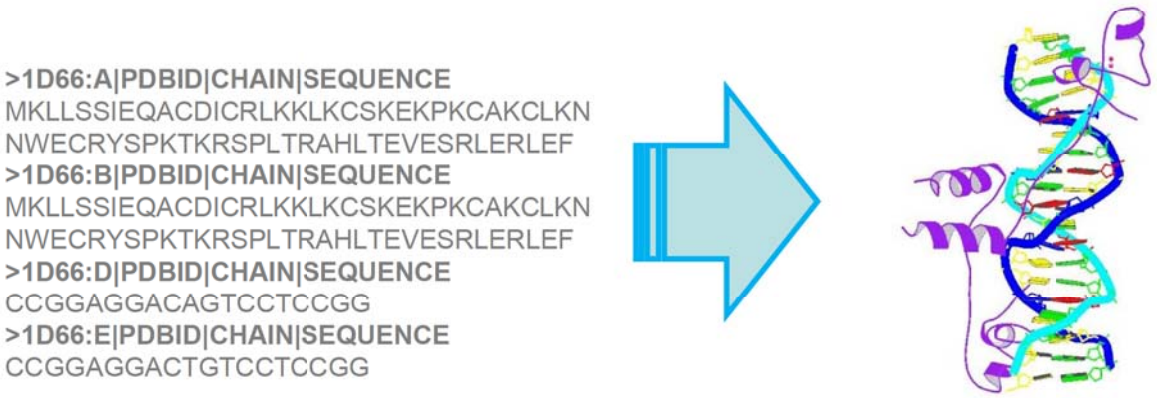


Databases for Protein Structure

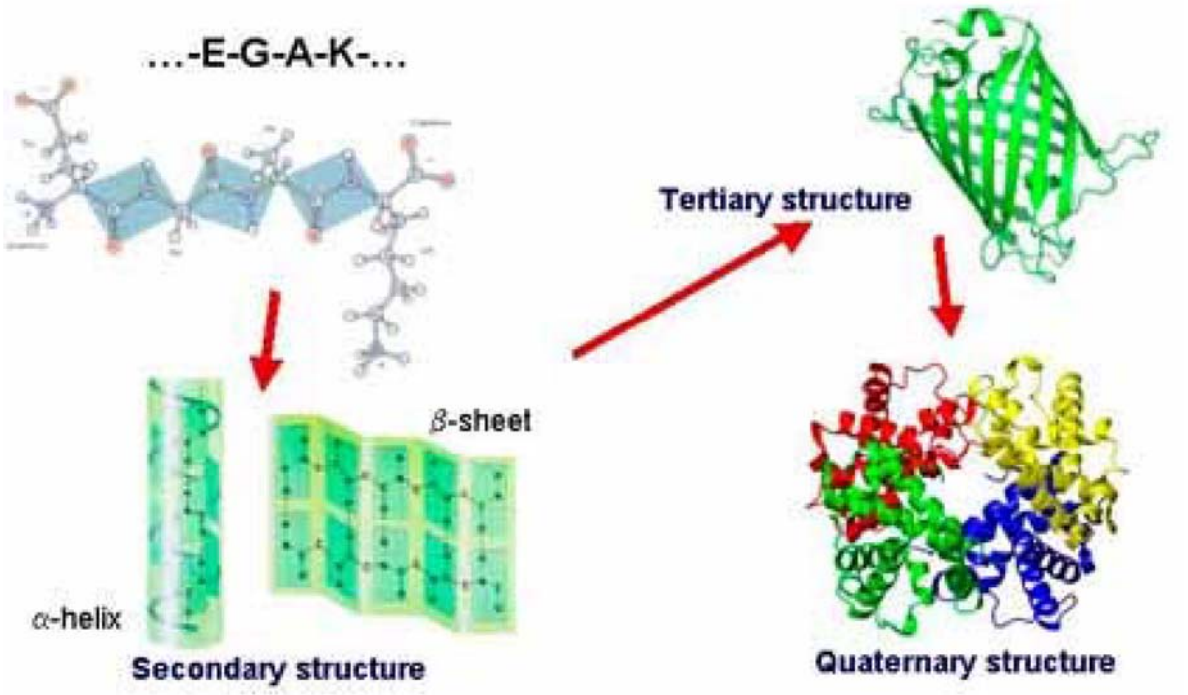
呂平江

國立清華大學

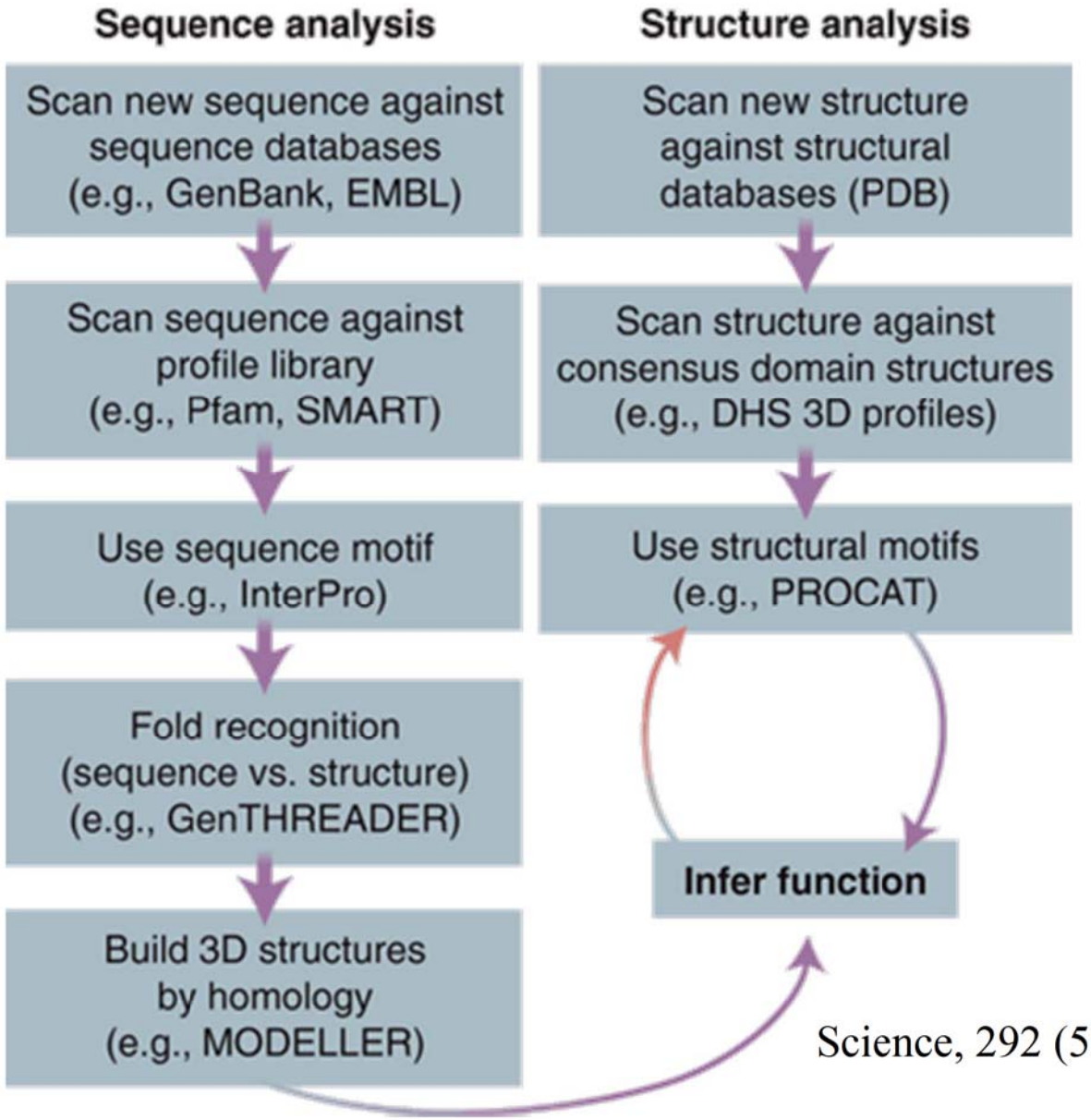
生命科學系/生物資訊與結構生物研究所

2013/06/26

From Sequence to Structure



From sequence and structure to function



Science, 292 (5524): 2095-2097 (2001)

