

# Homology modeling Tutorial

## Sequence to structure

# Homology modeling

## Principle

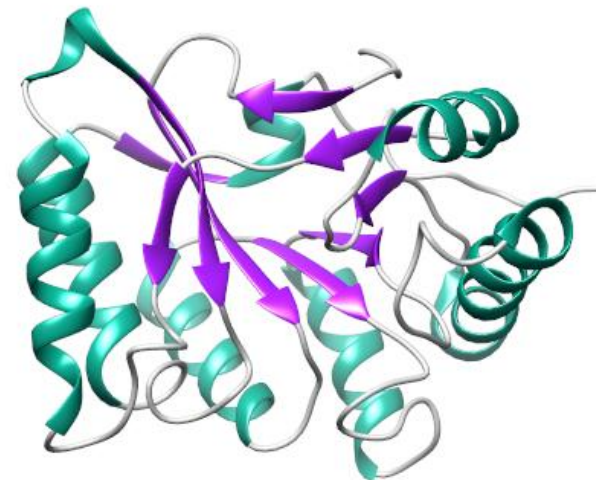
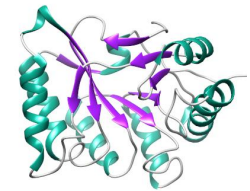
Evolutionary related protein tend to have similar structure

# Homology modeling

## Predicting structure from the sequence

```
89 SKSISFGGCLTQMYFMIALGNTDSYILAAMAYDRAVAIS 127
68 -FCAACHGCLFIACFVLVLTQSSI FSL LAIAIDRYIAIR 105
128 RPLHYTTIMSPRSCIWLIAGSWVIGNANALPHTLL-TAV 165
106 IPLRYNGLVTGTRAKGI I AICWVLSFAICLTP-MLG WNA 143
```

3d structure  
of template



# Homology modeling/Comparative modeling

TEMPLATES .....➤ TARGET

→ Predicts the three-dimensional structure of a given protein sequence (TARGET) based on an alignment to one or more known protein structures (TEMPLATES)

→ If similarity between the TARGET sequence and the TEMPLATE sequence is detected, structural similarity can be assumed.

Comparative Protein Models will be increasingly utilized to help solve biological problem

# Homology modeling

Basic steps in Homology modeling :

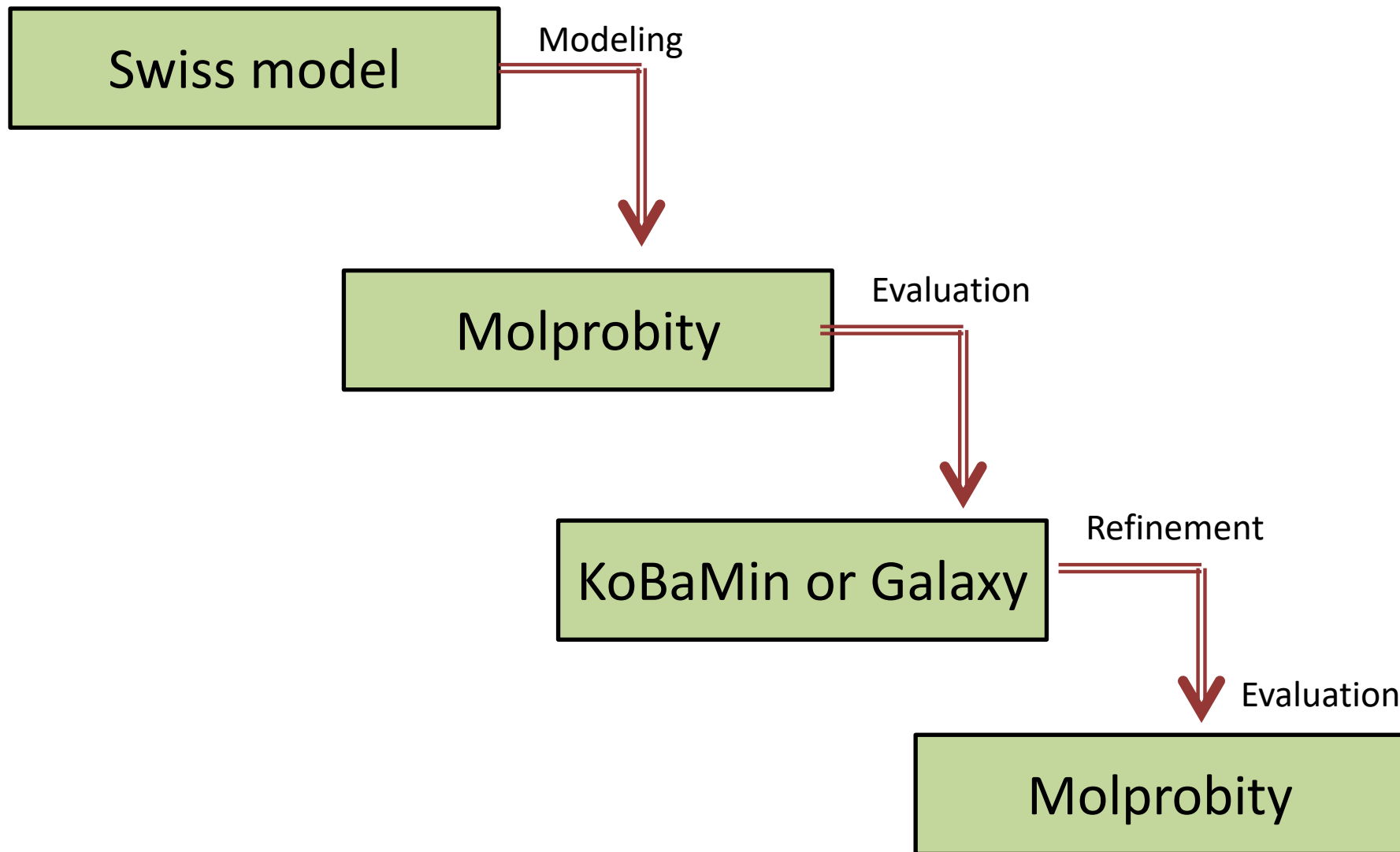
- i) Model building based on template
- ii) Refinement
- ii) Evaluation

