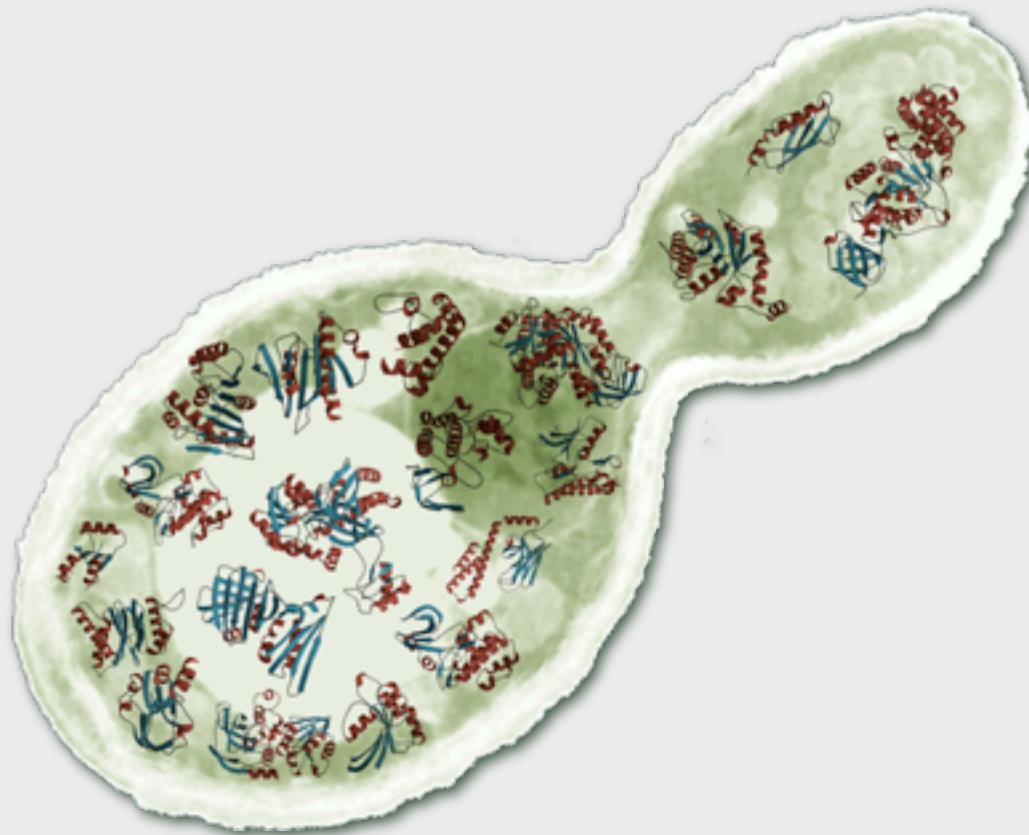


Comparative Protein Structure Prediction



Program

Intro to comparative
protein structure prediction

Template Search

Target – Template
Alignment

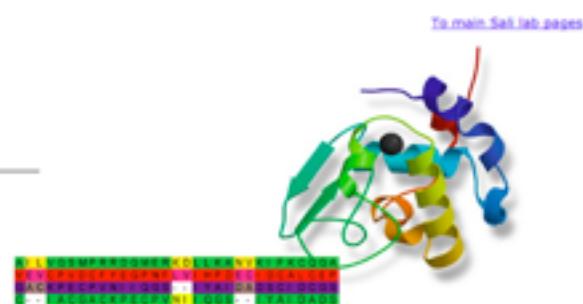
Model Building

Model Evaluation

<http://www.salilab.org/modeller/tutorial/>

Modeller

Program for Comparative Protein
Structure Modelling by Satisfaction
of Spatial Restraints



About MODELLER
MODELLER News
Download & Installation
Release Notes
Data file downloads
Registration
Accelrys licensing
Discussion Forum
Subscribe
Browse archives
Search archives
Documentation

Tutorial

MODELLER is used for homology or comparative modeling of protein three-dimensional structures. The user provides an alignment of a sequence to be modeled with known related structures and MODELLER automatically calculates a model containing all non-hydrogen atoms.

This web site presents a tutorial for the use of MODELLER 9v4 or newer (for older versions of MODELLER, use the [old MODELLER 7v7 tutorial](#)). There are 5 modeling examples that the user can follow:

1. [Basic Modeling](#). Model a sequence with high identity to a template.
This exercise introduces the use of MODELLER in a simple case where the template selection and target-template alignments are not a problem.

Objective

TO LEARN HOW-TO MODEL A
3D-STRUCTURE FROM A SEQUENCE
AND A KNOWN STRUCTURE

DISCLAIMER!

Structural Genomics @CNAG · CRG

Bioinformatics Resources

| Name | Type | World Wide Web address |
|------------------------|------|---|
| DATABASES | | |
| CATH | S | http://www.biochem.ucl.ac.uk/bsm/cath/ |
| DBAli | S | http://www.salilab.org/DBAli/ |
| GenBank | S | http://www.ncbi.nlm.nih.gov/Genbank/GenbankSearch.html |
| GeneCensus | S | http://bioinfo.mbb.yale.edu/genome |
| MODBASE | S | http://saliab.org/modbase/ |
| MSD | S | http://www.ebi.ac.uk/msd/ |
| NCBI | S | http://www.ncbi.nlm.nih.gov/ |
| PDB | S | http://www.rcsb.org/pdb/ |
| PSI | S | http://www.nigms.nih.gov/psi/ |
| Sacch3D | S | http://genome-www.stanford.edu/Sacch3D/ |
| SCOP | S | http://scop.mrc-lmb.cam.ac.uk/scop/ |
| TIGR | S | http://www.tigr.org/tdb/mdb/mdbcomplete.html |
| TrEMBL | S | http://srs.ebi.ac.uk/ |
| FOLD ASSIGNMENT | | |
| 123D | S | http://123d.ncifcrf.gov/ |
| 3D-PSSM | S | http://www.sbg.bio.ic.ac.uk/~3dpssm/index2.html |
| BIOINBGU | S | http://www.cs.bgu.ac.il/~bioinbgu/ |
| BLAST | S | http://www.ncbi.nlm.nih.gov/BLAST/ |
| DALI | S | http://www.ebi.ac.uk/dali/ |
| FASS | S | http://ffas.ljcrf.edu |
| FastA | S | http://www.ebi.ac.uk/fasta3/ |
| FRSVR | S | http://fold.doe-mbl.ucla.edu/ |

http://sgt.cnag.cat/www/software/?prot_resources

home
people
research
publications
presentations
Prot. resources
RNA resources

Nomenclature

Homology: Sharing a common ancestor, may have similar or dissimilar functions

Similarity: Score that quantifies the degree of relationship between two sequences.

Identity: Fraction of identical aminoacids between two aligned sequences (case of similarity).

Target: Sequence corresponding to the protein to be modeled.

Template: 3D structure/s to be used during protein structure prediction.

Model: Predicted 3D structure of the target sequence.

Nomenclature

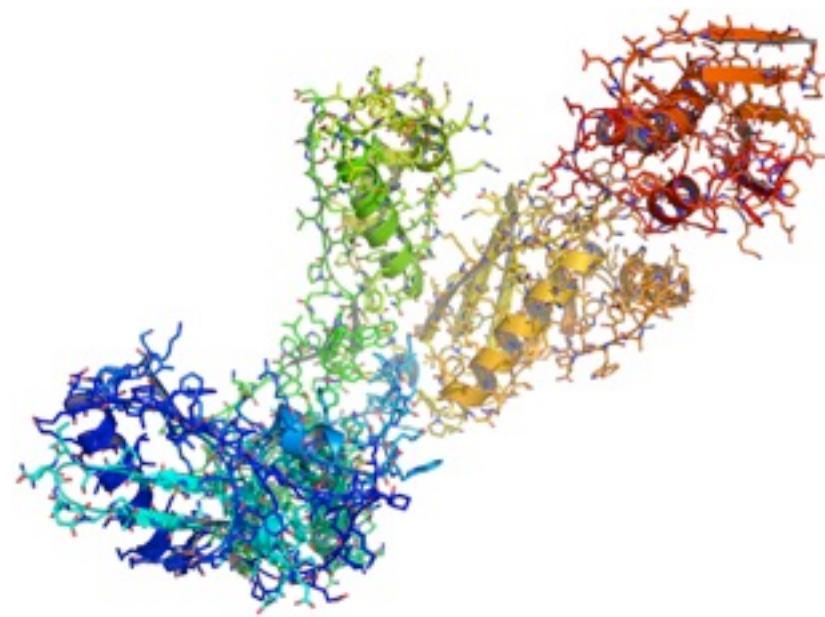
Fold: Three dimensional conformation of a protein sequence (usually at domain level).

Domain: Structurally globular part of a protein, which may independently fold.

Secondary Structure: Regular sub-domain structures composed by alpha-helices, beta-sheets and coils (or loops).

Backbone: Protein structure skeleton composed by the carbon, nitrogen and oxygen atoms.

Side-Chain: Specific atoms identifying each of the 20 residues types.



General References

Protein Structure Prediction:

Marti-Renom et al. Annu. Rev. Biophys. Biomol. Struct. 29, 291-325, 2000.
Baker & Sali. Science 294, 93-96, 2001.

Comparative Modeling:

Madhusudhan et al. The Proteomics Protocols Handbook. Ed. Walker. Humana Press Inc., Totowa, NJ. 831-860, 2005.