Molecular Biology Database Collection

~ **1380** databases

Nucleotide Sequence Databases
RNA sequence databases
Protein sequence databases
Structure Databases
- Small molecules
- Carbohydrates
- Nucleic acid structure
- Protein structure

Genomics Databases (non-vertebrate)
Metabolic and Signaling Pathways
Human and other Vertebrate Genomes
Human Genes and Diseases
Microarray Data and other Gene Expression Databases
Proteomics Resources
Other Molecular Biology Databases
Organelle databases
Plant databases
Immunological databases
Cell biology

Structure Databases

The 2012 Nucleic Acids Research Database Issue and the online Molecular Biology Database Collection
Nucleic Acids Research, **2012**, Vol. 40, Database issue **D1-D8**

- **Structure Databases**
  - Small molecules
    - AANT - Amino Acid - Nucleotide interaction database
    - ChEBI - Chemical Entities of Biological Interest
    - ChemBank
    - ChemDB
    - CSD - Cambridge Structural Database
    - DrugBank
    - Het-PDB Navi
    - HIC-Up
    - Klotho
    - LIGAND
    - PDB-Ligand
    - PubChem
    - R.E.DD.B.
    - SuperDrug
    - SuperNatural
  - Carbohydrates
    - BCSDB/Glycoscience
    - CCSD - Complex Carbohydrate Structure Database (CarbBank)
    - CSS - Carbohydrate Structure Suite
    - Glycan
    - Glycoconjugate Data Bank
    - GlycoMapsDB
    - GlycoSuiteDB
    - Monosaccharide Browser
    - SWEET-DB

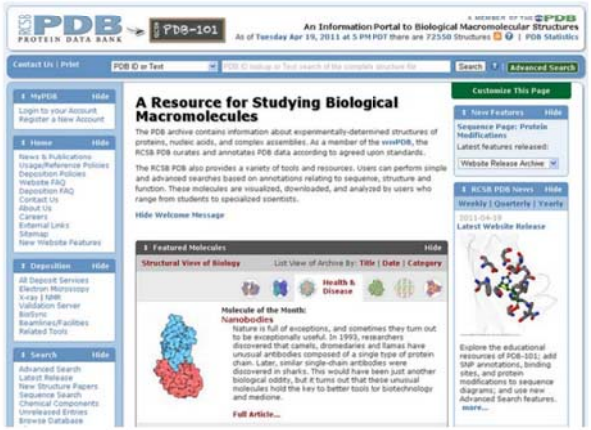
- **Structure Databases**
  - Nucleic acid structure
    - Greglist
    - GRSDB
    - ITS2
    - MeRNA
    - NCIR - Non-Canonical Interactions in RNA
    - NDB
    - NTDB
    - QuadBase
    - Rfam
    - RNA FRABASE
    - RNA SSTRAND
    - RNABase
    - RNAJunction
    - SARS-CoV RNA SSS
    - SCOR - Structural Classification Of RNA
    - Vir-Mir db
  - Protein structure
    - 3D-Genomics
    - 3DID - 3D interacting domains
    - ArchDB
    - ASTRAL
    - AutoPSI
    - BANMOKI
    - BioMagResBank
    - CADB - Conformational Angles DataBase of Proteins
    - CATH
    - CE
    - CoC Central
    - ColiSNP

- **Structure Databases**
  - Protein structure
    - Columba
    - CSA - Catalytic Site Atlas
    - Dali database
    - DBAli
    - Decoys-R-Us
    - DisProt - Database of Protein Disorder
    - DMAPS
    - Dockground
    - DomIns - Database of Domain Insertions
    - DSDBASE - Disulfide Database
    - DSMM - a Database of Simulated Molecular Motions
    - E-MSD - EBI-Macromolecular Structure Database
    - eF-site - Electrostatic surface of Functional site
    - EzCatDB
    - FireDB
    - FSN
    - Gene3D
    - Genomic Threading Database
    - GTOP - Genomes To Protein structures
    - HOMSTRAD - Homologous Structure Alignment Database
    - HotSprint
    - IMB Jena Image Library
    - IMGT/3Dstructure-DB
    - IMOTdb
    - MALISAM
    - LPFC
    - MegaMotifbase
    - MMDB
    - ModBase
    - MolMovDB - Database of Macromolecular Movements
    - PASS2