# Building the model

## Software for homology molecular modeling

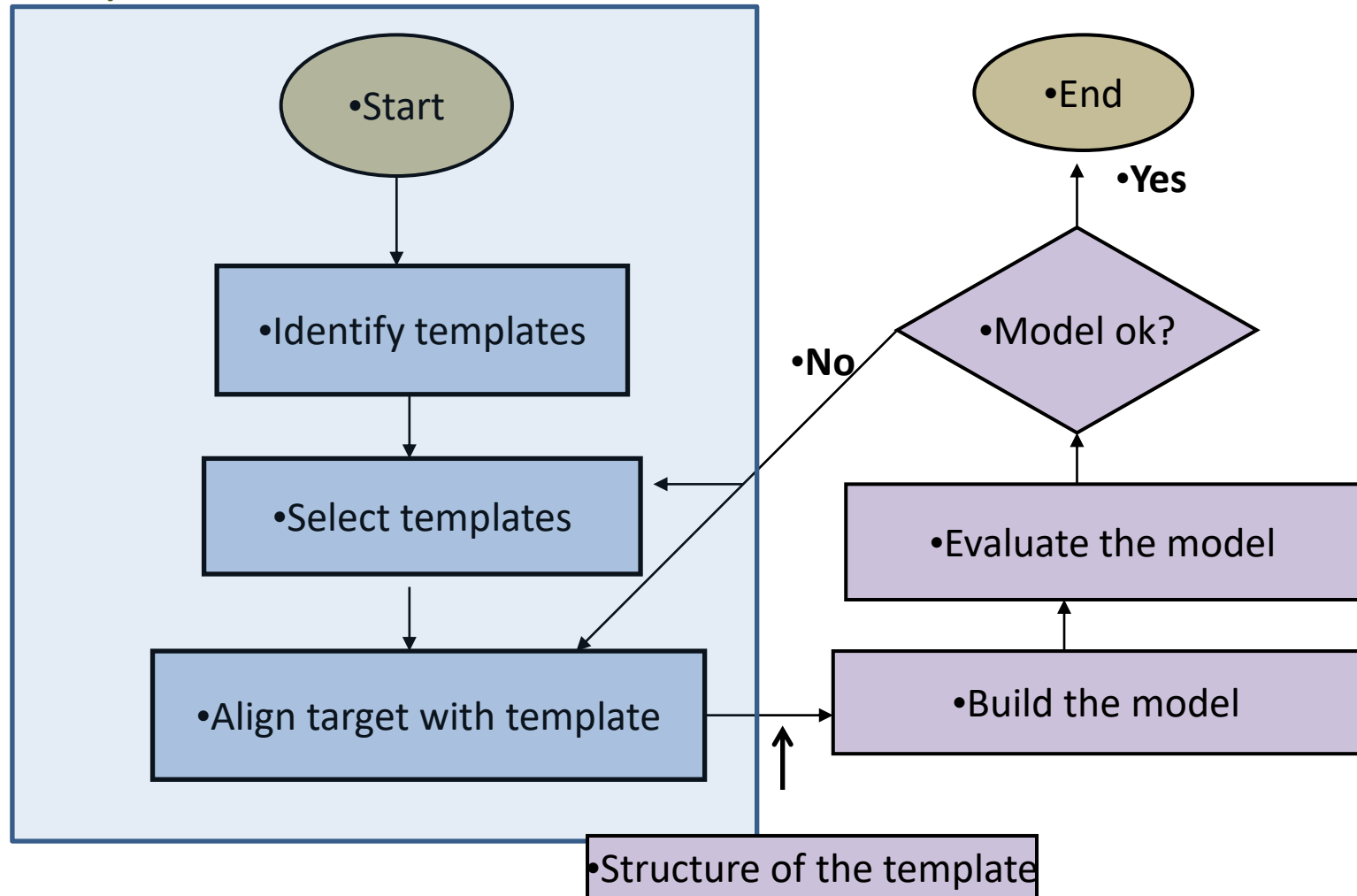
- Freeware: available for all OS
  - Downloadable
    - Modeller (Sali, 1998)
    - DeepView (SwissPDB viewer)
  - Web based:
    - **I-TASSER** (<http://zhanglab.ccmb.med.umich.edu/I-TASSER/SDSC1>)
    - **SWISS MODEL** server ([www.expasy.org/swissmod/SWISS-MODEL.html](http://www.expasy.org/swissmod/SWISS-MODEL.html) )
    - **Hhpred server** (<https://toolkit.tuebingen.mpg.de/tools/hhpred>)
    - **PSIPRED** (<http://bioinf.cs.ucl.ac.uk/psipred/>)

# Summary steps for modeling



# Basic Comparative Protein Modeling Procedures

## Step1





# Homology modeling/Comparative modeling

## Input for the modeling

- Target sequence- Sequence of the structure with unknown 3D structure
- 3D template- selected based on the highest sequence identity with the target sequence
- Alignment between the target and template

# Target selection

The screenshot shows the UniProt website with a navigation bar at the top containing links for Search, Blast, Align, Retrieve, and ID Mapping. Below this is a search bar with a dropdown menu set to 'Protein Knowledgebase (UniProtKB)' and buttons for 'Search', 'Advanced Search', and 'Clear'. The main content area is divided into several sections: 'WELCOME' with a mission statement, 'What we provide' with a table of services, 'NEWS' with a recent release announcement, 'SITE TOUR' with a thumbnail image, and 'PROTEIN SPOTLIGHT'.

Service	Description
UniProtKB	Protein knowledgebase, consists of two sections: <ul style="list-style-type: none"><li>★ Swiss-Prot, which is manually annotated and reviewed.</li><li>★ TrEMBL, which is automatically annotated and is not reviewed.</li></ul> Includes complete and reference proteome sets.
UniRef	Sequence clusters, used to speed up sequence similarity searches.
UniParc	Sequence archive, used to keep track of sequences and their identifiers.
Supporting data	Literature citations, taxonomy, keywords, subcellular locations, cross-referenced databases and more.

- Text search
- Sequence similarity searches (BLAST)
- Sequence alignments
- Batch retrieval

The screenshot shows the NCBI website with a navigation bar at the top containing links for Resources and How To. Below this is a search bar with a dropdown menu set to 'Protein' and a 'Search' button. The main content area is divided into several sections: 'Welcome to NCBI' with a mission statement, 'Get Started' with a list of links, 'Genotypes and Phenotypes' with a thumbnail image, 'Popular Resources' with a list of links, and 'NCBI Announcements' with a recent announcement. Two red arrows point from the 'Protein' dropdown menu to the 'Popular Resources' list.