MODELLER:

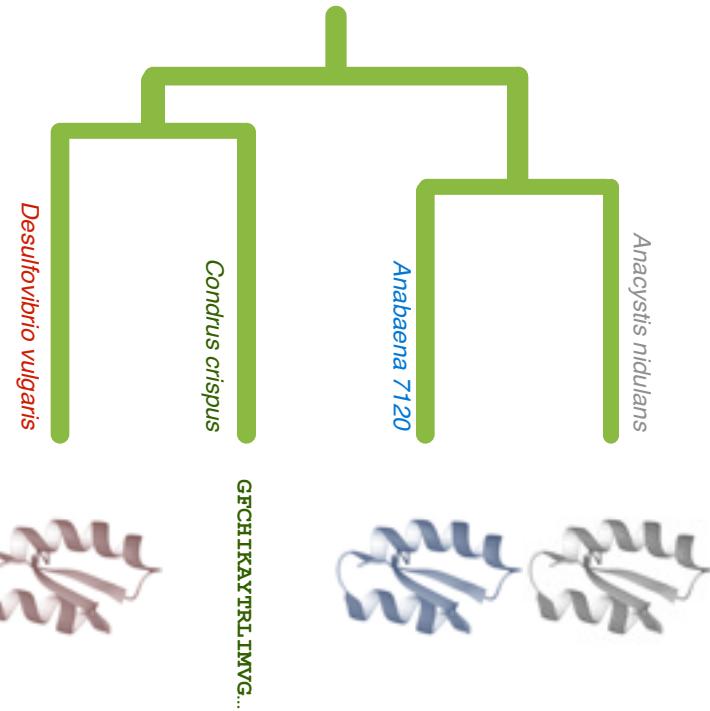
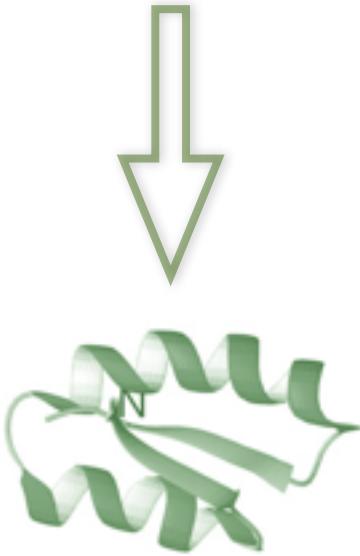
Sali & Blundell. J. Mol. Biol. 234, 779-815, 1993.
Eswar, M. A. et al. Comparative Protein Structure Modeling With MODELLER. Current Protocols in Bioinformatics, John Wiley & Sons, Inc., Supplement 15, 5.6.1-5.6.30, 2006.

Structural Genomics:

Sali. Nat. Struct. Biol. 5, 1029, 1998.
Burley et al. Nat. Genet. 23, 151, 1999.
Sali & Kuriyan. TIBS 22, M20, 1999.
Sanchez et al. Nat. Str. Biol. 7, 986, 2000.
Baker & Sali. Science 294, 93-96, 2001.
Terwilliger et al. Annu. Rev. Biophys. 38, 371-383, 2009.

Principles of protein structure

GFCHIKAYTRLIMVG...

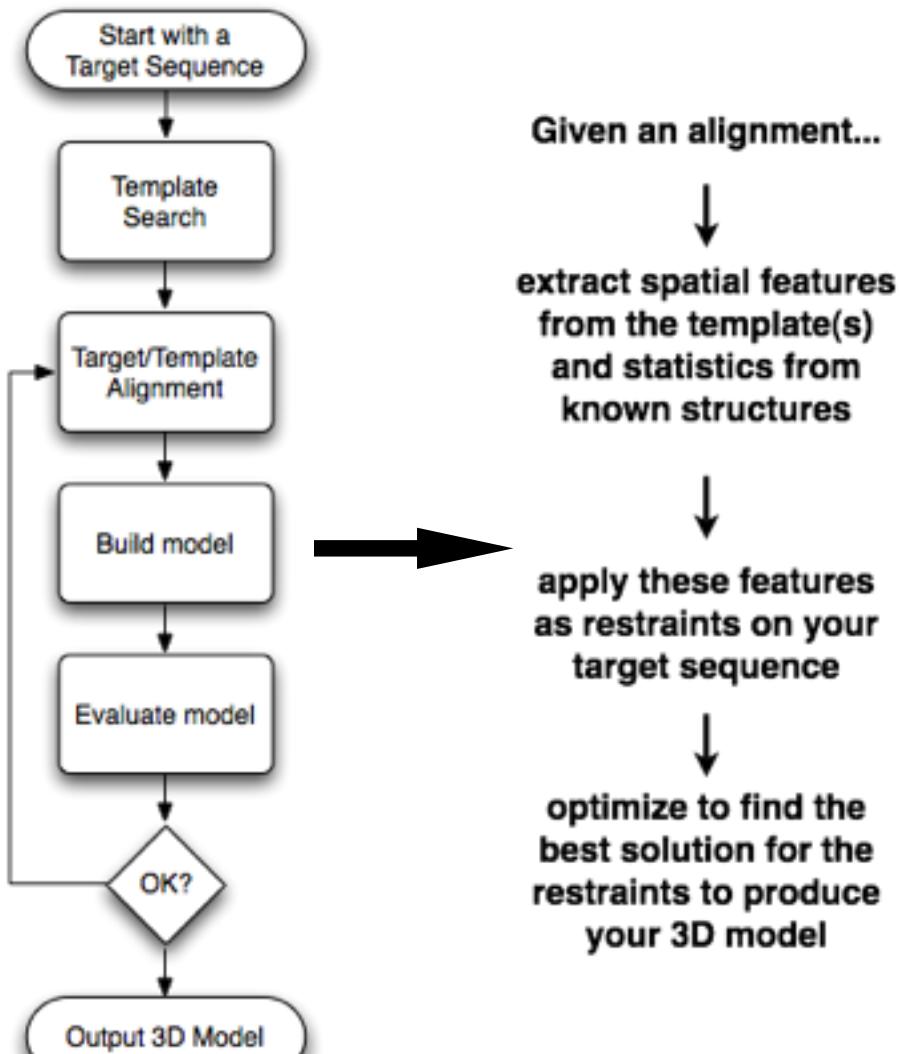


Folding (physics)
Ab initio prediction

Evolution (rules)
Threading
Comparative Modeling

D. Baker & A. Sali. Science 294, 93, 2001.

Comparative modeling by satisfaction of spatial restraints MODELLER

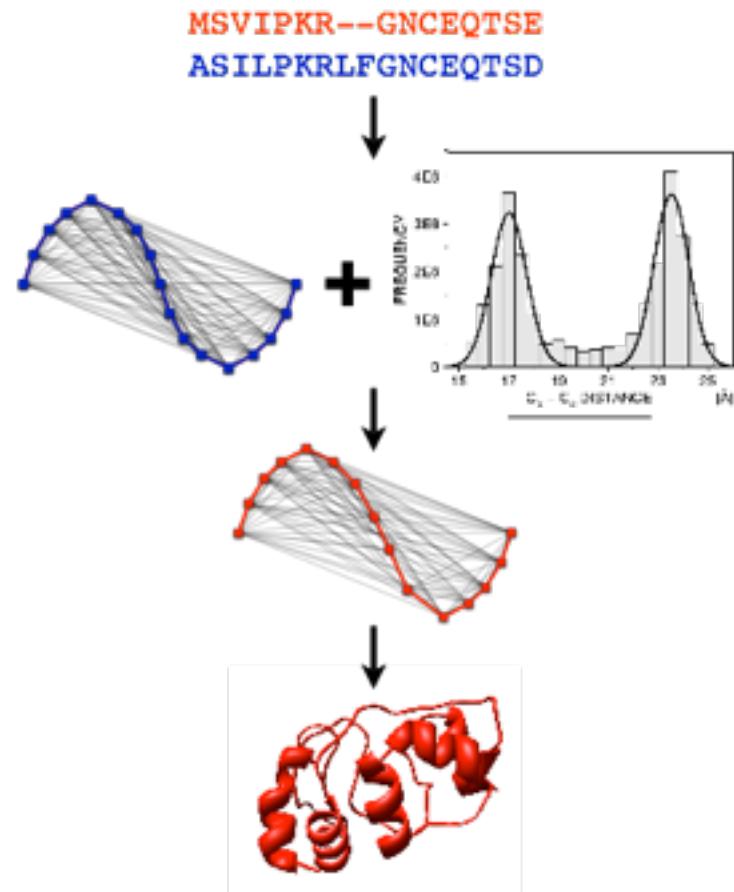


Given an alignment...

