COMPUTATIONAL STRUCTURAL BIOLOGY

STRUCTURE, SIMULATION, FUNCTION & PREDICTION

Lecture 3

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http://csb.stanford.edu/clas
LECTURE 3 CONTENTS

Helix-Helix Packing.
Helix-Sheet Packing.
Sheet-Sheet Packing.
Folding Unit Classification.
Sample Folds.
Classification Databases.
Helix-Helix Packing Concept 3.1
HELIX-HELIX-PACKING

Pairs of Alpha-Helices.

Helix Ridge Lines.

Common Helix Packings.

Helix Packing Omega=140 & -40.

Helix Packing Omega=20 & -160.

Common Helix Packings Revisited.
PAIRS OF ALPHA-HELICES

- $d$ is the separation of helix axes at that point (~12 Å).
- Omega ($\Omega$) is the dihedral angle about the line of closest approach.
HELIX RIDGE LINES

i to i+3 ridge

i to i+4 ridge
COMMON HELIX PACKINGS

$\Omega = 320^\circ$

or $\approx 40^\circ$

$\Omega = 140^\circ$

$\Omega = 20^\circ$
HELIX PACKING $\Omega = 140^\circ$ & $-40^\circ$

Inside view $(i, i+4)$  Outside view $(i, i+4)$

The sidechains in the pack well in both arrangements

$\Omega = 320^\circ$ or $-40^\circ$

$\Omega = 140^\circ$
HELIX PACKING $\Omega = 20^\circ$ & $-160^\circ$

Inside view $(i, i+3)$

Outside view $(i, i+4)$

$\Omega = 200^\circ$ or $-160^\circ$

Rare. The sidechains in the interface do not pack well. Not clear why.

Common. The sidechains in the interface pack well.
COMMON HELIX PACKINGS REVISITED

- The reason for the low frequency at $\Omega = -160^\circ$ (or $200^\circ$) is not clear?

Extra credit??
Helix and Sheet Packing

Concept 3.2
HELIX AND SHEET PACKING

α-Helix and β-Sheet.
Common Helix/Strand Packings.
Pair of Beta-Sheets.
Common Strand/Strand Packings.
ALPHA-HELIX AND BETA-SHEET

- End-on view (sheet orange, helices blue).
- Side view. Helices seem to follow strands not sheet.
COMMON HELIX/STRAND PACKINGS

(12, -20°)
This is preferred

(12, 160°)

Ω = 340°
or -20°

Ω = 160°

• Find that Ω = -20°
  not 0° is clearly most common.
PAIR OF BETA-SHEETS

- End-on view (sheet orange, helices blue).
- Top view. The two sheets in the sandwich are skewed by about \(-30^\circ\).
COMMON STRAND/STRAND PACKINGS

\( \Omega = 340^\circ \) or \(-20^\circ\)

\( \Omega = 155^\circ \)

(5Å, 340°)

(5Å, 155°)

(9Å, 130°)

Secondary peak due to second nearest neighbors.
Architectural Principles
Concept 3.3
ARCHITECTURAL PRINCIPLES

Hydrogen Bonding in Proteins.
Buried Waters in Proteins.
Close Packing in Proteins.
Cavities in Proteins.
Domains in Proteins.
Contact Order.
CLOSE PACKING IN PROTEINS

- Protein interiors are close-packed like the interiors of organic crystals.
- There are small cavities due to packing defects.
- Some of these are filled with a water molecule.

Aromatic residues are green. Other hydrophobic residues are cyan. The rest are gray.
HYDROGEN BONDING IN PROTEINS

• 90% of the hydrogen bonding groups in a protein form a bond to either another protein group or to a water molecule.

• This is done by making hydrogen bonds in the α-helix and β-sheet secondary structures.

• Unsatisfied hydrogen bonds remain at the ends of the α-helix, the edges of the β-sheet and in the polar side chains.

• These parts of the chain are generally on the outside in contact with the water.

• Sometimes hydrogen bonding is satisfied by burying a water molecule in the protein structure.
BURIED WATERS IN PROTEINS

- There are three water molecules buried in this protein (4pti.pdb).

- Protein polar groups point out to interact with water molecules.

- Buried water molecules also hydrogen bond.
CAVITIES IN PROTEINS

- There are many cavities in the protein.
- Most of the cavities are filled with water molecules.
DOMAINS IN PROTEINS 1

- The chain tends to stay in one spatial area.
- Very big proteins are often like a string of smaller proteins.
- Each unit is called a “domain”.

Michael Levitt 04
DOMAINS IN PROTEINS 2

T4 lysozyme with saccharide in active site
(148Lpdb)

- Often active sites are in the cleft between domains.
The contact order is the number of residues along the chain that separate two residues in close spatial contact.