- Tools: Analyze data using NCBI software
- Downloads: Get NCBI data or software
- How-To's: Learn how to accomplish specific tasks at NCBI
- Submissions: Submit data to GenBank or other NCBI databases

- PubMed
- Bookshelf
- PubMed Central
- PubMed Health
- BLAST
- Nucleotide
- Genome
- SNP
- Gene
- Protein
- PubChem

# Template selection

BLAST® Basic Local Alignment Search Tool

Home Recent Results Saved Strategies Help

My NCBI 12  
[Sign In] [Registered]

NCBI/ BLAST/ blastp suite Standard Protein BLAST

blastn blastp blastx tblastn tblastx

BLASTP programs search protein databases using a protein query. [more...](#) [Reset page](#) [Bookmark](#)

Enter Query Sequence

Enter accession number(s), gi(s), or FASTA sequence(s) [Clear](#)

Query subrange

From

To

Or, upload file  no file selected [?](#)

Job Title

Enter a descriptive title for your BLAST search [?](#)

☐ Align two or more sequences [?](#)

Choose Search Set

Database  [?](#)

Organism [Optional](#)

Enter organism name or id—completions will be suggested ☐ Exclude [?](#)

Enter organism common name, binomial, or tax id. Only 20 top taxa will be shown. [?](#)

Exclude [Optional](#)

☐ Models (XM/XP) ☐ Uncultured/environmental sample sequences

Entrez Query [Optional](#)

Enter an Entrez query to limit search [?](#)

Program Selection

Algorithm

☒ blastp (protein-protein BLAST)

☐ PSI-BLAST (Position-Specific Iterated BLAST)

☐ PHI-BLAST (Pattern Hit Initiated BLAST)

Choose a BLAST algorithm [?](#)

**BLAST** Search database Non-redundant protein sequences (nr) using Blastp (protein-protein BLAST)

☐ Show results in a new window

[+ Algorithm parameters](#)

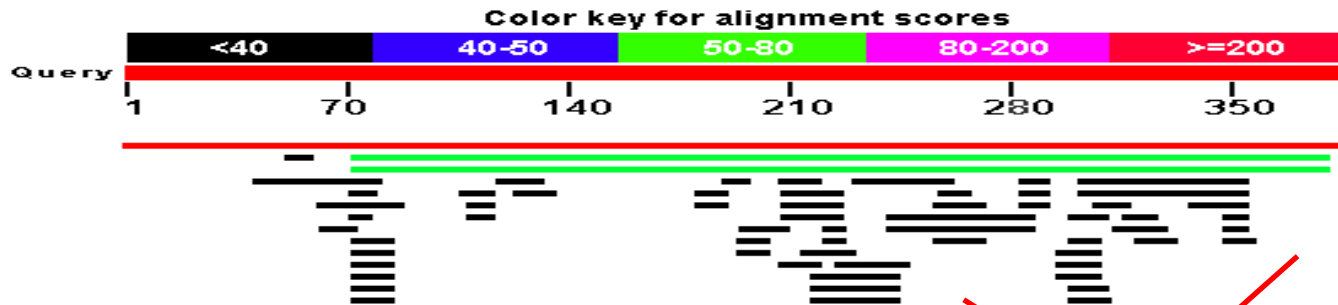
Sequence in the fasta format

Database selection

Protein data bank protein

Button to search

# 1V5C\_A Chain A, The Crystal Structure Of The Inactive Form Chi.. S=1164 E=0



Description	Max score	Total score	Query cover	E value	Ident	Accession	Select for PSI blast	Used to build PSSM
<input type="checkbox"/> Chain A, The Crystal Structure Of The Inactive Form Chitosanase From Bacillus Sp. K17 At Ph3.7 >qii58176988 pdb 1V5C A	1164	1164	100%	0.0	97%	<a href="#">qii58176988 1V5C_A</a>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
<input type="checkbox"/> Chain A, Endoglucanase A From Clostridium Thermocellum At Atomic Resolution >qii157830584 pdb 1CEM A Chain A, Endogluc	65.1	65.1	79%	1e-10	30%	<a href="#">qii157830584 1CEM_A</a>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
<input type="checkbox"/> Chain A, Atomic Resolution Structure Of An Inverting Glycosidase In Complex With Substrate	57.1	57.1	79%	4e-08	29%	<a href="#">qii201510901 KWE_A</a>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>



## Chain A, The Crystal Structure Of The Inactive Form Chitosanase From Bacillus Sp. K17 At Ph3.7

Sequence ID: [qii58176988|pdb|1V5C|A](#) Length: 386 Number of Matches: 1

► See 2 more title(s)

Range 1: 1 to 386		GenPept	Graphics	Next Match		Previous Match	
Score	Expect	Method	Identities	Positives	Gaps		
1164 bits(2737)	0.0	Composition-based stats.	376/386(97%)	378/386(97%)	0/386(0%)		
Query 1		AKEMKPFPPQVNYAGVIKPNHVTQESLNASVRSYYDNWKKKYLKNDLSSLPGGGYYVKGEI			60		
Sbjct 1		AKEMKPFPPQVNYAGVIKPNHVTQESLNASVRSYYDNWKKKYLKNDLSSLPGGGYYVKGEI			60		
Query 61		TGDADGFKPLGTSEGQGYGMIITVLMAGYDSNAQKIYDGLFKTARTFKSSQNPNLMGWV			120		
Sbjct 61		TGDADGFKPLGTSEGQGYGMIITVLMAGYDSNAQKIYDGLFKTARTFKSSQNPNLMGWV			120		
Query 121		ADSKKAQGHFDSATDGDLDIAYSLLLAHKQWGSNGAVNCLKEAQDMITKGIKASNVITNN			180		
Sbjct 121		ADSKKAQGHFDSATDGDLDIAYSLLLAHKQWGSNGV N LKEAQDMITKGIKASNVITNN			180		
Query 181		RLNLGDWDSKSSLDTRPSDWMMSHLRAFYEFTEGDKTWLTVINNLYDVYTQFSNKYSPNTG			240		
Sbjct 181		QLNLGDWDSKSSLDTRPSDWMMSHLRAFYEFTEGDKTWLTVINNLYDVYTQFSNKYSPNTG			240		
Query 241		LISDFVVKNPFPQAPKFL+SEYTNAYYYNARSVPRLRIVMDYAMYGEKRSKVISDKVSS			300		
Sbjct 241		LISDFVVKNPFPQAPKFLDESEYTNAYYYNARSVPRLRIVMDYAMYGEKRSKVISDKVSS			300		
Query 301		WIQNKINGNPSKIVDGYQLNGSNIGYPTAVFVSPFIAASITNSNNQKWNVSGWDWMKKNK			360		
Sbjct 301		WIQNKINGNPSKIVDGYQLNGSNIGSYPTAVFVSPFIAASITSSNNQKWNVSGWDWMKKNK			360		
Query 361		RESYFSDSYNLLTMLFIIGNWWKPIP	386				
Sbjct 361		RE YFSDSYNLLTMLFIIGNWWKPP	386				

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EBI > Tools > Multiple Sequence Alignment > ClustalW2

### ClustalW2 - Multiple Sequence Alignment

ClustalW2 is a general purpose multiple sequence alignment program for DNA or proteins.

New version! Clustal Omega is now available for protein sequences - give it a try!

Use this tool

**STEP 1 - Enter your input sequences**  
Enter or paste a set of (Protein) sequences in any supported format:

Or, upload a file:  no file selected

**STEP 2 - Set your Pairwise Alignment Options**  
Alignment Type: ☒ Slow ☐ Fast  
The default settings will fulfill the needs of most users and, for that reason, are not visible.  
 (Click here, if you want to view or change the default settings.)

**STEP 3 - Set your Multiple Sequence Alignment Options**  
The default settings will fulfill the needs of most users and, for that reason, are not visible.  
 (Click here, if you want to view or change the default settings.)