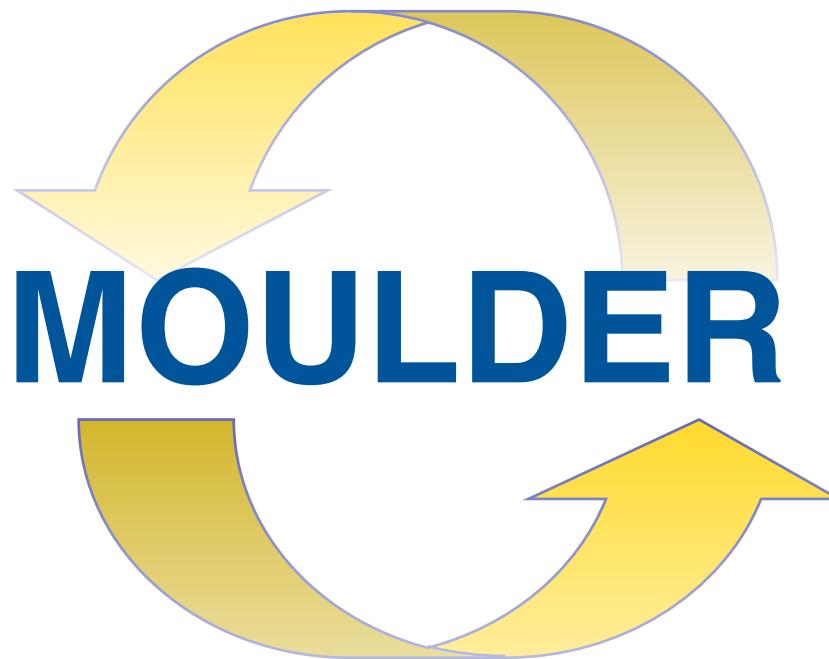
extract spatial features from the template(s) and statistics from known structures

apply these features as restraints on your target sequence

optimize to find the best solution for the restraints to produce your 3D model

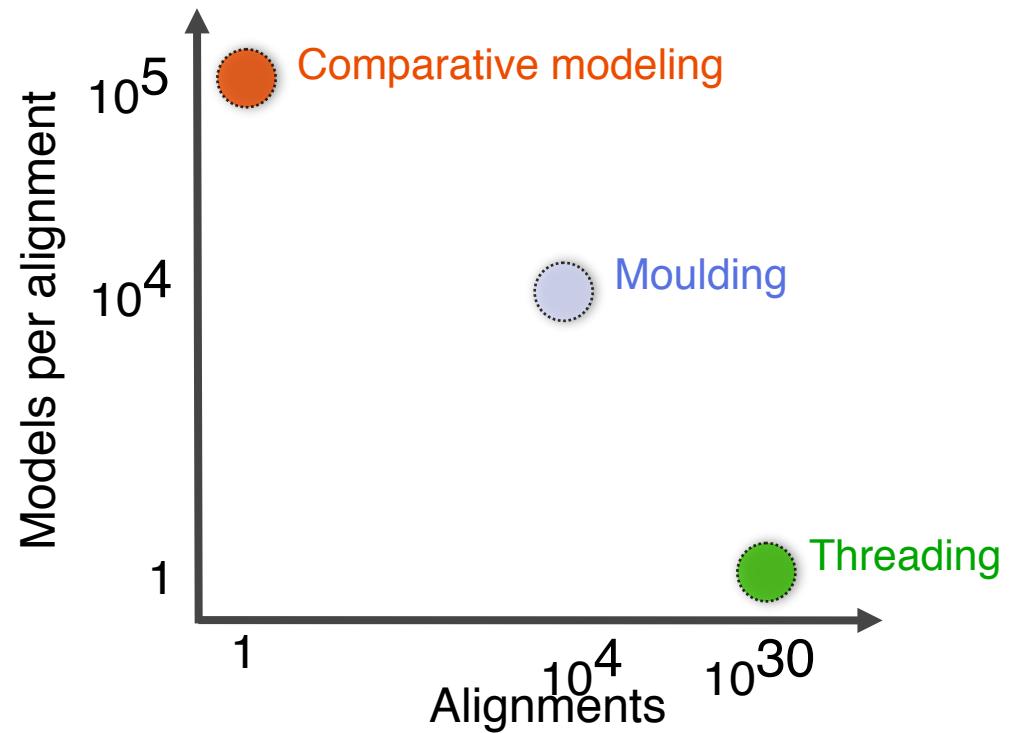
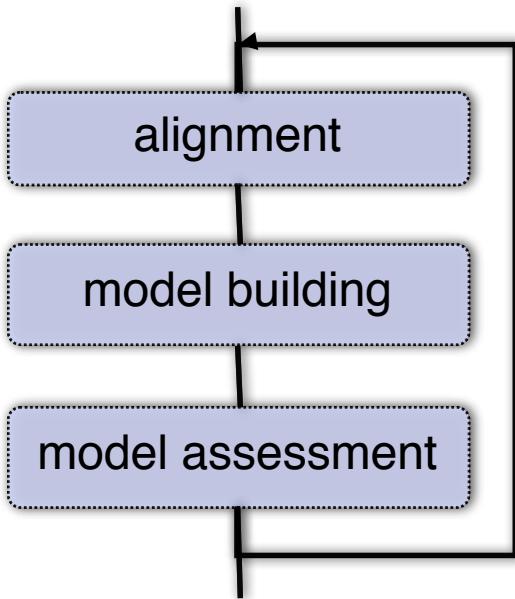


A. Šali & T. Blundell, J. Mol. Biol. 234, 779, 1993.
J.P. Overington & A. Šali, Prot. Sci. 3, 1582, 1994.
A. Fiser, R. Do & A. Šali, Prot. Sci., 9, 1753, 2000.



John, Sali (2003). NAR pp31 3982

Moulding: iterative alignment, model building, model assessment



Genetic algorithm operators

Single point cross-over

...TSSQ—N**MKLGVFWGY**—...
..V—SSCN—**GDLHMKVGV**...



...TSSQ—N**MK**—**LGVFWGY**...
..V—SSCN**GDLHMKV**—**GV**...

...TSSQN**MK**—**LGVFWGY**...
..VSSCN**GDLHMKV**—**GV**...

...TSSQN**MKLGVFWGY**—...
..VSSCN—**GDLHMKVGV**...

Gap insertion

...TSSQN**MKLGVFWG**Y...
..VSSCN**GDLHMKVGV**...



...TSSQN—**MKLGVFWG**Y...
..VSSC**N****GDLHMKVGV**—V...

Gap shift

...**T**—S**SQNMKLGVFWGY**...
..VSSC**NGDLHMKVGV**—...



...—**T**—S**SQNMKLGVFWGY**...
..VSSC**NGDLHMKVGV**—...

...**T**—S—**SQNMKLGVFWGY**...
..VSSC**NGDLHMKVGV**—...

...—**T**S—**SQNMKLGVFWGY**...
..VSSC**NGDLHMKVGV**—...

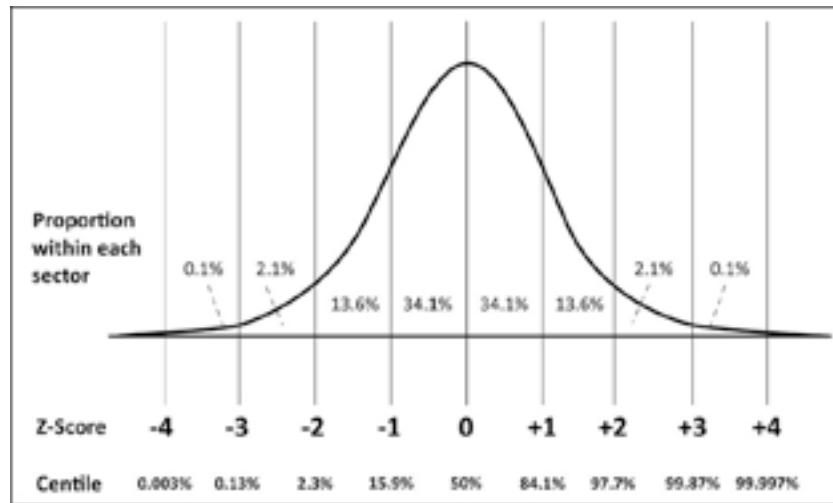
...**TS**—**SQNMKLGVFWGY**...
..VSSC**NGDLHMKVGV**—...

Also, “two point crossover” and “gap deletion”.

Composite model assessment score

- Weighted linear combination of several structural properties:

$$Z = 0.17 Z(P_p) + 0.02 Z(P_s) + 0.10 Z(S_c) + 0.26 Z(H_a) + 0.45 (A_s)$$



John, Sali (2003). NAR pp31 3982

Application to a difficult modeling case

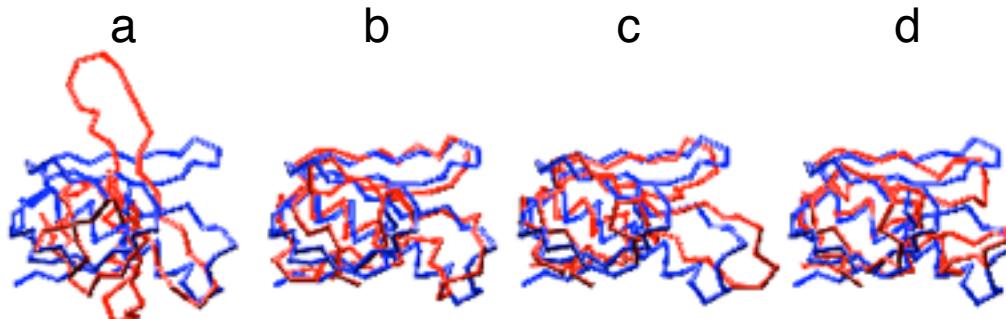
1BOV-1LTS

Best Z

Sequence identity 4.4%

Initial model C α RMSD 10.1 \AA

Final model C α RMSD 3.6 \AA



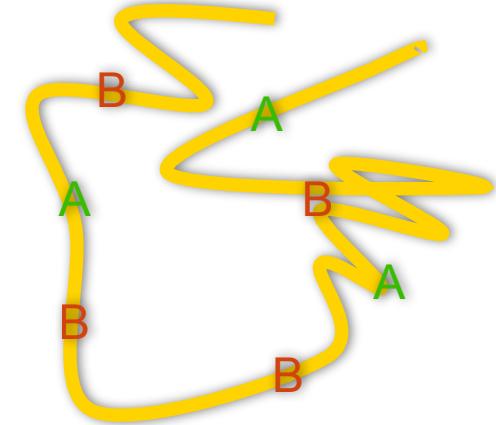
Benchmark with the “very difficult” test set