- **Structure Databases**
  - Protein structure
    - PDB
    - PDB-REPRDB
    - PDBselect
    - PDBsum
    - PDB_TM
    - PepConfDB
    - PFD - Protein Folding Database
    - Phospho3D
    - PIDD
    - PMDB - Protein Model Database
    - Structure Superposition Database
    - ProSAS
    - PROTCOM
    - PRTAD
    - RESID
    - S4: Structure-based Sequence Alignments of SCOP Superfamilies
    - SCOP - Structural Classification Of Proteins
    - SCOPPI
    - SitesBase
    - SNAPPI
    - SSToSS - Sequence-Structural Templates of Single-member Superfamilies
    - STINGreport
    - SUPERFAMILY
    - SURFACE
    - SWISS-MODEL Repository
    - TargetDB
    - TMBETA-GENOME
    - TOPOFIT-DB
    - TOPS - Topology Of Protein Structures

Protein Data Bank (PDB)

- http://**www.pdb.org/**
- Structure data determined by X-ray crystallography and NMR
- The data include the atom coordinate, reference, sequence, secondary structure, disulfide bond ……etc.



The number of protein structure and the last update date

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Everything | Author | Macromolecule | Sequence | Ligand
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91550 Structures
Last Update: Jun 18, 2013

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82347 Structures
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Full Description

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Structural View of Biology | List View

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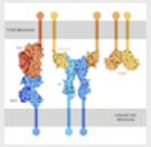
Molecule of the Month
Dermcidin

Bacteria are a constant threat, so our bodies have many defenses to protect us from infection. One of our first lines of defense is a collection of small peptides, termed antimicrobial peptides, that are secreted from our cells. These peptides are toxic to a broad spectrum of bacteria, binding to their membranes and disrupting their function. For instance, dermcidin is an antimicrobial peptide secreted by sweat glands that attacks any bacteria on our skin.

Full Article



Protein Structure Initiative Featured System
Tuning Immune Response with Costimulation

The job of the immune system is tricky, requiring a careful balance. The immune system must seek out and destroy viruses, bacteria and cancer cells using an army of aggressive cells and molecules. But at the same time, this response must be held in check, to ensure that the immune system does not attack our healthy cells and cause autoimmune diseases. PSI researchers are studying molecules that stimulate and inhibit our immune response, ensuring that it is activated only when necessary.

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Organism | Taxonomy | Exp. Method | X-ray Resolution | Release Date | Polymer Type

Organism
- Homo sapiens (22834)
- Escherichia coli (4729)
- Mus musculus (3914)

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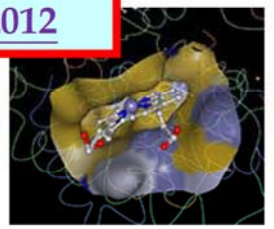
arterly | Yearly
Resolution