**STEP 4 - Submit your job**  
☐ Be notified by email (Tick this box if you want to be notified by email when the results are available)

If you plan to use these services during a course please contact us.  
[Request a free 30-day trial or ask for help from our support staff.](#)

Fasta format sequences

Button to start the alignment

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EBI > Tools > Multiple Sequence Alignment > ClustalW2

### ClustalW2 Results

[Alignments](#) [Result Summary](#) [Guide Tree](#) [Submission Details](#) [Submit Another Job](#)

**Alignment**

CLUSTAL 2.1 multiple sequence alignment

sp   P08100   OPDS_HUMAN	MNQTGPGNFYVPFSSNAGGVVSPFEYPOYYLAEPQFQSMIAAYMFLILVL	50
gi   157880263   pdb   1U19   A	MNQTGPGNFYVPFSSNAGGVVSPFEYPOYYLAEPQFQSMIAAYMFLILVL	50
*****		
sp   P08100   OPDS_HUMAN	GFFINFLTLVTVQHKRLTPLNYILLNLAVADLFMVLCGFTSTLYTSLH	100
gi   157880263   pdb   1U19   A	GFFINFLTLVTVQHKRLTPLNYILLNLAVADLFMVLCGFTSTLYTSLH	100
*****		
sp   P08100   OPDS_HUMAN	GYFVFGPTGTCNLEGFFATLGGEIALWSLVLAIERYVVVCKPMSNFRFGE	150
gi   157880263   pdb   1U19   A	GYFVFGPTGTCNLEGFFATLGGEIALWSLVLAIERYVVVCKPMSNFRFGE	150
*****		
sp   P08100   OPDS_HUMAN	NHAIMGVAF TWMALACAAPLAGWSRYIPEGLQCSGIDYYTLKPEVNN	200
gi   157880263   pdb   1U19   A	NHAIMGVAF TWMALACAAPPLVGWSRYIPEGMQCSGIDYYTPHEETNN	200
*****		
sp   P08100   OPDS_HUMAN	ESFVIYMFVVHFTIPMIIIFCYGQLVFTVKEAAAQQQESATTQKAEKEV	250
gi   157880263   pdb   1U19   A	ESFVIYMFVVHFTIPLIVIFFCYGQLVFTVKEAAAQQQESATTQKAEKEV	250
*****		
sp   P08100   OPDS_HUMAN	TRMVIIMVIAFLICWVPYASVAFYIFTHQGSNFGPIFMTIPAFFAKSAAI	300
gi   157880263   pdb   1U19   A	TRMVIIMVIAFLICWLPYAGVAFYIFTHQGSDFGPIFMTIPAFFAKTSAV	300
*****		
sp   P08100   OPDS_HUMAN	YNPVIYIMMNKQFRNCMLTTICCGKNPLGDDEASATVSKTETSQVAPA	348
gi   157880263   pdb   1U19   A	YNPVIYIMMNKQFRNCMTTLCCKGNPLGDDEASTTVSKTETSQVAPA	348
*****		

Alignment

# Rules for Template selection


- The quality of the homology model is dependent on the quality of the sequence alignment and template structure
- Model quality declines with decreasing sequence identity.
- The approach can be complicated by the presence of alignment gaps that indicate a structural region present in the target but not in the template
- Is an X-ray crystallography structure (NMR structure are usually much less resolved)?
- All the atoms are resolved in the selected structure?
- Is the chosen structure the best resolved one (typical good resolution is smaller than 2Å)

*As a rule of thumb we should never use template with an E value larger than 0.1.*



# Building the model

- I-TASSER
- QUARK
- LOMETS
- COACH
- COFACTOR
- MUSTER
- SEGMENT
- FG-MD
- ModRefiner
- REMO
- SPRING
- COTH
- BSpred
- SVMSEQ
- ANGLO
- BSP-SLIM
- SAXSTER
- ThreaDom
- EvoDesign
- TM-score
- TM-align
- MM-align
- NY-align
- EDTSurf
- MVD



## I-TASSER ONLINE

Protein Structure & Function Predictions

(The server completed predictions for [176105 proteins](#) submitted by [45006 users](#) from [115 countries](#))  
(The template library was updated on [2014/04/10](#))

I-TASSER server is an on-line platform for protein structure and function predictions. 3D models are built based on multiple-threading alignments by [LOMETS](#) and iterative template fragment assembly simulations; function insights are derived by matching the 3D models with [BioLiP protein function database](#). I-TASSER (as 'Zhang-Server') was ranked as the No 1 server for protein structure prediction in recent [CASP7](#), [CASP8](#), [CASP9](#), and [CASP10](#) experiments. It was also ranked as the best for function prediction in [CASP9](#). The server is in active development with the goal to provide the most accurate structural and function predictions using state-of-the-art algorithms. The server is only for non-commercial use. Please report problems and questions at [I-TASSER message board](#) and some members will study and answer the questions asap. ([>> More about the server ...](#))

**Download I-TASSER Standalone Package (Version 3.0) NEW**

[\[Queue\]](#) [\[Forum\]](#) [\[Download\]](#) [\[Example\]](#) [\[Search\]](#) [\[Registration\]](#) [\[About\]](#) [\[Statistics\]](#) [\[Remove\]](#) [\[Potential\]](#) [\[Decoys\]](#) [\[News\]](#)

Copy and paste your sequence here (<1,500 residues, in [FASTA format](#)):


Or upload the sequence from your local computer:

No file selected.

Email: (mandatory, where results will be sent to)

Password: (mandatory, please click [here](#) if you do not have a password)

# Building the model

 **SWISS-MODEL**  
molecular Life Sciences

Modelling Tools Repository Docu

myWorkspace  
Automated Mode  
**Alignment Mode**  
DeepView Project Mode


## Welcome to SWISS-MODEL


SWISS-MODEL is a fully automated protein structure homology-modelling server, accessible via the ExPASy web (Pdb-Viewer). The purpose of this server is to make Protein Modelling accessible to all biochemists and molecular biologists worldwide.

[Start Modelling](#)

SWISS-MODEL has recently had a face lift! You can still access the [familiar version here](#).