D. Fischer threading test set of 68 structural pairs (a subset of 19)

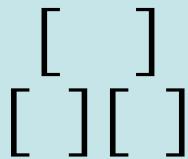
| Target -template | Sequence identity [%] | Coverage [% aa] | Initial prediction | | Final prediction | | Best prediction | |
|------------------|--------------------------|--------------------|----------------------------|-------------------|----------------------------|-------------------|----------------------------|-------------------|
| | | | C _α RMSD [Å] | CE overlap [%] | C _α RMSD [Å] | CE overlap [%] | C _α RMSD [Å] | CE overlap [%] |
| 1ATR-1ATN | 13.8 | 94.3 | 19.2 | 20.2 | 18.8 | 20.2 | 17.1 | 24.6 |
| 1BOV-1LTS | 4.4 | 83.5 | 10.1 | 29.4 | 3.6 | 79.4 | 3.1 | 92.6 |
| 1CAU-1CAU | 18.8 | 96.7 | 11.7 | 15.6 | 10.0 | 27.4 | 7.6 | 47.4 |
| 1COL-1CPC | 11.2 | 81.4 | 8.6 | 44.0 | 5.6 | 58.6 | 4.8 | 59.3 |
| 1LFB-1HOM | 17.6 | 75.0 | 1.2 | 100.0 | 1.2 | 100.0 | 1.1 | 100.0 |
| 1NSB-2SIM | 10.1 | 89.2 | 13.2 | 20.2 | 13.2 | 20.1 | 12.3 | 26.8 |
| 1RNH-1HRH | 26.6 | 91.2 | 13.0 | 21.2 | 4.8 | 35.4 | 3.5 | 57.5 |
| 1YCC-2MTA | 14.5 | 55.1 | 3.4 | 72.4 | 5.3 | 58.4 | 3.1 | 75.0 |
| 2AYH-1SAC | 8.8 | 78.4 | 5.8 | 33.8 | 5.5 | 48.0 | 4.8 | 64.9 |
| 2CCY-1BBH | 21.3 | 97.0 | 4.1 | 52.4 | 3.1 | 73.0 | 2.6 | 77.0 |
| 2PLV-1BBT | 20.2 | 91.4 | 7.3 | 58.9 | 7.3 | 58.9 | 6.2 | 60.7 |
| 2POR-2OMF | 13.2 | 97.3 | 18.3 | 11.3 | 11.4 | 14.7 | 10.5 | 25.9 |
| 2RHE-1CID | 21.2 | 61.6 | 9.2 | 33.7 | 7.5 | 51.1 | 4.4 | 71.1 |
| 2RHE-3HLA | 2.4 | 96.0 | 8.1 | 16.5 | 7.6 | 9.4 | 6.7 | 43.5 |
| 3ADK-1GKY | 19.5 | 100.0 | 13.8 | 26.6 | 11.5 | 37.7 | 7.7 | 48.1 |
| 3HHR-1TEN | 18.4 | 98.9 | 7.3 | 60.9 | 6.0 | 66.7 | 4.9 | 79.3 |
| 4FGF-81IB | 14.1 | 98.6 | 11.3 | 24.0 | 9.3 | 30.6 | 5.4 | 41.2 |
| 6XIA-3RUB | 8.7 | 44.1 | 10.5 | 14.5 | 10.1 | 11.0 | 9.0 | 34.3 |
| 9RNT-2SAR | 13.1 | 88.5 | 5.8 | 41.7 | 5.1 | 51.2 | 4.8 | 69.0 |
| AVERAGE | 14.2 | 85.2 | 9.6 | 36.7 | 7.7 | 44.8 | 6.3 | 57.8 |

Model Assessment

(Potentials of Mean Force)



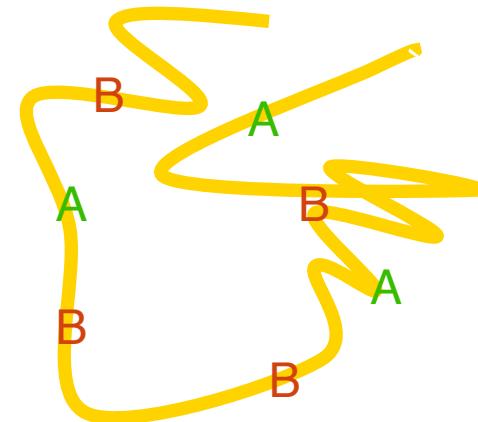
Scoring Statistical Potential (inspiration)



From statistical physics, we know that energy difference between two states (ΔE) and the ratio of their occupancies ($N_1:N_2$) are related [9]:

$$\Delta E = -kT \ln \left(\frac{N_1}{N_2} \right) \quad (1)$$

in which T is the absolute temperature and k is the Boltzmann's constant. As we are interested in an interaction energy between two amino acid side chains, it would seem natural to define N_1 as the number of interactions between these two residues types in a group of real protein structures, a number which is readily available from simple database analysis. But this number must be compared with the number of interactions in some other system, N_2 , to obtain the energy difference between them.

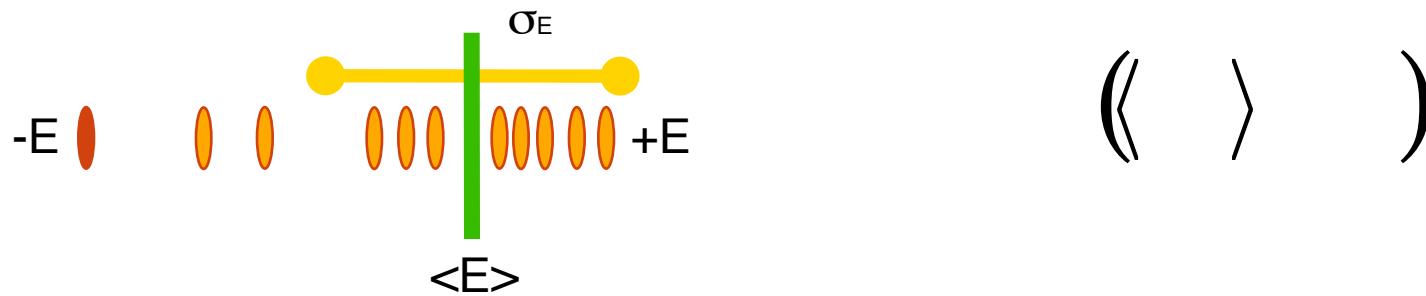


Tanaka and Sheraga (1975) PNAS, 72 pp3802
Sippl, (1990) J.Mo.Biol. 213 pp859
Godzik, (1996) Structure 15 pp363

Scoring

Significance of an alignment (score)

“Energy” Z-score the model with respect the energy of random models (or rest of decoys).

