60		GO	Alignment	<i>f</i> View Sup
2q68A	153.8	27	65		GO	All	<i>f</i> View Sup

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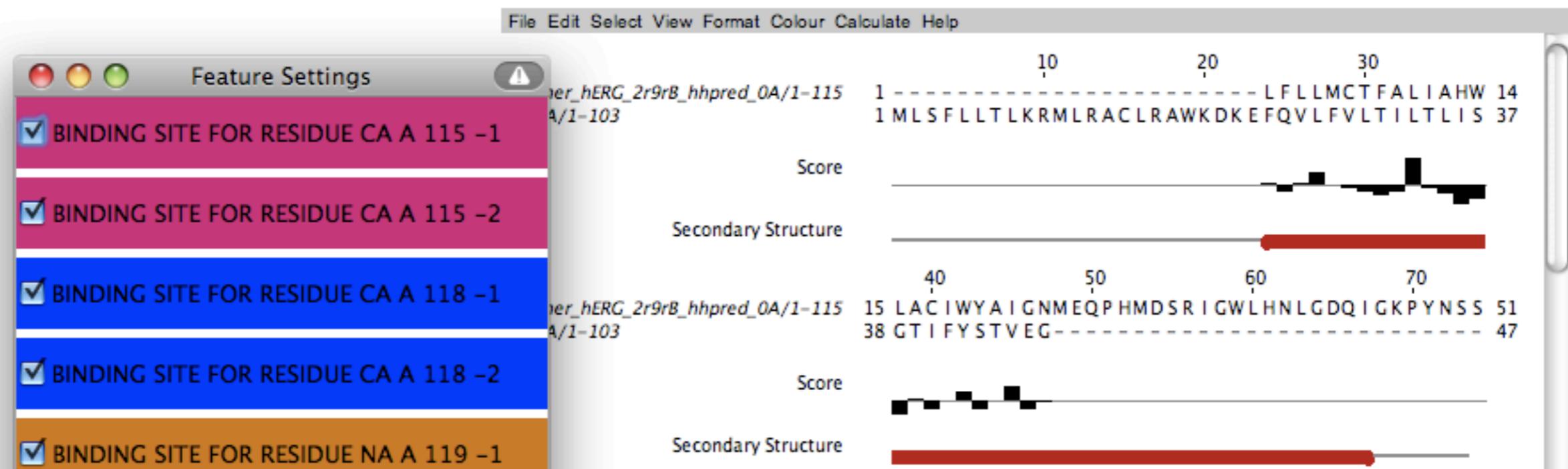
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Alignment between **spanner_hERG_2r9rB_hhpred_0A** and **2q68A**

Query: **spanner_hERG_2r9rB_hhpred_0A**
Templ: [**2q68A**](#)
Score: **163.1**
Seq ID (aligned residues): **26%**



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Template	Score	Identity	Coverage	Domain	Annot	Alignment	Superposition
2q68A	163.1	26	65		GO	Alignment	<i>f</i> View Sup
2q67A	163.1	27	63		GO	Alignment	<i>f</i> View Sup
2q69B	162.7	27	65		GO	Alignment	<i>f</i> View Sup
2q69A	162.2	27	61		GO	Alignment	<i>f</i> View Sup
2a79B	161.3	20	76		GO	Alignment	View Sup
2ahyA	159.3	27	65		GO	Alignment	<i>f</i> View Sup
2q6aB	158.8	27	65		GO	Alignment	<i>f</i> View Sup
2ahyB	158.2	27	65		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2ahzA	154.4	27	66		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q6aA	153.9	27	60		GO	Alignment	<i>f</i> View Sup
2q68A	153.8	27	65		GO	All	<i>f</i> View Sup

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2q67A	163.1	27	63		GO	Alignment	<i>f</i> View Sup
2q69B	162.7	27	65		GO	Alignment	<i>f</i> View Sup
2q69A	162.2	27	61		GO	Alignment	<i>f</i> View Sup
2a79B	161.3	20	76		GO	Alignment	View Sup
2ahyA	159.3	27	65		GO	Alignment	<i>f</i> View Sup
2q6aB	158.8	27	65		GO	Alignment	<i>f</i> View Sup
2ahyB	158.2	27	65		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2ahzA	154.4	27	66		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q6aA	153.9	27	60		GO	Alignment	<i>f</i> View Sup
2q68A	153.8	27	65		GO	All	<i>f</i> View Sup