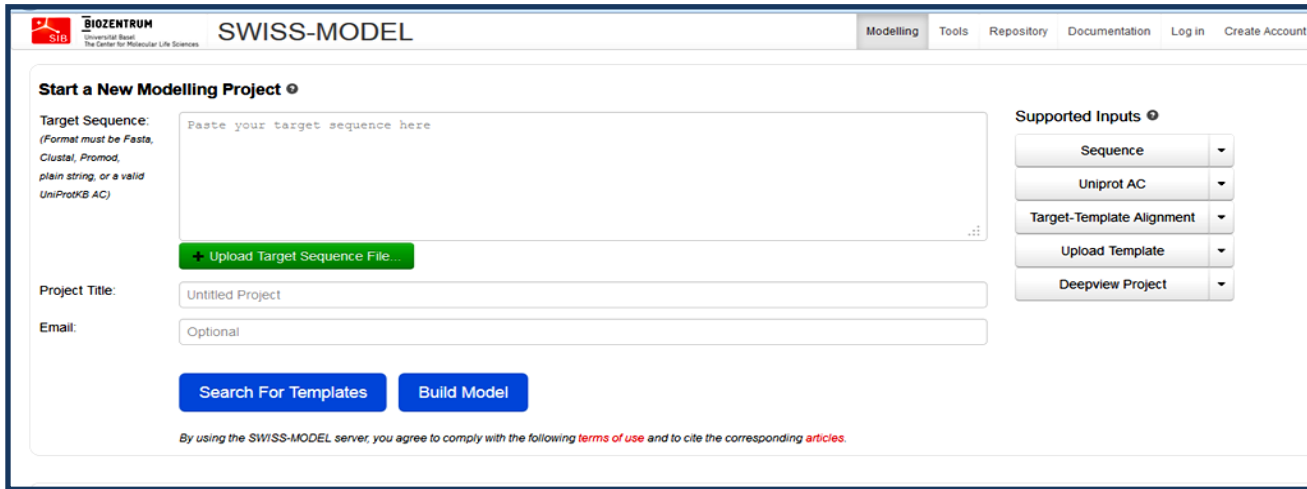
**Protein Structure Bioinformatics Group**  
c/o Prof. Torsten Schwede  
Swiss Institute of Bioinformatics  
Biozentrum, University of Basel  
Klingelbergstrasse 50/70  
CH-4056 Basel / Switzerland  
[help-swissmodel@unibas.ch](mailto:help-swissmodel@unibas.ch)

**BIOZENTRUM**  
Universität Basel  
The Center for Molecular Life Sciences

**SIB**  
Swiss Institute of Bioinformatics



# Building the model



**BIOZENTRUM**  
Universität Basel  
The Center for Molecular Life Sciences

**SWISS-MODEL**

Modelling Tools Repository Documentation Log in Create Account

### Start a New Modelling Project

**Target Sequence:**  
(Format must be Fasta, Clustal, Promod, plain string, or a valid UniProtKB AC)

Paste your target sequence here

[+ Upload Target Sequence File...](#)

**Project Title:** Untitled Project

**Email:** Optional

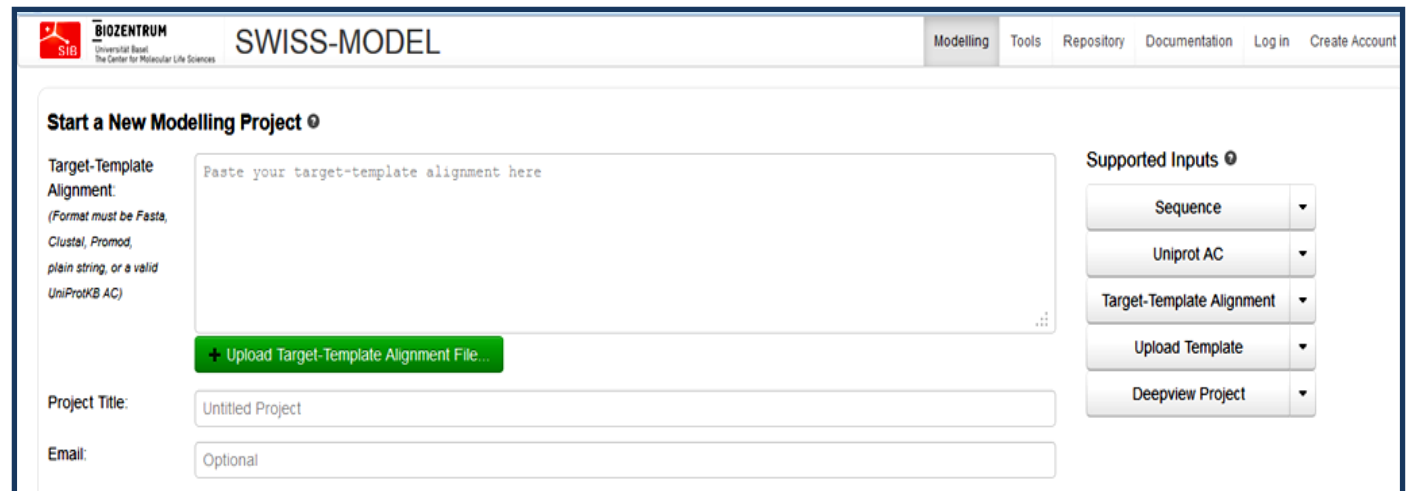
[Search For Templates](#) [Build Model](#)

By using the SWISS-MODEL server, you agree to comply with the following [terms of use](#) and to cite the corresponding [articles](#).

**Supported Inputs**

- Sequence
- Uniprot AC
- Target-Template Alignment
- Upload Template
- Deepview Project

Automated mode



**BIOZENTRUM**  
Universität Basel  
The Center for Molecular Life Sciences

**SWISS-MODEL**

Modelling Tools Repository Documentation Log in Create Account

### Start a New Modelling Project

**Target-Template Alignment:**  
(Format must be Fasta, Clustal, Promod, plain string, or a valid UniProtKB AC)

Paste your target-template alignment here

[+ Upload Target-Template Alignment File...](#)

**Project Title:** Untitled Project

**Email:** Optional

**Supported Inputs**

- Sequence
- Uniprot AC
- Target-Template Alignment
- Upload Template
- Deepview Project