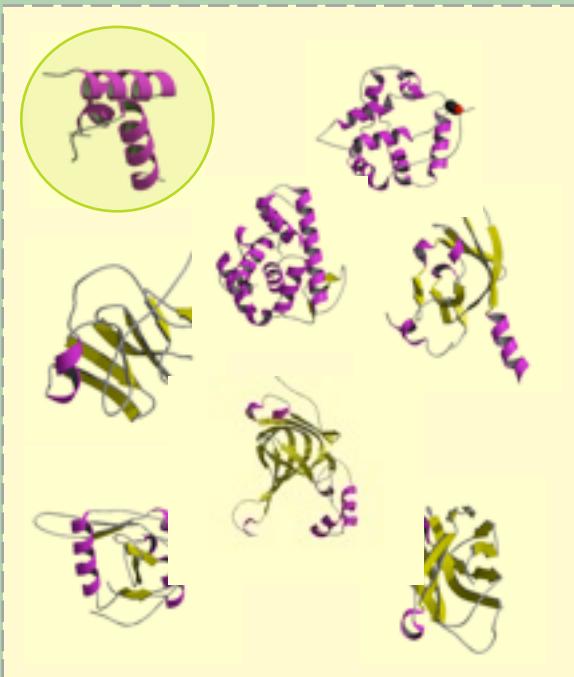


ProSa

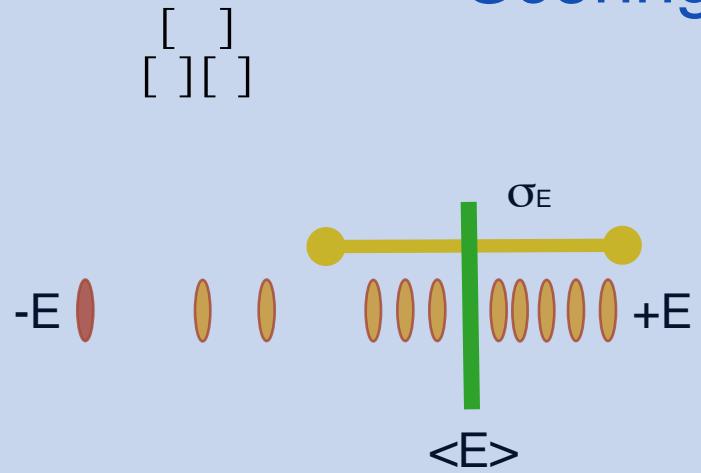
<http://www.came.sbg.ac.at/prosa.php>

Deriving

Structural space



Scoring



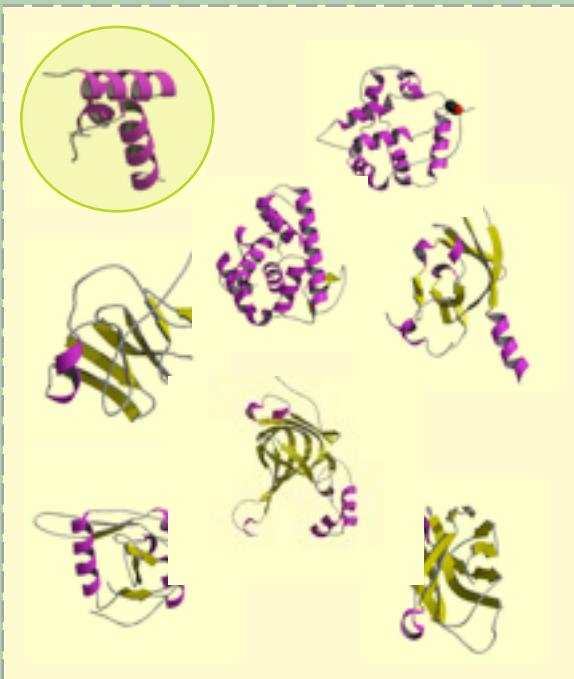
$$Zscore = \frac{(\langle E \rangle - E_m)}{\sigma_E}$$

DFIRE/DFIRE2

<http://sparks.informatics.iupui.edu/yueyang/DFIRE/dDFIRE-service>

Deriving

Structural space



Scoring

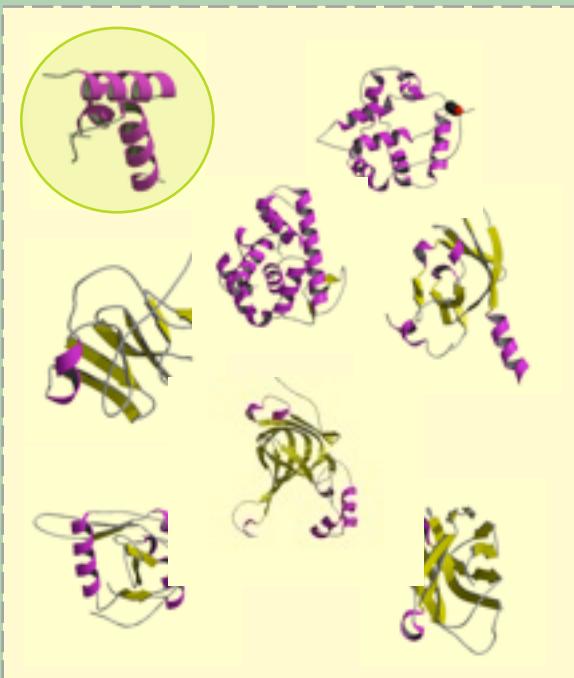
Pseudo-Energy
with respect a
ideal gas-phase
reference state

DOPE (MODELLER)

<http://www.salilab.org/modeller/>

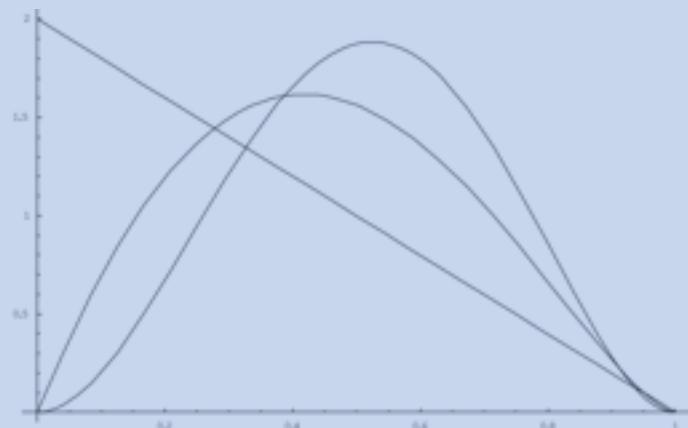
Deriving

Structural space



Scoring

Pseudo-Energy with respect a ideal spherical protein as a reference state

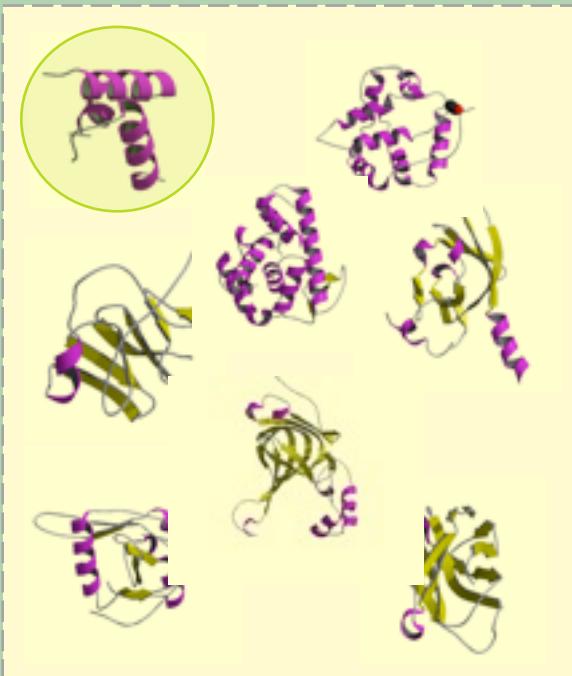


Verify3D

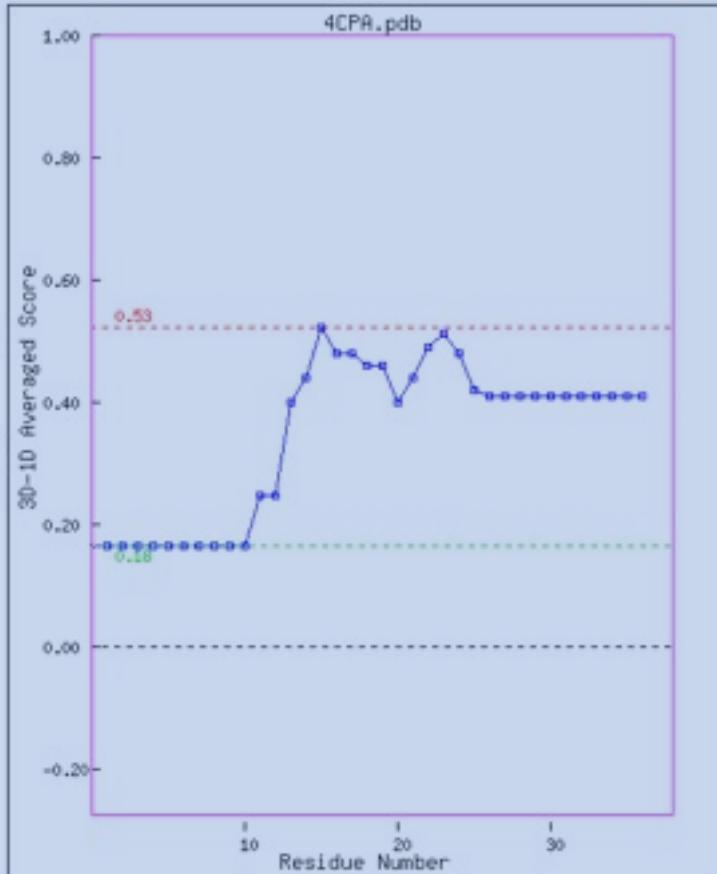
http://nihserver.mbi.ucla.edu/Verify_3D/

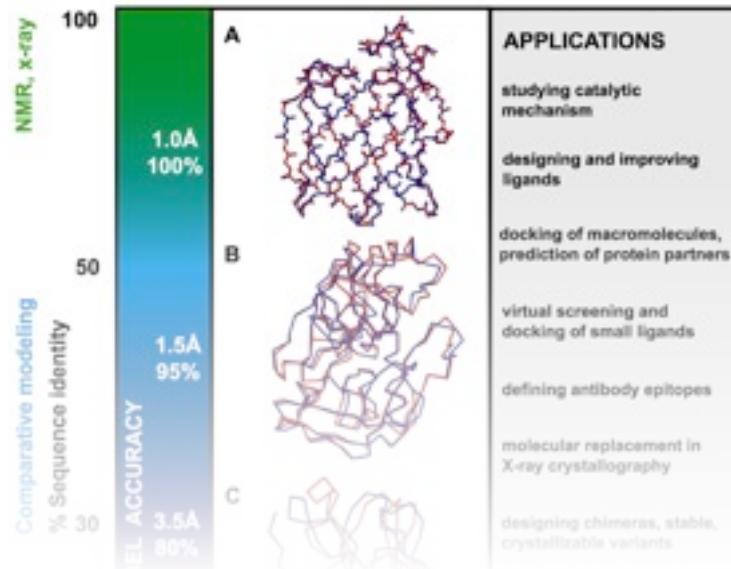
Deriving

Structural space



Scoring





Accuracy and applicability of comparative models

Comparative modeling by satisfaction of spatial restraints Types of errors and their impact