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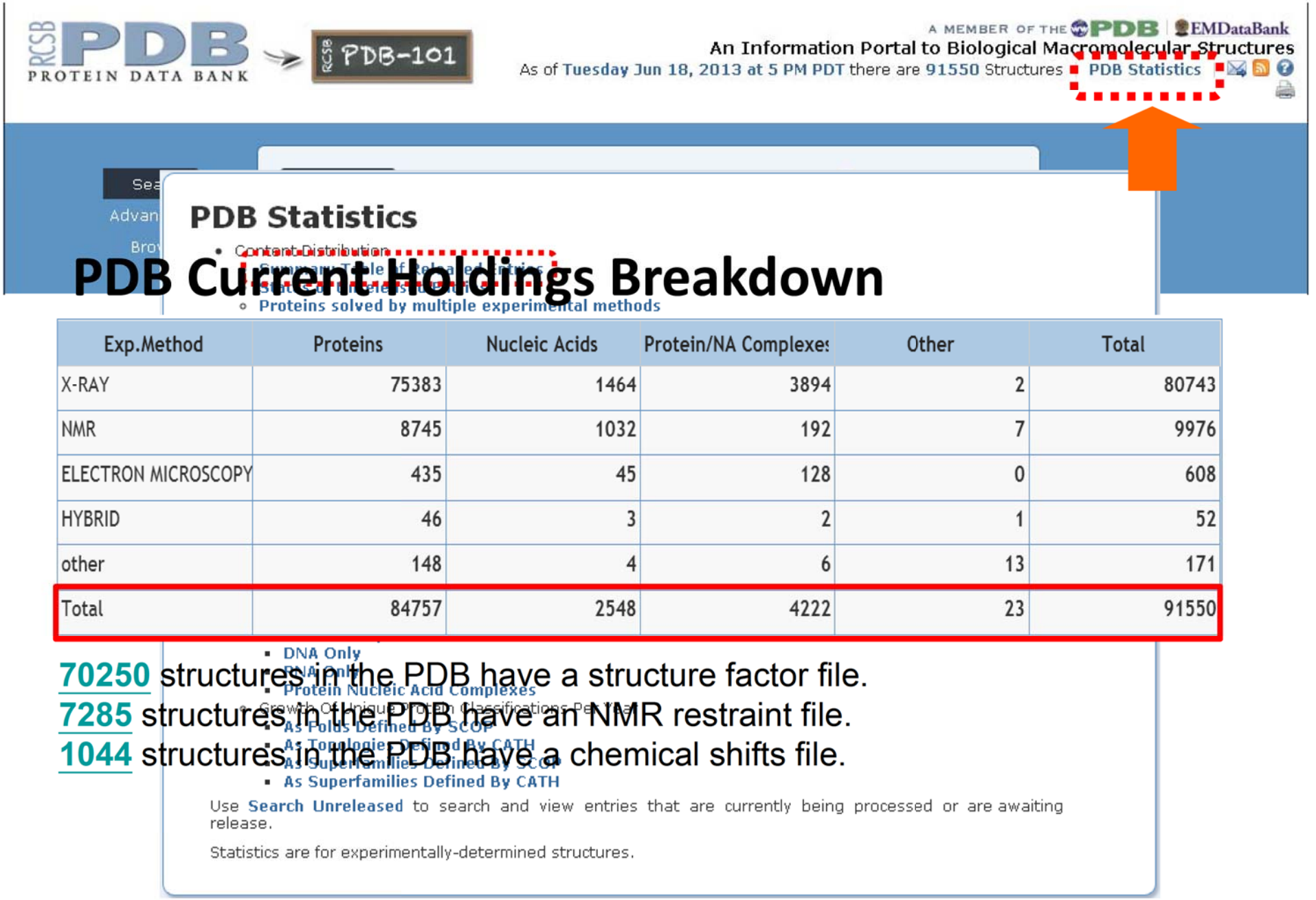

PDB Current Holdings Breakdown

Exp.Method	Proteins	Nucleic Acids	Protein/NA Complexes	Other	Total
X-RAY	75383	1464	3894	2	80743
NMR	8745	1032	192	7	9976
ELECTRON MICROSCOPY	435	45	128	0	608
HYBRID	46	3	2	1	52
other	148	4	6	13	171
Total	84757	2548	4222	23	91550

70250 structures in the PDB have a structure factor file.
7285 structures in the PDB have an NMR restraint file.
1044 structures in the PDB have a chemical shifts file.