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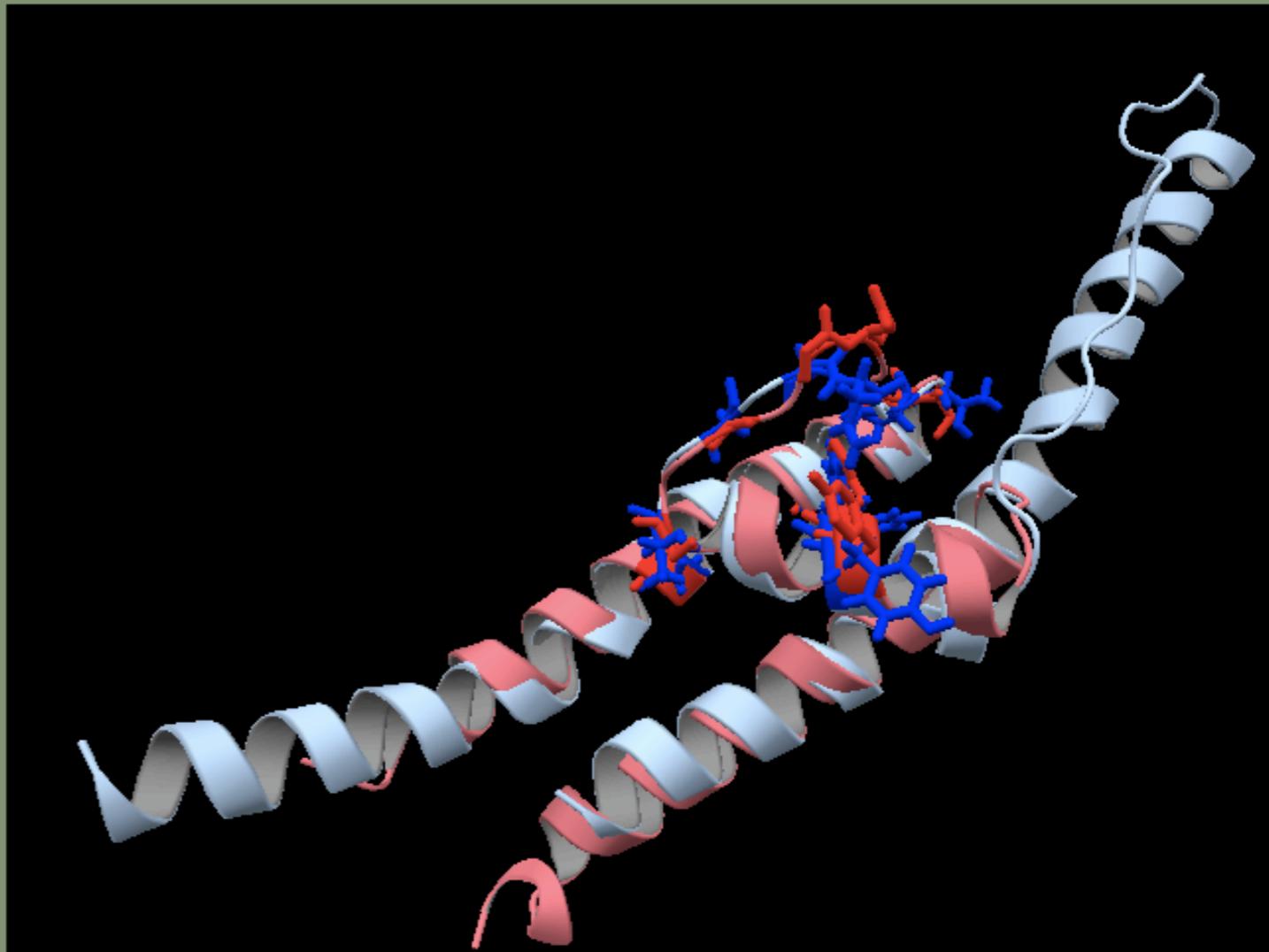
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Aligned residue pairs