Experimentally, proteins with the smallest average contact order fold fastest. This is thought to be because residues close along the chain collide more frequently.
Folding Unit Classification
Concept 3.4
FOLDING UNIT CLASSIFICATION

Folding Units.
All-α Proteins.
All-β Proteins.
α/β Proteins.

β/β Chirality.
βαβ Chirality: Why?
α+β Proteins.
FOLDING UNITS

- Folding units are small assemblies of secondary structure that occur often in folded globular proteins.

- They were first identified in 1976 (Levitt & Chothia, Nature, 261, 552)

- Stabilized by packing & hydrophobic interactions

- Stabilized by hydrogen bonds

- There is now evidence that these units may sometimes be stable in isolation.
ALL-ALPHA PROTEINS 1

Built from α-helices packed together

- Folding diagrams allow one to visualize a complicated three dimensional fold in a 2-D sketch.
- Try to view the α-helices (or β-strands) end on.
- Show chain connections.

Myohemerythrin (2mhr.pdb)
ALL-ALPHA PROTEINS 2

Top

Myohemerythrin (2mhr.pdb)

End-on

End-on
ALL-BETA PROTEINS 1

Built mainly from β-strands packed together

RUB
IGC
IGV
PBN

Circle hairpins in red

SDM
CON
CHT

*Strands form hairpins, hairpins form sheets, sheets form layers (sandwiches). All is twisted.

End-on views are distorted
ALL-\( \text{BETA} \) PROTEINS 2
ALPHA/BETA PROTEINS 1

Flavodoxin (3fm pdb)
ALPHA/BETA PROTEINS 2

Built from α-helices and β-strands that alternate

- TRX
- FLN
- AKN
- PGM
- TIM
- SUB
- CPA
- LDH
- PGK
- HKN
- GPD
- TIM

- The sheets are mainly parallel due to the βββ folding units.

[Image of protein structures]
ALPHA/BETA PROTEINS 3

All the βαβ folding units circled in red have something in common. What is it?
EXPLAIN BETA-BARREL

- The TIM β-barrel fold recurs in seemingly unrelated SCOP superfamilies.
- The active site is always at the N-terminus of the parallel helices (the C-terminus of the stands).
- This is convergent evolution. It shows that this fold is both very stable and also easily adapted to a wide variety of functions.

Picture shows a monomer of 6tim pdb with 3-phosphoglycerol
BAB CHIRALITY

- Left-handed BAB is common.
- Right-handed BAB is very rare.

Anti-clockwise

Why? Clockwise
BAB CHIRALITY WHY

* Left-handed ββ has short path.

* Right-handed ββ has long path. Ends trapped!
ALPHA+BETA PROTEINS

Built from α-helices and β-strands that segregate

- PTI
- LZN
- TLS

- The sheets are mainly antiparallel due to the β hairpin folding units.
- α+β like a mix of all-α & all-β.
Sample Folds

Concept 3.5
SOME EXAMPLES

Small Proteins.
Coiled-coil Proteins.
Membrane Proteins.
Simple All-α Fold.
All-β with Long β-hairpins.
Antiparallel All-β Fold.
Parallel All-β Fold.
Simple α/β Fold.
SMALL PROTEINS

End-On View

1ctf.pdb

1p6b.pdb

Top view

2cro.pdb

4icb.pdb
COILED-COIL PROTEINS

• 5 parallel α-helices each with 46 residues in a parallel five helix coiled-coil.

• Coiled coils are normally just two α-helices.

The cross-section is well-packed
MEMBRANE PROTEINS

Porin from Escherichia coli

- Outer membrane of bacteria is permeable thanks to porin.

Side view

Top view (from outside)
SIMPLE ALL-ALPHA FOLD

70 kDa soluble lytic transglycosylase (1sly.pdb)

- 2 curved layers: right-handed α/α superhelix.
- 26 α-helices and 450 residues.
ALL-BETA WITH LONG BETA-HAIRPINS

Human Bactericidal Protein (1bp1.pdb)

Just show strands not helices
ANTIPARALLEL ALL-BETA FOLD

Outer surface protein A from Lyme disease spirochete (1osp.pdb)

- β-hairpin repeats with 21 strands in single sheet.
- Sheet bends on itself.
- Middle part exposed to solvent on both sides.
PARALLEL ALL-BETA FOLD

P22 tailspike protein from Salmonella typhimurium phage p22

- Huge beta-helix with 16 turns.
- Each turn is three strands that form well-packed core.
SIMPLE ALPHA/BETA FOLD

- Sequence has 16 α/β repeats.
- The cross-section is well-packed helix aligns to strand.