RCSB PDB PROTEIN DATA BANK → RCSB PDB-101

An Infor

As of Tuesday Jun 18, 2013 at 5 I

Sea

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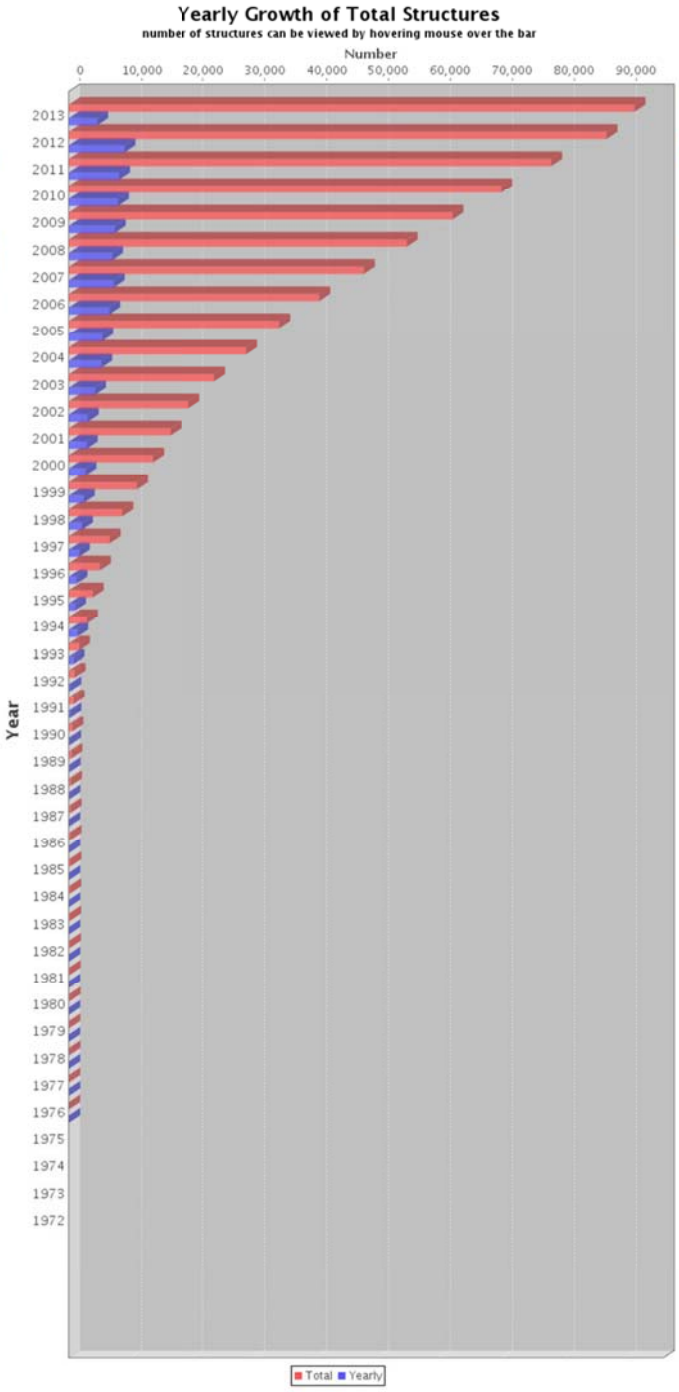
PDB Statistics

- Content Distribution
  - Summary Table of Released Entries
  - Status of Unreleased Entries
  - Proteins solved by multiple experimental methods
  - Redundancy based on sequence similarity
  - By Resolution
  - By Space Group
  - By Natural Source Organism
  - By Gene Source Scientific Organism
  - By Top 100 Journals
  - By Structural Genomics Centers
  - By Structure Molecular Weight
  - By Enzyme Classification

- Content Growth
  - Growth of Released Structures Per Year
  - Growth of Released Structures Per Year by Experimental Method
    - X-ray
    - NMR
    - Electron Microscopy
  - Growth of Released Structures Per Year By Molecular Type
    - Protein Only
    - DNA Only
    - RNA Only
    - Protein Nucleic Acid Complexes
  - Growth Of Unique Protein Classifications Per Year
    - As Folds Defined By SCOP
    - As Topologies Defined By CATH
    - As Superfamilies Defined By SCOP
    - As Superfamilies Defined By CATH

Use Search Unreleased to search and view entries that are currentl release.

Statistics are for experimentally-determined structures.



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Health & Disease

Dermcidin

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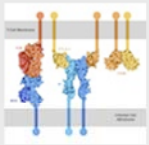
Full Article



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Organism | Taxonomy | Exp. Method | X-ray Resolution | Release Date | Polymer Type

Organism

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- Escherichia coli (4729)
- Mus musculus (3914)

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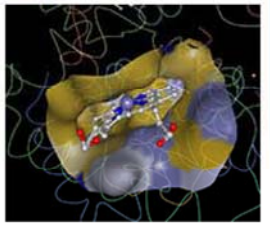