spanner_hERG_2r9rB_hhpred_0A	2q68A	Show	Hide	Score
P83	P71	<input checked="" type="radio"/>	<input type="radio"/>	10.0
Y67	Y55	<input checked="" type="radio"/>	<input type="radio"/>	9.2
F91	F79	<input checked="" type="radio"/>	<input type="radio"/>	8.0
F68	F56	<input checked="" type="radio"/>	<input type="radio"/>	7.9
G77	G65	<input checked="" type="radio"/>	<input type="radio"/>	7.8
G99	G87	<input checked="" type="radio"/>	<input type="radio"/>	7.7
G79	G67	<input checked="" type="radio"/>	<input type="radio"/>	7.6
N80	N68	<input checked="" type="radio"/>	<input type="radio"/>	6.6
T74	T62	<input checked="" type="radio"/>	<input type="radio"/>	6.4
T85	T73	<input checked="" type="radio"/>	<input type="radio"/>	6.4
K89	K77	<input type="radio"/>	<input type="radio"/>	6.2
L4	L27	<input type="radio"/>	<input type="radio"/>	6.0
V76	V64	<input type="radio"/>	<input type="radio"/>	5.7
A65	A53	<input type="radio"/>	<input type="radio"/>	5.6
I93	I81	<input type="radio"/>	<input type="radio"/>	5.4
L73	L61	<input type="radio"/>	<input type="radio"/>	5.4
L66	L54	<input type="radio"/>	<input type="radio"/>	5.3
L10	L33	<input type="radio"/>	<input type="radio"/>	5.3
I98	I86	<input type="radio"/>	<input type="radio"/>	5.2
I90	I78	<input type="radio"/>	<input type="radio"/>	5.2
I114	V102	<input type="radio"/>	<input type="radio"/>	3.8
V63	I51	<input type="radio"/>	<input type="radio"/>	3.6

Superposition of spanner_hERG_2r9rB_hhpred_0A (blue) and 2q68A (red)



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2q68A	163.1	26	65		GO	Alignment	<i>f</i> View Sup
2q67A	163.1	27	63		GO	Alignment	<i>f</i> View Sup
2q69B	162.7	27	65		GO	Alignment	<i>f</i> View Sup
2q69A	162.2	27	61		GO	Alignment	<i>f</i> View Sup
2a79B	161.3	20	76		GO	Alignment	View Sup
2ahyA	159.3	27	65		GO	Alignment	<i>f</i> View Sup
2q6aB	158.8	27	65		GO	Alignment	<i>f</i> View Sup
2ahyB	158.2	27	65		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2q67A	156.1	27	63		GO	Alignment	<i>f</i> View Sup
2ahzA	154.4	27	66		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q69A	154.2	27	61		GO	Alignment	<i>f</i> View Sup
2q6aA	153.9	27	60		GO	Alignment	<i>f</i> View Sup
2q68A	153.8	27	65		GO	All	<i>f</i> View Sup