Alignment mode

# Building the model

Summary Templates **38** Models **0**

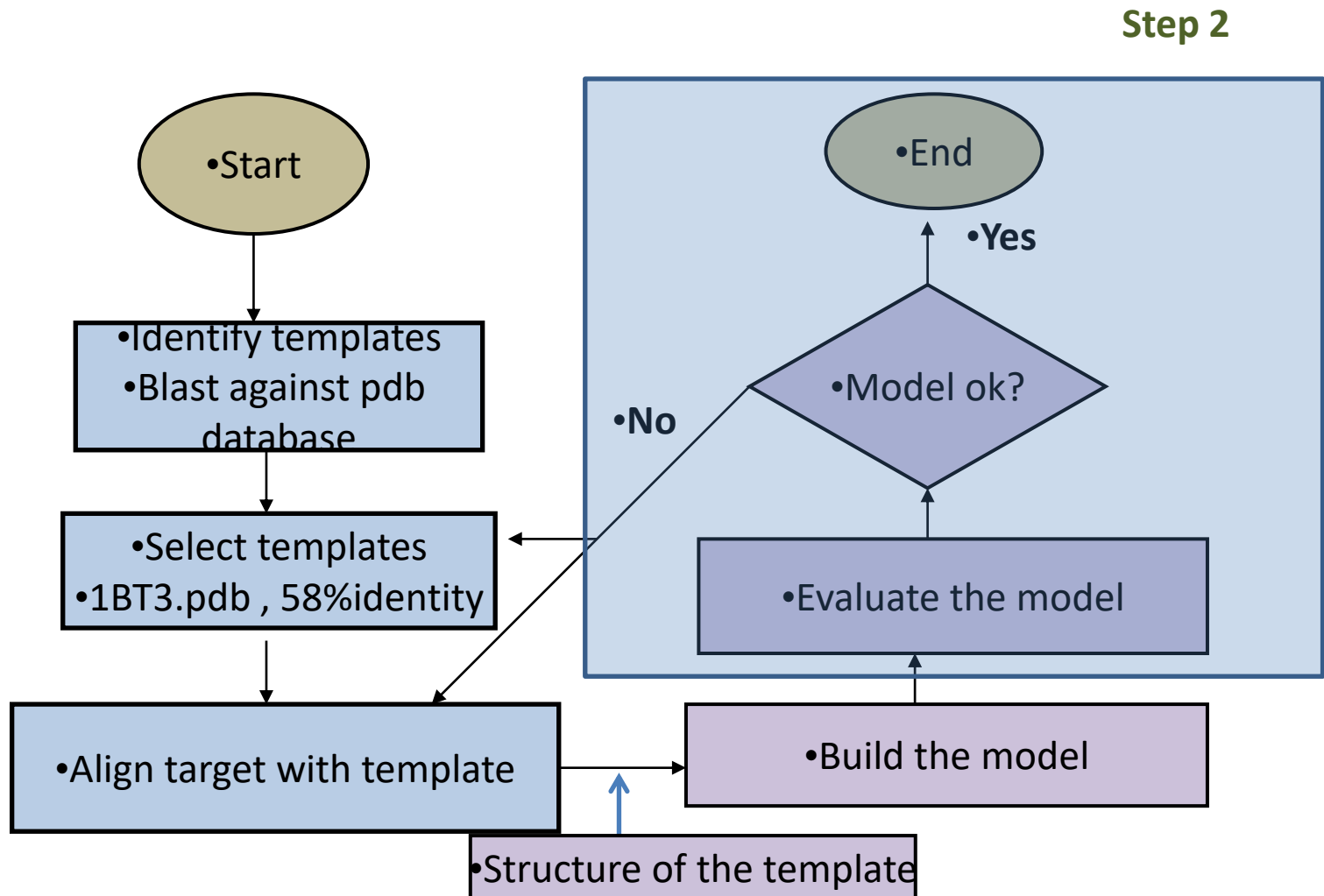
## Template Results

Templates Sequence Similarity Alignment of Selected Templates More

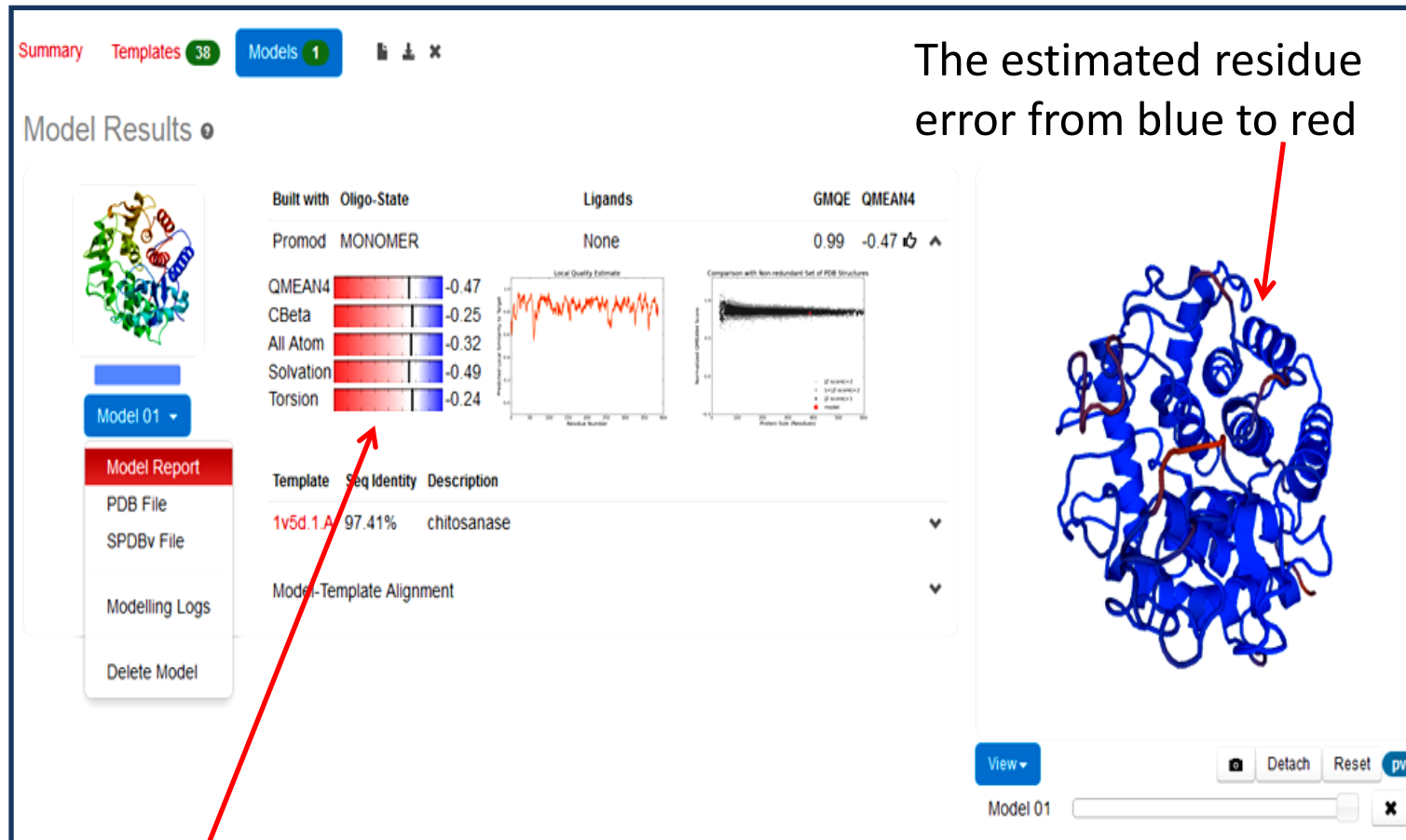
Name	Title	Coverage	Identity	Method	Oligo State	Ligands
<input checked="" type="checkbox"/> 1v5d.1.A	chitosanase		97.41	X-ray, 1.5Å	monomer	None
<input type="checkbox"/> 1cem.1.A	CELLULASE CELA (1,4-BETA-D-GLUCAN-GLUCANOHYDROLASE)		30.86	X-ray, 1.6Å	monomer	None
<input type="checkbox"/> 1kwf.1.A	Endoglucanase A		30.29	X-ray, 0.9Å	monomer	None
<input type="checkbox"/> 1cem.1.A	CELLULASE CELA (1,4-BETA-D-GLUCAN-GLUCANOHYDROLASE)		33.63	X-ray, 1.6Å	monomer	None
<input type="checkbox"/> 1kwf.1.A	Endoglucanase A		33.03	X-ray, 0.9Å	monomer	None
<input type="checkbox"/> 1h13.1.A	ENDO-1,4-BETA-XYLANASE		19.54	X-ray, 1.3Å	monomer	None
<input type="checkbox"/> 1xw1.1.A	endo-1,4-beta-xylanase		19.54	X-ray, 1.3Å	monomer	None
<input type="checkbox"/> 1xw2.1.A	Endo-1,4-beta-Xylanase		19.25	X-ray, 1.8Å	monomer	None
<input type="checkbox"/> 1h14.1.A	ENDO-1,4-BETA-XYLANASE		18.97	X-ray, 1.5Å	monomer	None
<input type="checkbox"/> 2a8z.1.A	endo-1,4-beta-xylanase		18.97	X-ray, 3.2Å	monomer	None
<input type="checkbox"/> 2drr.1.A	Xylanase Y		17.20	X-ray, 1.6Å	monomer	1 x Ni <sup>2+</sup>
<input type="checkbox"/> 1xw6.1.A	xylanase Y		16.62	X-ray, 1.4Å	monomer	1 x YVP-YVP <sup>2+</sup> 1 x Ni <sup>2+</sup>