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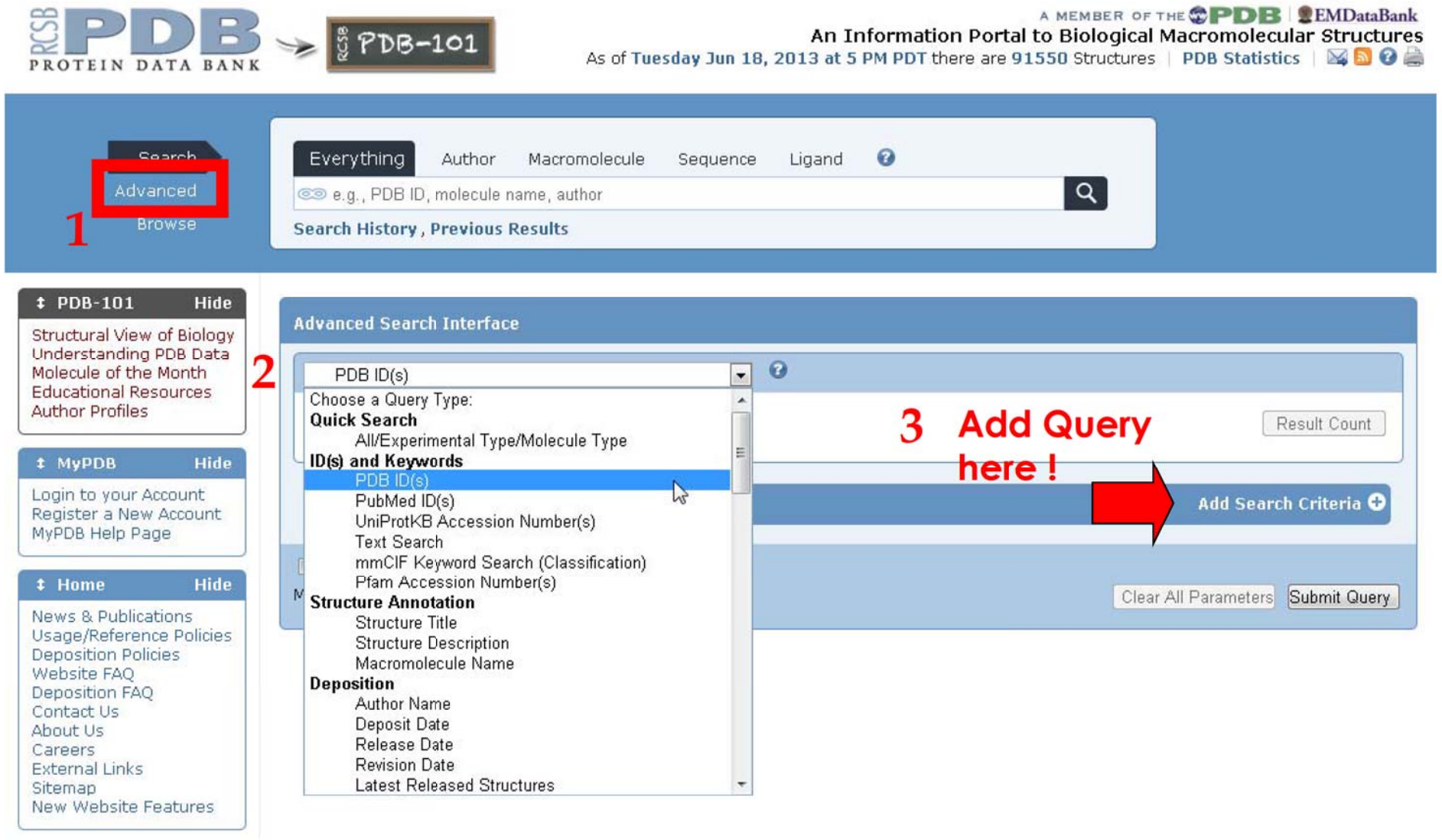

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DNA RECOGNITION BY GAL4: STRUCTURE OF A PROTEIN/DNA COMPLEX

PDB ID 1D66

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Primary Citation

DNA recognition by GAL4: structure of a protein-DNA complex.

Marmorstein, R., Carey, M., Ptashne, M., Harrison, S.C.