SeSAW considers both sequence and structure

Template	Score	Identity	Coverage	Domain	Annot	Alignment	Superposition
2q68A	163.1	26	65		GO	Alignment	View Sup
2q67A	163.1	27	63		GO	Alignment	View Sup
2q69B	162.7	27	65		GO	Alignment	View Sup
2q69A	162.2	27	61		GO	Alignment	View Sup
2a79B	161.3	20	76		GO	Alignment	View Sup
2ahyA	159.3	27	65		GO	Alignment	View Sup
2q6aB	158.8	27	65		GO	Alignment	View Sup
2ahyB	158.2	27	65		GO	Alignment	View Sup
2q67A	156.1	27	63		GO	Alignment	View Sup
2q67A	156.1	27	63		GO	Alignment	View Sup
2ahzA	154.4	27	66		GO	Alignment	View Sup
2q69A	154.2	27	61		GO	Alignment	View Sup
2q69A	154.2	27	61		GO	Alignment	View Sup
2q6aA	153.9	27	60		GO	Alignment	View Sup
2q68B	153.2	25	65		GO	Alignment	View Sup
2q67B	152.8	27	63		GO	Alignment	View Sup
3e86A	150.0	26	60		GO	Alignment	View Sup
3e86A	150.0	26	60		GO	Alignment	View Sup
3e8hA	149.9	30	57		GO	Alignment	View Sup
2ahzB	149.9	27	59		GO	Alignment	View Sup
2ahzA	149.5	27	62		GO	Alignment	View Sup
2ahzA	149.5	27	62		GO	Alignment	View Sup
3e8fA	149.5	30	57		GO	Alignment	View Sup
3e89A	149.5	30	57		GO	Alignment	View Sup
3e8hA	149.4	26	60		GO	Alignment	View Sup
3e8hA	149.4	26	60		GO	Alignment	View Sup
2a01B	149.3	26	66		GO	Alignment	View Sup
3e8fA	149.2	26	60		GO	Alignment	View Sup
3e8fA	149.2	26	60		GO	Alignment	View Sup
3e8bA	149.1	26	61		GO	Alignment	View Sup
3e8bA	149.1	26	61		GO	Alignment	View Sup
3e86A	148.5	29	59		GO	Alignment	View Sup
3e89A	148.3	26	60		GO	Alignment	View Sup
3e89A	148.3	26	60		GO	Alignment	View Sup
3e8gA	147.2	30	57		GO	Alignment	View Sup
2zd9C	147.1	16	70		GO	Alignment	View Sup
3e83A	147.0	29	59		GO	Alignment	View Sup
3e8bA	146.8	29	59		GO	Alignment	View Sup
2q69B	146.8	27	63		GO	Alignment	View Sup
2q69B	146.8	27	63		GO	Alignment	View Sup
3e86B	146.8	26	57		GO	Alignment	View Sup
3behC	146.6	16	73		GO	Alignment	View Sup
2q6aA	145.9	26	60		GO	Alignment	View Sup
2q6aA	145.9	26	60		GO	Alignment	View Sup
3e86B	145.8	26	57		GO	Alignment	View Sup
3e8gB	145.7	26	57		GO	Alignment	View Sup
3e8gB	145.7	26	57		GO	Alignment	View Sup
2q6aB	145.5	27	61		GO	Alignment	View Sup
2q6aB	145.5	27	61		GO	Alignment	View Sup
2q67B	144.8	27	63		GO	Alignment	View Sup
2q67B	144.8	27	63		GO	Alignment	View Sup
3e8fB	144.7	26	59		GO	Alignment	View Sup
3e8fB	144.7	26	59		GO	Alignment	View Sup

2ahyA	144.3	27	62	GO	Alignment	View Sup	
2ahyA	144.3	27	62	GO	Alignment	View Sup	
2ahyB	143.4	27	62	GO	Alignment	View Sup	
2ahyB	143.4	27	62	GO	Alignment	View Sup	
2a01A	142.2	26	66	GO	Alignment	View Sup	
2zd9A	142.0	18	70	GO	Alignment	View Sup	
2q68B	141.9	26	63	GO	Alignment	View Sup	
2q68B	141.9	26	63	GO	Alignment	View Sup	
3behD	141.7	18	70	GO	Alignment	View Sup	
2q68A	141.6	26	66	GO	Alignment	View Sup	
2q68A	141.6	26	66	GO	Alignment	View Sup	
2zd9B	141.3	16	73	GO	Alignment	View Sup	
3behB	138.4	16	71	GO	Alignment	View Sup	
1lnqH	137.7	18	57	SCOP:f.14.1.1	GO	Alignment	View Sup
3e8bB	137.0	26	58	GO	Alignment	View Sup	
3e8bB	136.0	26	58	GO	Alignment	View Sup	
2ahzB	134.6	26	66	GO	Alignment	View Sup	
2ahzB	134.6	26	66	GO	Alignment	View Sup	
2zd9D	133.8	16	72	GO	Alignment	View Sup	
1lnqF	132.1	18	56	SCOP:f.14.1.1	GO	Alignment	View Sup
1lnqD	132.1	18	56	SCOP:f.14.1.1	GO	Alignment	View Sup
1lnqG	131.5	18	56	SCOP:f.14.1.1	GO	Alignment	View Sup
3behA	131.1	17	70	GO	Alignment	View Sup	
1zwiC	128.5	15	72	CATH:1.10.287.70	GO	Alignment	View Sup
3e83A	128.5	25	65	GO	Alignment	View Sup	
3e83A	128.5	25	65	GO	Alignment	View Sup	
2r9rH	125.8	20	54	Alignment	View Sup	Alignment	View Sup
2r9rB	125.7	20	54	Alignment	View Sup	Alignment	View Sup
3e89B	124.7	25	63	GO	Alignment	View Sup	
3e89B	123.7	25	63	GO	Alignment	View Sup	
3e8gA	120.9	25	66	GO	Alignment	View Sup	
3e8gA	120.9	25	66	GO	Alignment	View Sup	
3e8hB	120.9	25	64	GO	Alignment	View Sup	
3e8hB	120.9	25	64	GO	Alignment	View Sup	
2qksB	120.6	17	50	GO	Alignment	View Sup	
2qksA	120.2	18	48	GO	Alignment	View Sup	
3e83B	119.9	25	63	GO	Alignment	View Sup	
3e83B	118.9	25	63	GO	Alignment	View Sup	
2a9hC	116.2	17	69	CATH:1.10.287.70	GO	Alignment	View Sup
1x16B	112.6	15	64	SCOP:f.14.1.1	GO	Alignment	View Sup
2qtoC	112.6	13	70	CATH:1.10.287.70	GO	Alignment	View Sup
2ih1C	112.4	14	71	CATH:1.10.287.70	GO	Alignment	View Sup
2p7tC	111.5	14	75	CATH:1.10.287.70	GO	Alignment	View Sup
2hj1C	111.1	15	72	SCOP:f.14.1.1	GO	Alignment	View Sup
4-1-C	110.1	20	60	SCOP:f.14.1.1	GO	Alignment	View Sup