**Build Models 1** Clear Selection

# Basic Comparative Protein Modeling Procedures



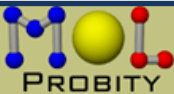
# Model Evaluation



reflecting the predicted model reliability

# Model Evaluation

<http://molprobiy.biochem.duke.edu/>



## Main page

**Main page**

- About hydrogens
- Evaluate X-ray
- Evaluate NMR
- Fix up structure
- Work with kins

View & download files

**FILE UPLOAD/RETRIEVAL (MORE OPTIONS)**

PDB/NDB code:

No file selected.

type: PDB coords

---

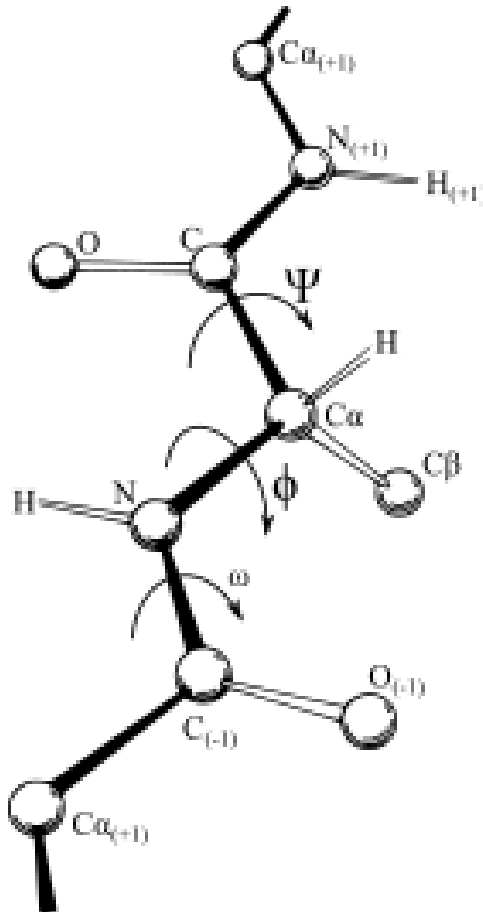
type: PDB coords

Protein Geometry	Poor rotamers	2	0.60%	Goal: <1%
	Ramachandran outliers	0	0.00%	Goal: <0.05%
	Ramachandran favored	374	97.40%	Goal: >98%
	C $\beta$ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	25 / 3149	0.79%	Goal: 0%
	Bad backbone angles:	29 / 4275	0.68%	Goal: <0.1%

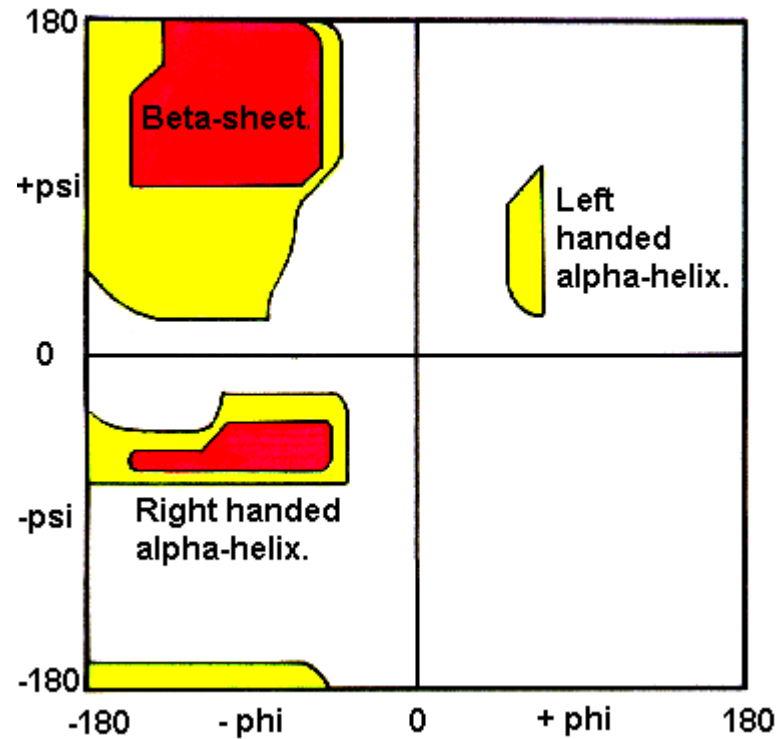
In the two column results, the left column gives the raw count, right column gives the percentage.