Wrong fold



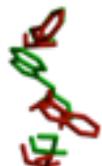
Miss alignments



Loop regions

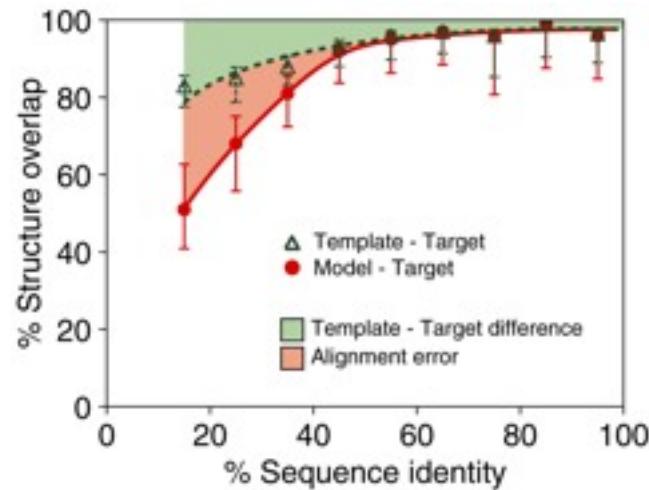
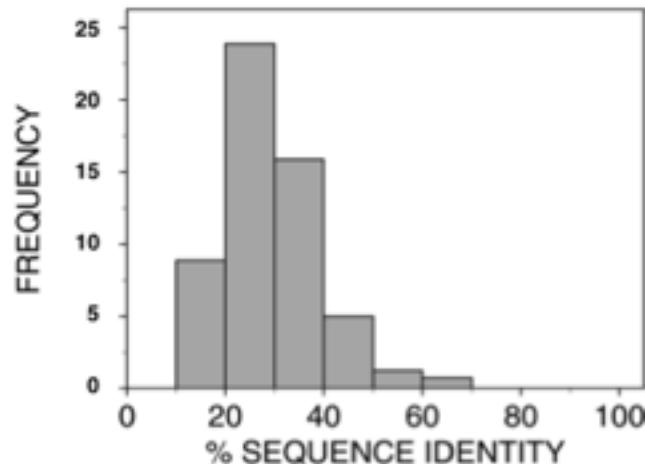


Rigid body distortions



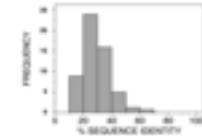
Side-chain packing

Template - Model - Real Structure



Marti-Renom et al. Ann Rev Biophys Biomol Struct (2000) 29, 291

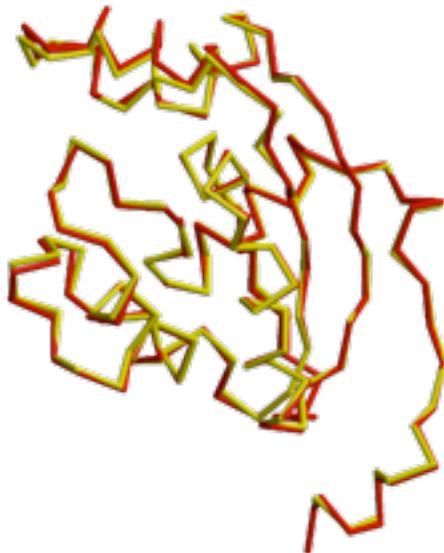
Model Accuracy



HIGH ACCURACY (2/10) MEDIUM ACCURACY (3/10) LOW ACCURACY (5/10)

NM23 Seq id 77%

C α equiv 147/148
RMSD 0.41Å

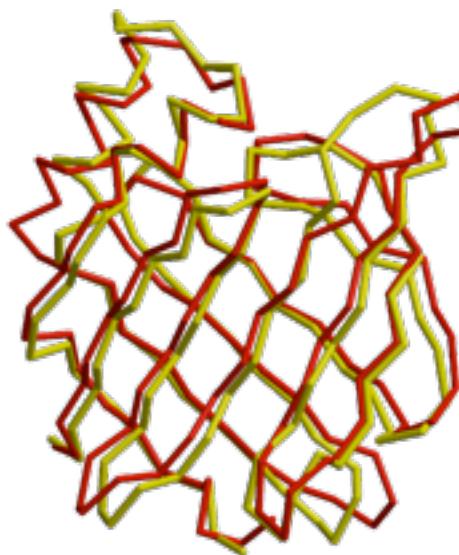


Sidechains
Core backbone
Loops

X-RAY / MODEL

CRABP Seq id 41%

C α equiv 122/137
RMSD 1.34Å



Sidechains
Core backbone
Loops
Alignment

EDN Seq id 33%

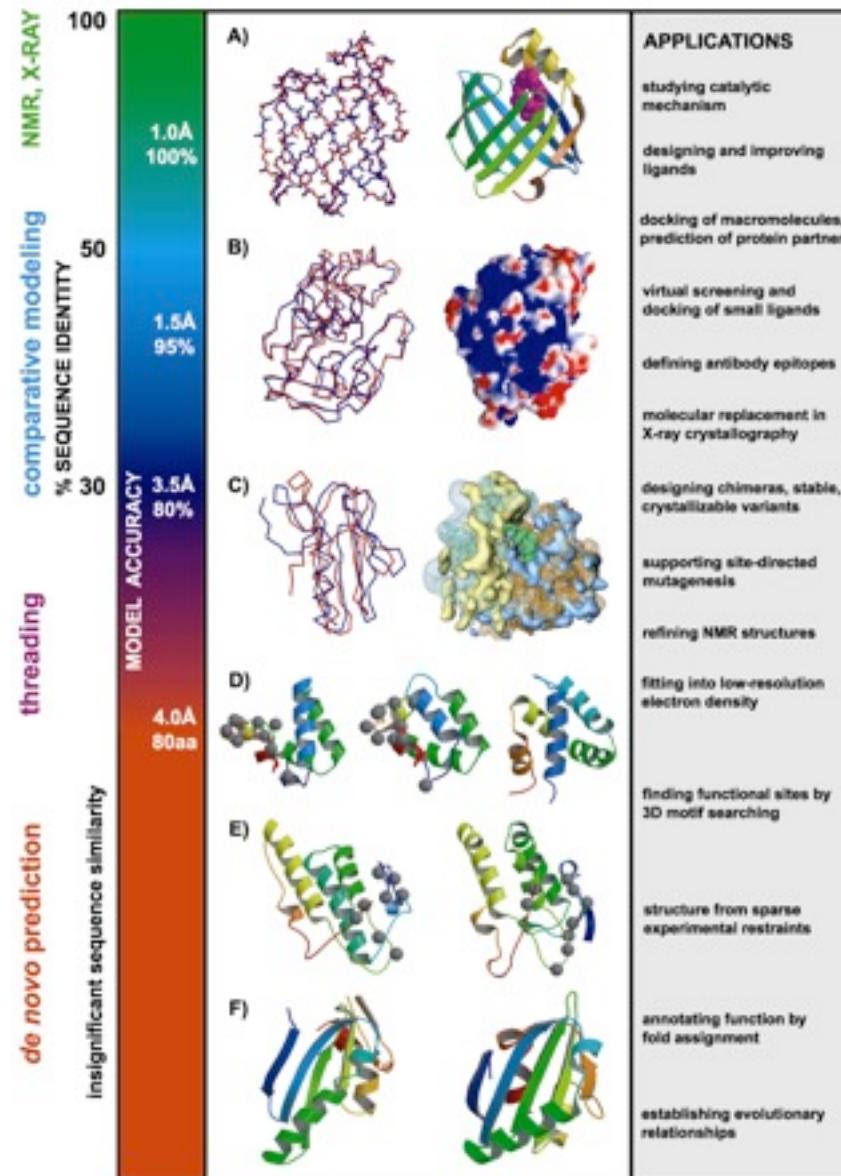
C α equiv 90/134
RMSD 1.17Å



Sidechains
Core backbone
Loops
Alignment
Fold assignment

Marti-Renom et al. Annu. Rev. Biophys. Biomol. Struct. 29, 291-325, 2000.

Utility of protein structure models, despite errors



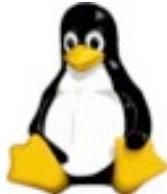
Comparative Protein Structure Prediction

MODELLER tutorial

```
$>mod9v11 model.py
```

Obtaining MODELLER and related information

- ◆ MODELLER (9v11) web page
- ◆ <http://www.salilab.org/modeller/>
 - ◆ Download Software (Linux/Windows/Mac)
 - ◆ HTML Manual
 - ◆ Join Mailing List



Using MODELLER

- ◊ No GUI! ☹
- ◊ Controlled by command file ☹☹
- ◊ Script is written in PYTHON language ☺
- ◊ You may know Python language is simple ☺☺

“MINIMAL” MODELLER

◆ INPUT:

- ◆ **Target Sequence** (FASTA/PIR format)
- ◆ **Template Structure** (PDB format)
- ◆ **Python script file**

◆ OUTPUT:

- ◆ **Target-Template Alignment**
- ◆ **Model** in PDB format
- ◆ Additional data (in .log)

Modeling of BLBP

Input

- ◆ Target: Brain lipid-binding protein (BLBP)
- ◆ BLBP sequence in PIR (MODELLER) format:

blbp.seq

```
>P1;blbp
sequence:blbp::::::::::
VDAFCATWKLTDSQNFDEYMKALGVGFATRQGNVTKPTVIISQEGGKVVIRTQCTFKNTEINFQLGEFEETSIDDRNCKSVVRLDGD
KLIHVQKWDGKETNCTREIKDGKMWVTLTFGDIVAVRCYEKA*
```