SeSAW considers both sequence and structure

Template	Score	Identity	Coverage	Domain	Annot	Alignment	Superposition
2q68A	163.1	26	65		GO	Alignment	View Sup
2q67A	163.1	27	63		GO	Alignment	View Sup
2q69B	162.7	27	65		GO	Alignment	View Sup
2q69A	162.2	27	61		GO	Alignment	View Sup
2a79B	161.3	20	76		GO	Alignment	View Sup
2ahyA	159.3	27	65		GO	Alignment	View Sup
2q6aB	158.8	27	65		GO	Alignment	View Sup
2ahyB	158.2	27	65		GO	Alignment	View Sup
2q67A	156.1	27	63		GO	Alignment	View Sup
2q67A	156.1	27	63		GO	Alignment	View Sup
2ahzA	154.4	27	66		GO	Alignment	View Sup
2q69A	154.2	27	61		GO	Alignment	View Sup
2q69A	154.2	27	61		GO	Alignment	View Sup
2q6aA	153.9	27	60		GO	Alignment	View Sup
2q68B	153.2	25	65		GO	Alignment	View Sup
2q67B	152.8	27	63		GO	Alignment	View Sup
3e86A	150.0	26	60		GO	Alignment	View Sup
3e86A	150.0	26	60		GO	Alignment	View Sup
3e8hA	149.9	30	57		GO	Alignment	View Sup
2ahzB	149.9	27	59		GO	Alignment	View Sup
2ahzA	149.5	27	62		GO	Alignment	View Sup
2ahzA	149.5	27	62		GO	Alignment	View Sup
3e8fA	149.5	30	57		GO	Alignment	View Sup
3e89A	149.5	30	57		GO	Alignment	View Sup
3e8hA	149.4	26	60		GO	Alignment	View Sup
3e8hA	149.4	26	60		GO	Alignment	View Sup
2a0lB	149.3	26	66		GO	Alignment	View Sup
3e8fA	149.2	26	60		GO	Alignment	View Sup
3e8fA	149.2	26	60		GO	Alignment	View Sup
3e8bA	149.1	26	61		GO	Alignment	View Sup
3e8bA	149.1	26	61		GO	Alignment	View Sup
3e86A	148.5	29	59		GO	Alignment	View Sup
3e89A	148.3	26	60		GO	Alignment	View Sup
3e89A	148.3	26	60		GO	Alignment	View Sup
3e8gA	147.2	30	57		GO	Alignment	View Sup
2zd9C	147.1	16	70		GO	Alignment	View Sup
3e83A	147.0	29	59		GO	Alignment	View Sup
3e8bA	146.8	29	59		GO	Alignment	View Sup
2q69B	146.8	27	63		GO	Alignment	View Sup
2q69B	146.8	27	63		GO	Alignment	View Sup
3e86B	146.8	26	57		GO	Alignment	View Sup
3behC	146.6	16	73		GO	Alignment	View Sup
2q6aA	145.9	26	60		GO	Alignment	View Sup
2q6aA	145.9	26	60		GO	Alignment	View Sup
3e86B	145.8	26	57		GO	Alignment	View Sup
3e8gB	145.7	26	57		GO	Alignment	View Sup
3e8gB	145.7	26	57		GO	Alignment	View Sup
2q6aB	145.5	27	61		GO	Alignment	View Sup
2q6aB	145.5	27	61		GO	Alignment	View Sup
2q67B	144.8	27	63		GO	Alignment	View Sup
2q67B	144.8	27	63		GO	Alignment	View Sup
3e8fB	144.7	26	59		GO	Alignment	View Sup
3e8fB	144.7	26	59		GO	Alignment	View Sup

Original template does not have highest score!