#	Alt	Res	High B	Ramachandran	Rotamer	C $\beta$ deviation	Bond lengths	Bond angles
			Avg: 0.85	Outliers: 0 of 384	Poor rotamers: 2 of 334	Outliers: 0 of 357	Outliers: 17 of 386	Outliers: 17 of 386
A 1		ALA	0.71	-	-	0.052Å	-	-
A 2		LYS	0.6	Favored (18.81%) General / 61.3,29.8	96.1% ( <i>mttt</i> ) chi angles: 298.4,185.6,177.2,185.8	0.036Å	-	-
A 3		GLU	0.72	Favored (58.09%) General / -60.4,137.7	25.4% ( <i>mp0</i> ) chi angles: 286.3,67.3,34	0.075Å	-	-
A 4		MET	0.75	Favored (17.3%) General / -99.5,-18.6	77.8% ( <i>mtm</i> ) chi angles: 293.2,180.9,285.3	0.014Å	-	-
A 5		LYS	0.76	Favored (11.06%) Pre-proline / -127.7,53.7	45.7% ( <i>mmtm</i> ) chi angles: 290,293.6,190.6,297.9	0.071Å	-	-
A 6		PRO	0.83	Favored (81.68%) Trans-proline / -63.6,141.8	98.7% ( <i>Cg_endo</i> ) chi angles: 30.5	0.029Å	-	-
A 7		PHE	0.85	Favored (96.43%) Pre-proline / -65.7,137.8	54% ( <i>t80</i> ) chi angles: 181.9,273.7	0.069Å	-	-
A 8		PRO	0.88	Favored (3.55%) Cis-proline / -97.9,137.2	33.5% ( <i>Cg_endo</i> ) chi angles: 37.1	0.06Å	-	-
A 9		GLN	0.76	Favored (43.56%) General / -79.0,-28.3	26.6% ( <i>mm100</i> ) chi angles: 287.4,299.5,108.8	0.051Å	-	-

# Ramachandran PLOT



The Ramachandran Plot.



# Homology Modeling Results

## Many places can go wrong:

- Bad template - it doesn't have the same structure as the target
- Bad alignment (a very common problem)
- Bad loop construction
- Bad side chain positioning

# Model Refinement

→ Side chain optimization

KOBAMIN server, GALAXY webserver

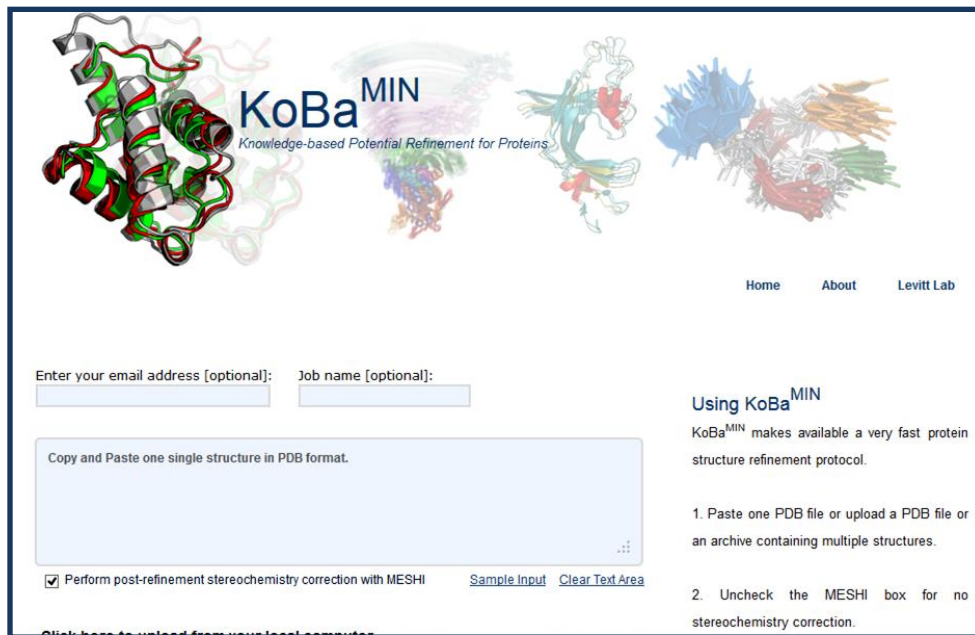
→ Loop modeling

MODLOOP



# Model optimization

<http://csb.stanford.edu/kobamin/>



**KoBa<sup>MIN</sup>**  
Knowledge-based Potential Refinement for Proteins

Home About Levitt Lab

Enter your email address [optional]:  Job name [optional]:

Copy and Paste one single structure in PDB format.

☒ Perform post-refinement stereochemistry correction with MESHI [Sample Input](#) [Clear Text Area](#)

[Click here to upload from your local computer](#)

**Using KoBa<sup>MIN</sup>**  
KoBa<sup>MIN</sup> makes available a very fast protein structure refinement protocol.

1. Paste one PDB file or upload a PDB file or an archive containing multiple structures.
2. Uncheck the MESHI box for no stereochemistry correction.

+ Table is sortable by clicking on the field titles.

Model	KB Energy (kcal/mol)	RMSD (Initial)	RMSD (Reference)	GDT-TS (Reference)	GDT-HA (Reference)	Time Spent (s)	View in Jmol
<a href="#">01</a>	-8799.3917	0.260	0.260	1.000	0.997	126	<input type="button" value="Load"/>

Show  entries

+ Table is sortable by clicking on the field titles.

# Model optimization

<http://galaxy.seoklab.org/cgi-bin/submit.cgi?type=REFINE>

## GalaxyWEB

A web server for protein structure prediction, refinement, and related methods  
Computational Biology Lab, Department of Chemistry, Seoul National University

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### GalaxyRefine

Model structures generated by protein structure prediction methods can be refined. **No gaps are allowed in the middle of initial protein structure.**

#### User Information

Job name

E-mail address (Optional)

#### Model Structure to be refined

PDB File  No file selected.  
( $\leq 500$  AA) Protein Structure File (allowed file extensions: pdb, txt)

#### Refinement options

Refinement method ☒ Both mild and aggressive relaxation (takes more time)  
☐ Mild relaxation only

Refinement region ☒ Whole protein  
☐ Fragments (residue ranges, example: 24-45, 72-80)

#### Submit

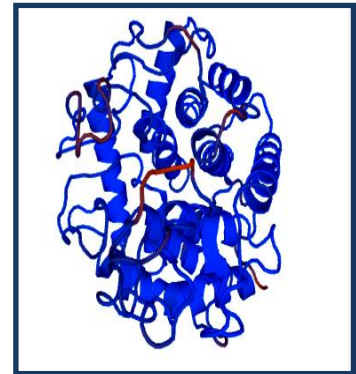
#### Help


- [Information](#)
- PDB File: [File Format](#)
- E-mail: Average run time is 1~2h.  
If e-mail address is given, the server sends notifications automatically. **If not, the user has to bookmark the report page.**

#### Example

- PDB file: [TR747.pdb](#)
- Report: [\[View\]](#)

# Model optimization



 **ModLoop**

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## ModLoop: Modeling of Loops in Protein Structures

ModLoop is a web server for automated modeling of loops in protein structures. The server relies on the loop modeling routine in MODELLER that predicts the loop conformations by satisfaction of spatial restraints, without relying on a database of known protein structures.

**Developer:**  
Andras Fiser

**Acknowledgements:**  
Ben Webb  
Ursula Pieper  
Andrej Sali  
Version r194

**General information** ?  
Email address (optional) ?   
Modeller license key ?   
Upload coordinate file ?  No file selected.

**Enter loop segments** ?

**Name your model** ?

Key

Residues for  
model

# Excercise

Generate 3D model using SWISS-PDB and evaluate your model