Modeling of BLBP

STEP 1: Align blbp and 1hms sequences

Python script for target-template alignment

```
# Example for: alignment.align()

# This will read two sequences, align them, and write the alignment
# to a file:

log.verbose()
env = environ()

aln = alignment(env)
mdl = model(env, file='1hms')
aln.append_model(mdl, align_codes='1hms')
aln.append(file='blbp.seq', align_codes=('blbp'))

# The as1.sim.mat similarity matrix is used by default:
aln.align(gap_penalties_1d=(-600, -400))
aln.write(file='blbp-1hms.ali', alignment_format='PIR')
aln.write(file='blbp-1hms.pap', alignment_format='PAP')
```

Run by typing mod9v11 align.py in the directory where you have the python file.
MODELLER will produce a align.log file

Modeling of BLBP

STEP 1: Align blbp and 1hms sequences

Python script for target-template alignment

```
# Example for: alignment.align()

# This will read two sequences, align them, and write the alignment
# to a file:

log.verbose()
env = environ()

aln = alignment(env)
mdl = model(env, file='1hms')
aln.append_model(mdl, align_codes='1hms')
aln.append(file='blbp.seq', align_codes=('blbp'))

# The as1.sim.mat similarity matrix is used by default:
aln.align(gap_penalties_1d=(-600, -400))
aln.write(file='blbp-1hms.ali', alignment_format='PIR')
aln.write(file='blbp-1hms.pap', alignment_format='PAP')
```

Run by typing `mod9v11 align.py` in the directory where you have the python file.
MODELLER will produce a `align.log` file

Modeling of BLBP

STEP 1: Align blbp and 1hms sequences

Python script for target-template alignment

```
# Example for: alignment.align()

# This will read two sequences, align them, and write the alignment
# to a file:

log.verbose()
env = environ()

aln = alignment(env)
mdl = model(env, file='1hms')
aln.append_model(mdl, align_codes='1hms')
aln.append(file='blbp.seq', align_codes='blbp')

# The as1.sim.mat similarity matrix is used by default:
aln.align(gap_penalties_1d=(-600, -400))
aln.write(file='blbp-1hms.ali', alignment_format='PIR')
aln.write(file='blbp-1hms.pap', alignment_format='PAP')
```

Run by typing `mod9v11 align.py` in the directory where you have the python file.
MODELLER will produce a `align.log` file

Modeling of BLBP

STEP 1: Align blbp and 1hms sequences

Python script for target-template alignment

```
# Example for: alignment.align()

# This will read two sequences, align them, and write the alignment
# to a file:

log.verbose()
env = environ()

aln = alignment(env)
mdl = model(env, file='1hms')
aln.append_model(mdl, align_codes='1hms')
aln.append(file='blbp.seq', align_codes=('blbp'))

# The as1.sim.mat similarity matrix is used by default:
aln.align(gap_penalties_1d=(-600, -400))
aln.write(file='blbp-1hms.ali', alignment_format='PIR')
aln.write(file='blbp-1hms.pap', alignment_format='PAP')
```

Run by typing `mod9v11 align.py` in the directory where you have the python file.
MODELLER will produce a `align.log` file

Modeling of BLBP

STEP 1: Align blbp and 1hms sequences

Output

blbp-1hms.ali

```
>P1;1hms
structureX:1hms: 1 :A: 131 :A:undefined:undefined:-1.00:-1.00
VDAFLGTWKLVDSKNFDDYMKSLGVGFATRQVASMTKPTTIEKNGDILTLKTHSTFKNTEISFKLGVEFDETTA
DDRKVKSIVTLDGGKLVLQKWDGQETTLVRELIDGLILTLHGTAVCTRTRYEKE*
>P1;blbp
sequence:blbp:   : :   : : : : 0.00: 0.00
VDAFCATWKLTDSQNFDAYMKALGVGFATRQVGNVTKPTVIISQEGGKVIRTQCTFKNTEINFQLGEEFEETSI
DDRNCKSVVRLDGDKLIHVQKWDGKETNCTREIKDGKMWVTLFGDIVAVRCYEKA*
```

Modeling of BLBP

STEP 1: Align blbp and 1hms sequences

Output

```
>P1;1hms
structureX:1hms: 1 : : 131 : : undefined:undefined:-1.00:-1.00
VDAFLGTWKLVDNSKNFDDYMKSLGVGFATRQVASMTKPTTIEKNGDILTLKTHSTFKNTEISFKLGVEFDETTA
DDRKVKSIVTLDGGKLVLQKWDGQETTLVRELIDGKLILTLHGTAVCTRTRYEKE*
>P1;blbp
sequence:blbp:      : :      : : : : 0.00: 0.00
VDAFCATWKLTDSQNFDEYMKALGVGFATRQVGNVTKPTVIISQEGGKVVIRTQCTFKNTEINFQLGEEFEETSI
DRRNCKSVVRLDGDKLIHVQKWDGKETNCTREIKDGKMWVTLFGDIVAVRCYEKA*
```

Modeling of BLBP

STEP 1: Align blbp and 1hms sequences

Output

blbp-1hms.pap

```
_aln.pos      10          20          30          40          50          60
1hms        VDAFLGTWKLVDSKNFDDYMKS LGVGFA TRQVASMTKPTT IIEKNGDIL TLKTHSTFKNTE ISFKLGV
blbp        VDAFCATWKLTDSONFDE YMKA LGVGFA TRQVG NVTKPTVI ISQEGGKV VIRTQCTFKNTE INFQLGE
_consrvd    *****  *****  **  ***  ***  *****  *****  *  *  *  *****  *  **

_aln.p       70          80          90         100         110         120         130
1hms        EFD ETTADD RKVKSIVTLDGGKL VHLQ KWDGQETTLV RELI DGLI LT LTHGTAVC TRTYEKE
blbp        EFE ETSID DRNCKS VVR LDGD KLIHV QKWDG KETN CTR EIKDG KMV VT LTF GDI VAVRCYEKA
_consrvd    **  **  ***  **  *  ***  *  *  *****  *  **  *  ***  *  *  *  *
```

Modeling of BLBP

STEP 2: Model the blbp structure using the alignment from step 1.

Python script for model building

```
# Homology modelling by the automodel class
from modeller.automodel import *          # Load the automodel class
log.verbose()                            # request verbose output
env = environ()                          # create a new MODELLER environment

# directories for input atom files
env.io.atom_files_directory = './:/.../atom_files'

a = automodel(env,
               alnfile  = 'blbp-1hms.ali',      # alignment filename
               knowns   = '1hms',              # codes of the templates
               sequence = 'blbp')             # code of the target

a.starting_model= 1                      # index of the first model
a.ending_model  = 1                      # index of the last model
                                         # (determines how many models to calculate)
a.make()                                 # do the actual homology modelling
```

Run by typing `mod9v11 model.py` in the directory where you have the python file.
MODELLER will produce a `model.log` file

Modeling of BLBP

STEP 2: Model the blbp structure using the alignment from step 1.

Python script for model building

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env = environ()                       # create a new MODELLER environment

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                                    # (determines how many models to calculate)
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Modeling of BLBP

STEP 2: Model the blbp structure using the alignment from step 1.

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    alnfile  = 'blbp-1hms.ali',        # alignment filename
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Run by typing `mod9v11 model.py` in the directory where you have the python file.
MODELLER will produce a `model.log` file

Modeling of BLBP

STEP 2: Model the blbp structure using the alignment from step 1.

Python script for model building

PDB file

Can be viewed with Chimera

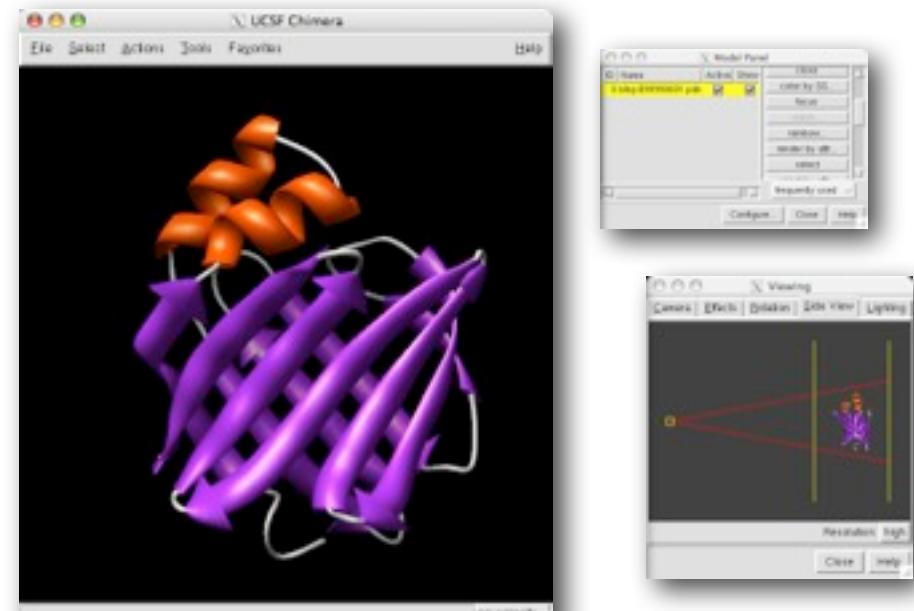
<http://www.cgl.ucsf.edu/chimera/>

PyMol

<http://www.pymol.org>

Rasmol

<http://www.openrasmol.org>



- Model file →
blbp.B99990001.pdb

In 15 days!