2ahyA	144.3	27	62	GO	Alignment	View Sup	
2ahyA	144.3	27	62	GO	Alignment	View Sup	
2ahyB	143.4	27	62	GO	Alignment	View Sup	
2ahyB	143.4	27	62	GO	Alignment	View Sup	
2a0lA	142.2	26	66	GO	Alignment	View Sup	
2zd9A	142.0	18	70	GO	Alignment	View Sup	
2q68B	141.9	26	63	GO	Alignment	View Sup	
2q68B	141.9	26	63	GO	Alignment	View Sup	
3behD	141.7	18	70	GO	Alignment	View Sup	
2q68A	141.6	26	66	GO	Alignment	View Sup	
2q68A	141.6	26	66	GO	Alignment	View Sup	
2zd9B	141.3	16	73	GO	Alignment	View Sup	
3behB	138.4	16	71	GO	Alignment	View Sup	
1lnqH	137.7	18	57	SCOP:f.14.1.1	GO	Alignment	View Sup
3e8bB	137.0	26	58	GO	Alignment	View Sup	
3e8bB	136.0	26	58	GO	Alignment	View Sup	
2ahzB	134.6	23	66	GO	Alignment	View Sup	
2ahzB	134.6	26	66	GO	Alignment	View Sup	
2zd9D	133.8	16	72	GO	Alignment	View Sup	
1lnqF	132.1	18	56	SCOP:f.14.1.1	GO	Alignment	View Sup
1lnqD	132.1	18	56	SCOP:f.14.1.1	GO	Alignment	View Sup
1lnqG	131.5	18	56	SCOP:f.14.1.1	GO	Alignment	View Sup
3behA	131.1	17	70	GO	Alignment	View Sup	
1zwiC	128.5	15	72	CATH:1.10.287.70	GO	Alignment	View Sup
3e83A	128.5	25	65	GO	Alignment	View Sup	
3e83A	128.5	25	65	GO	Alignment	View Sup	
2r9rH	125.8	20	54	Alignment		View Sup	
2r9rB	125.7	20	54	Alignment		View Sup	
3e89B	124.7	25	63	GO	Alignment	View Sup	
3e89B	123.7	25	63	GO	Alignment	View Sup	
3e8gA	120.9	25	66	GO	Alignment	View Sup	
3e8gA	120.9	25	66	GO	Alignment	View Sup	
3e8hB	120.9	25	64	GO	Alignment	View Sup	
3e8hB	120.9	25	64	GO	Alignment	View Sup	
2qksB	120.6	17	50	GO	Alignment	View Sup	
2qksA	120.2	18	48	GO	Alignment	View Sup	
3e83B	119.9	25	63	GO	Alignment	View Sup	
3e83B	118.9	25	63	GO	Alignment	View Sup	
2a9hC	116.2	17	69	CATH:1.10.287.70	GO	Alignment	View Sup
1x16B	112.6	15	64	SCOP:f.14.1.1	GO	Alignment	View Sup
2qtoC	112.6	13	70	CATH:1.10.287.70	GO	Alignment	View Sup
2ih1C	112.4	14	71	CATH:1.10.287.70	GO	Alignment	View Sup
2p7tC	111.5	14	75	CATH:1.10.287.70	GO	Alignment	View Sup
2hj1C	111.1	15	72	SCOP:f.14.1.1	GO	Alignment	View Sup
411C	110.1	20	60	SCOP:f.14.1.1	GO	Alignment	View Sup

Acknowledgements

Prof. Haruki Nakamura (PDBj, Osaka Univ.)

Mr. Mieszko Lis (MIT)

Assoc. Prof Akira Kinjo (PDBj, Osaka Univ.)

Ms. Reiko Yamashita (PDBj)

Mr. Atsuro Yoshihara (PDBj)