Ribonuclease Inhibitor (2bnh.pdb)
Classification Databases

Concept 3.6
CLASSIFICATION DATABASES

CATH.

CATH Mainly Alpha.

CATH Mainly Beta.

CATH Mixed Alpha-beta.

CATH Few Secondary Structures.

CATH Drill Down To A Level.

CATH Drill Down To H Level.

CATH Hierarchy.

CATH The Numbers.

Other Databases SCOP, DALI.
CATH

4 top-level Categories

Mainly Alpha
Mainly Beta
Mixed Alpha-Beta
Few Secondary Structures

CATH is:
C: Class
A: Architecture
T: Topology
H: Homology

Janet Thornton
CATH MAINLY ALPHA

Mainly Alpha Tree

C: Class 1
A: Architecture 5
T: Topology 228
H: Homology 433
CATH MAINLY BETA

Mainly Beta Tree

C: Class 1
A: Architecture 19
T: Topology 139
H: Homology 286
CATH MIXED ALPHA-BETA

Mixed Alpha-Beta Tree

C: Class 1
A: Architecture 12
T: Topology 361
H: Homology 659
CATH FEW SECONDARY STRUCTURES

Few Secondary Structures Tree

A: Architecture  1
B: Architecture  1
C: Class  1
D: Class  1
E: Class  1
F: Class  1
G: Class  1
H: Homology  89
I: Homology  85
J: Homology  85
K: Homology  85
L: Homology  85
M: Homology  85
N: Homology  85
O: Homology  85
P: Homology  85
Q: Homology  85
R: Homology  85
S: Homology  85
T: Topology  85
U: Topology  85
V: Topology  85
W: Topology  85
X: Topology  85
Y: Topology  85
Z: Topology  85

Levels

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Display all levels (1 matches)
CATH DRILL DOWN TO A LEVEL

CATH is:
C: Class
A: Architecture
T: Topology
H: Homology
CATH DRILL DOWN TO H LEVEL

Homologous Superfamily (3.15.10.10)

Bactericidal permeability-increasing protein; domain 1

Classification

- Class: 3
  - Alpha Beta
- Architecture: 3.15
  - Super Roll
- Topology: 3.15.10
  - Bactericidal permeability-increasing protein; domain 1
- Homologous Superfamily: 3.15.10.10
  - Bactericidal permeability-increasing protein; domain 1

Summary

The following table provides an overview of the number of levels found further through the hierarchy.

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<td>Horseshoe</td>
<td>Roll</td>
<td>Barrel</td>
<td>HIV-1 Transactivator Protein</td>
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<td>Alpha solenoid</td>
<td>Barrel</td>
<td>2 Layer Sandwich</td>
<td>Omega-AgatoxinIV</td>
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## CATH THE NUMBERS

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OTHER DATABASES SCOP

Cyrus Chothia
Alexei Murzin
Steven Brenner

- SCOP is manually curated
- SCOP actively maintained
- SCOP Hierarchy
  CLASS 11
  FOLD 800
  SUPERFAMILY 1294
  FAMILY 2327

First Web Database
Perl cgi.pl
# OTHER DATABASES DALI 1

**Dali: Structural Neighbours in PDB90**

- **Fold index:** A tree is constructed by average linkage clustering of the structural similarity score. The tree is cut at Dali Z-score levels 2, 4, 8, 16, 32 and 64. The first level (Z>2) can be used as an operational definition of folds.
- **PDB code:** The list includes all chains in PDB90. PDB90 is a representative subset of the PDB, where no two chains share more than 90% sequence identity. The domain number is appended as _n. Domains are numbered 1,2,3,... Proteins with a domain number 0 have not been assigned by the structural domain decomposition algorithm but are assigned as single-domain structures by default.
- **Adda:** Adda sequence families are defined independently of structure information based on Blast searches and sequence-profile similarities, using relatively conservative cutoffs. Structural neighbours in the same Adda family are evolutionarily related, but some superfamilies are split into many Adda families. The number of the corresponding Adda domain family is given, where the structural and sequence-based domain definitions agree.
- **Browse:** Click on the link to view the list of structural neighbours of the representative and their alignments.
- **Compound:** The COMPND record from PDB.

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- **Built automatically using DALI structure comparison.**
- **More for computers than people.**

Click on “interact” to see more.
OTHER DATABASES DALI 2

Dali database: select structural neighbours of 1e2aA


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- Protein with PDB code 1e2aA is very similar to itself.
- 1e2aA also similar to 1dn1B.

FSSP has multi-sequence alignments.
# Comparing CATH SCOP DALI

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**Date**
- CATH: v2.5.1 25-Nov-03
- SCOP: v1.65 1-Aug-03
- DALI: May-03

- Very different even from the simplest point of view.

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