<http://www.salilab.org/modeller/tutorial/>

The screenshot shows a web browser window titled "Tutorial" displaying the MODELLER website at <http://salilab.org/modeller/tutorial/>. The page features a large red "Modeller" logo. Below it, a subheader reads: "Program for Comparative Protein Structure Modelling by Satisfaction of Spatial Restraints". To the right is a 3D ribbon model of a protein structure with a green and blue color scheme. Below the ribbon is a sequence alignment diagram showing two sequences: "A I L V G E M P R D Q D O M E R K D I L K A N V K I F X C O S A" and "Y E V C P Y D C T Y E G P Y S L V I H P D E C I D C A C E P". A yellow arrow points from the left margin towards the "Tutorial" section.

Tutorial

MODELLER is used for homology or comparative modeling of protein three-dimensional structures. The user provides an alignment of a sequence to be modeled with known related structures and MODELLER automatically calculates a model containing all non-hydrogen atoms.

This web site presents a tutorial for the use of MODELLER 9v2 or newer (for older versions of MODELLER, use the [old MODELLER 7v7 tutorial](#)). There are 5 modeling examples that the user can follow:

1. [Basic Modeling](#). Model a sequence with high identity to a template.
This exercise introduces the use of MODELLER in a simple case where the template selection and target-template alignments are not a problem.
2. [Advanced Modeling](#). Model a sequence based on multiple templates and bound to a ligand.
This exercise introduces the use of multiple templates, ligands and loop refinement in the process of model building with MODELLER.

FULLY AUTOMATIC MODWEB

<http://salilab.org/modweb>

The screenshot shows a web browser window for the ModWeb Server. The URL in the address bar is <https://modbase.compbio.ucsf.edu/scgi/modweb.cgi>. The page title is "ModWeb Server". The main content area features a logo of a blue triangle with a white "S" and the text "ModWeb Server". Below the logo is a navigation menu with links: Sali Lab Home, ModWeb, ModLoop, ModBase, IMP, ModPipe, LS-SNP. Underneath the menu are links for Help, User Login, ModBase Datasets for User Anonymous, Contact, News, Current ModWeb queue, and ModWeb Home.

News:

- New Chimera - Modeller Module for interactive modeling!
 - In Chimera's daily build starting Sept 15, 2010
- Additional functionality for registered users:
 - Template based modeling
 - Access to all user's ModWeb datasets
 - Email notification for User's ModBase updates
- Developers:
Eswar Narayanan
Ursula Pieper
Ben Webb
- Acknowledgements:
David Eramian
Mailur S. Madhusudhan
Marc A. Marti-Renom
Min-Yi Shen
Andrey Sali

ModWeb: A Server for Protein Structure Modeling
Welcome to the new ModWeb (old version)

General information

Name: [Input field]
Email address: [Input field]
Modeller license key: [Input field] (Not necessary for ModBase updates)
Dataset name (optional): [Input field]
Availability: Add to academic dataset

Input data

Input protein sequences: [Large input area]
or upload sequences file (FASTA Format): [Choose File] no file selected
 Calculate Models Reset

Model selection criteria

Best scoring model
 Longest well scoring model
 Upload models to ModBase

Other options

Very Fast: [Dropdown menu]

MODBASE

<http://salilab.org/modbase>

Search Page

UCSF - University of California, San Francisco | About UCSF | UCSF Medical Center

Home User Login ModBase Search Page ModWeb Modelling Server Help Current Logins

**MOD
BASE**

Database of Comparative Protein Structure Models

Welcome to ModBase, a database of three-dimensional protein models calculated by comparative modeling.
[Old ModBase Interface](#)

General Information

Statistics

Project Pages

Documentation

Authors and Acknowledgements

Publications

Todo List

Related Resources

Note:
MODBASE contains theoretically calculated models, not experimentally determined structures. The models may contain significant errors.

ModBase search form

Search type: Model(Default) Display type: Model detail (graphical)

All available datasets are selected Select specific dataset(s)

Search by properties Property: All Organism: All Advanced search

Model Details

UCSF - University of California, San Francisco | About UCSF | UCSF Medical Center

Home User Login ModBase Search Page ModWeb Modelling Server Help Current Logins

**MOD
BASE**

Sequence Information

Primary Database Link: P43602 (K0254_HUMAN)
Organism: Homo sapiens
Annotation: killer cell immunoglobulin-like receptor 2ds4 precursor (mhc class i dce nk cell receptor) (natural killer associated transcript 8) (nktr-8dce) (p58 natural killer cell receptor clone cl-39) (p58 nk
Sequence Length: 304
Model Information:

Perform action on this model: Select option

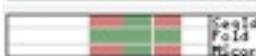
Sequence Model Coverage: 

Sequence Identity: 88.00%
E-Value: 2e-43
Model Score: 1.00
Target Region: 27-321
Protein Length: 304
Template PDB: 1mX
Code: 1mX
Template Region: 6-200
Dataset: spr-human2

Filtered models for current sequence (Show all models)

Cross-references

Sequence Overview

| | | | | |
|---|------------------------|------------------------------|--|------|
|  | Q8G8A6 | hypothetical protein | Pseudomonas aeruginosa | 3738 |
|  | Q8G9W1 | hypothetical protein | Escherichia coli | 1140 |
|  | Q8CY62 | hypothetical protein spr1965 | Streptococcus pneumoniae , Streptococcus pneumoniae R6 | 1038 |

Model Overview

| | | | | | | | | | | | |
|---|--|----------------------|--|------|-----------|-----|-------|-------|------|-----------------------|--------|
|  |  Q8G8C7 | hypothetical protein | Pseudomonas aeruginosa | 4996 | 2089-2158 | 70 | 37.00 | 7e-14 | 1.00 | 1dnvA | 8-78 |
|  |  Q8G8C7 | hypothetical protein | Pseudomonas aeruginosa | 4996 | 492-1017 | 526 | 36.00 | 1e-82 | 1.00 | 1amuA | 19-529 |
|  |  Q8G9W1 | hypothetical protein | Escherichia coli | 1140 | 349-1135 | 787 | 35.00 | 0 | 1.00 | 1r9dA | 6-783 |

- Pieper et al. (2004) Nucleic Acids Research 32, D217-D222

Modeling RNA

MC-FOLD / MC-SYM

<http://www.major.iric.ca/MajorLabEn/MC-Tools.html>

<http://www.major.iric.ca/MC-Sym/>



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IN IMMUNOLOGY AND CANCER



Messages:

- Please note that Working directories are erased 7 days after the last change made.

Pipeline page

MC-Sym's [user's guide](#) | [FAQ](#) | [wiki](#)

MC-SYM

1. Input File

- Make sure that your input file contains only printable ASCII characters
- Do not use Microsoft Word to edit the script; use WordPad instead

2. Local File (Option)

Browse ...

3. Directory Key (Option)

remove previous models

4. Email Address (Option)

Provide your email address to receive notifications about:

- Job completion
- Directory removal (48h notice)

- Coarse-grained model
- Fragment-based approach
- Fully automated
- Slow
- Sampling bottleneck
- Relative poor accuracy

ROSIE

http://rosie.rosettacommons.org/rna_denovo

Welcome to ROSIE

Rosetta Online Server that Includes Everyone

Welcome Queue Documentation Support

Login Create an account

Rosetta RNA_Denovo Protocol



[\[Submit RNA_Denovo task\]](#)

| Current Status | Protocol | Task ID | Created | Last Update |
|----------------|------------|---------|---------------------|---------------------|
| Queued | RNA_Denovo | task1 | 2023-03-27 10:00:00 | 2023-03-27 10:00:00 |
| Queued | RNA_Denovo | task2 | 2023-03-27 10:00:00 | 2023-03-27 10:00:00 |
| Queued | RNA_Denovo | task3 | 2023-03-27 10:00:00 | 2023-03-27 10:00:00 |
| Queued | RNA_Denovo | task4 | 2023-03-27 10:00:00 | 2023-03-27 10:00:00 |

[\[RNA Denovo Queue\]](#)



[\[RNA Denovo Documentation\]](#)

Please cite the following article when referring to results from our RNA_Denovo server:

- Das, R., Karanicolas, J., Baker., D. "Atomic accuracy in predicting and designing noncanonical RNA structure". *Nature Methods* 7:291–294. (2010).
[Online](#) | [PDF](#)

MODERNA

<http://iimcb.genesisilico.pl/modernaserver/>



Laboratory of Bioinformatics and Protein Engineering

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Homepage

ModeRNA server

A server for RNA structure modeling and analysis

by Magdalena Rother, Kaja Milanowska, Tomasz Puton, Kristian Rother, and Janusz M. Bujnicki.

<http://iimcb.genesisilico.pl/modernaserver/>

What is the ModeRNA server?



This service is based on the ModeRNA software for RNA 3D structure prediction, analysis, and manipulation.

Currently, the server allows you to:

- **build a model** (requires a pairwise sequence alignment and a structural template).
- **find template** (looks for potential templates using ParAlign and Rfam).
- **align sequences** (prepares an alignment between two RNA sequences using R-coffee).
- **convert PDB naming** (changes nomenclature in a PDB file).
- **clean up a structure** (remove water, ions, and ligands, adds missing P atoms and changes "*" into "" in ribose).

- Comparative RNA modeling
- Able to handle 115 nucleotide modifications