Journal: (1992) Nature **356:** 408-414

PubMed: 1557122
DOI: 10.1038/356408a0
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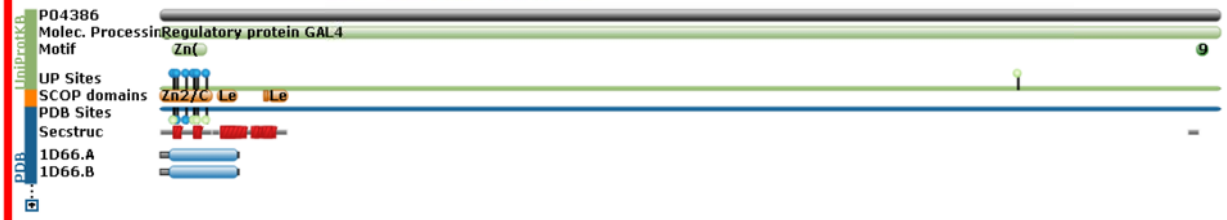
PubMed Abstract:

A specific DNA complex of the 65-residue, N-terminal fragment of the yeast transcriptional activator, GAL4, has been analysed at 2.7 A resolution by X-ray crystallography. The protein binds as a dimer to a symmetrical 17-base-pair sequence. A small, Zn(2+)-containing domain... [Read More & Search PubMed Abstracts]

Molecular Description Hide

Classification: Transcription/dna
Structure Weight: 27737.04

Molecule:	DNA (5'-D(*CP*CP*GP*GP*AP*GP*GP*AP*CP*AP*GP*TP*CP*CP*TP*CP*C P*GP*G)-3')				
Polymer:	1	**Type:**	dna	**Length:**	19
Chains:	D				
Molecule:	DNA (5'-D(*CP*CP*GP*GP*AP*GP*GP*AP*CP*TP*GP*TP*CP*CP*TP*CP*C P*GP*G)-3')				
Polymer:	2	**Type:**	dna	**Length:**	19
Chains:	E				
Molecule:	PROTEIN (GAL4)				
Polymer:	3	**Type:**	protein	**Length:**	66
Chains:	A, B				
Organism	Saccharomyces cerevisiae				
Gene Names	GAL4 YPL248C				
UniProtKB:	Protein Feature View | Search PDB | P04386				



Source Hide

Polymer: 1
Scientific Name: Synthetic construct — Taxonomy

Polymer: 2
Scientific Name: Synthetic construct — Taxonomy

Polymer: 3

Ligand Chemical Component Hide

Identifier	Formula	Name	Interactions
CD Search Download	Cd	CADMIUM ION	Ligand Explorer

Biological Assembly

View in 3D More Images...

Biological assembly 1 assigned by authors

Downloadable viewers:
Simple Viewer Protein Workshop
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Deposition Summary Hide

Authors: Marmorstein, R., Carey, M., Ptashne, M., Harrison, S.C.

Deposition:	1992-03-06
Release:	1992-03-06
Last Modified (REVDAT):	2009-02-24

Revision History Hide

Mouse over text for details
2011-07-13
Version format compliance

Experimental Details Hide

Method: X-RAY DIFFRACTION
Exp. Data:
N/A

Resolution[Å]:	2.70
R-Value:	0.230 (obs.)
R-Free:	n/a
Space Group:	P 43 21 2

Unit Cell:

Length [Å]	Angles [°]
a = 80.85	α = 90.00
b = 80.85	β = 90.00
c = 73.70	γ = 90.00

DNA recognition by GAL4: structure of a protein–DNA complex

Ronen Marmorstein, Michael Carey*, Mark Ptashne & Stephen C. Harrison†

Harvard University, Department of Biochemistry and Molecular Biology, and † Howard Hughes Medical Institute, 7 Divinity Avenue, Cambridge, Massachusetts 02138, USA

A specific DNA complex of the 65-residue, N-terminal fragment of the yeast transcriptional activator, GAL4, has been analysed at 2.7 Å resolution by X-ray crystallography. The protein binds as a dimer to a symmetrical 17-base-pair sequence. A small, Zn^{2+}-containing domain recognizes a conserved CCG triplet at each end of the site through direct contacts with the major groove. A short coiled-coil dimerization element imposes 2-fold symmetry. A segment of extended polypeptide chain links the metal-binding module to the dimerization element and specifies the length of the site. The relatively open structure of the complex would allow another protein to bind coordinately with GAL4.

THE yeast protein GAL4 activates transcription of genes required for catabolism of galactose and melibiose[1-3]. The DNA sequences recognized by GAL4 are 17 base pairs (bp) in length[4-6], and each site binds a dimer of the protein[7]. Four such sites, similar but not identical in sequence, are found in the upstream activating sequence (UAS_G) that mediates GAL4 activation of the GAL1 and GAL10 genes, for example[8].

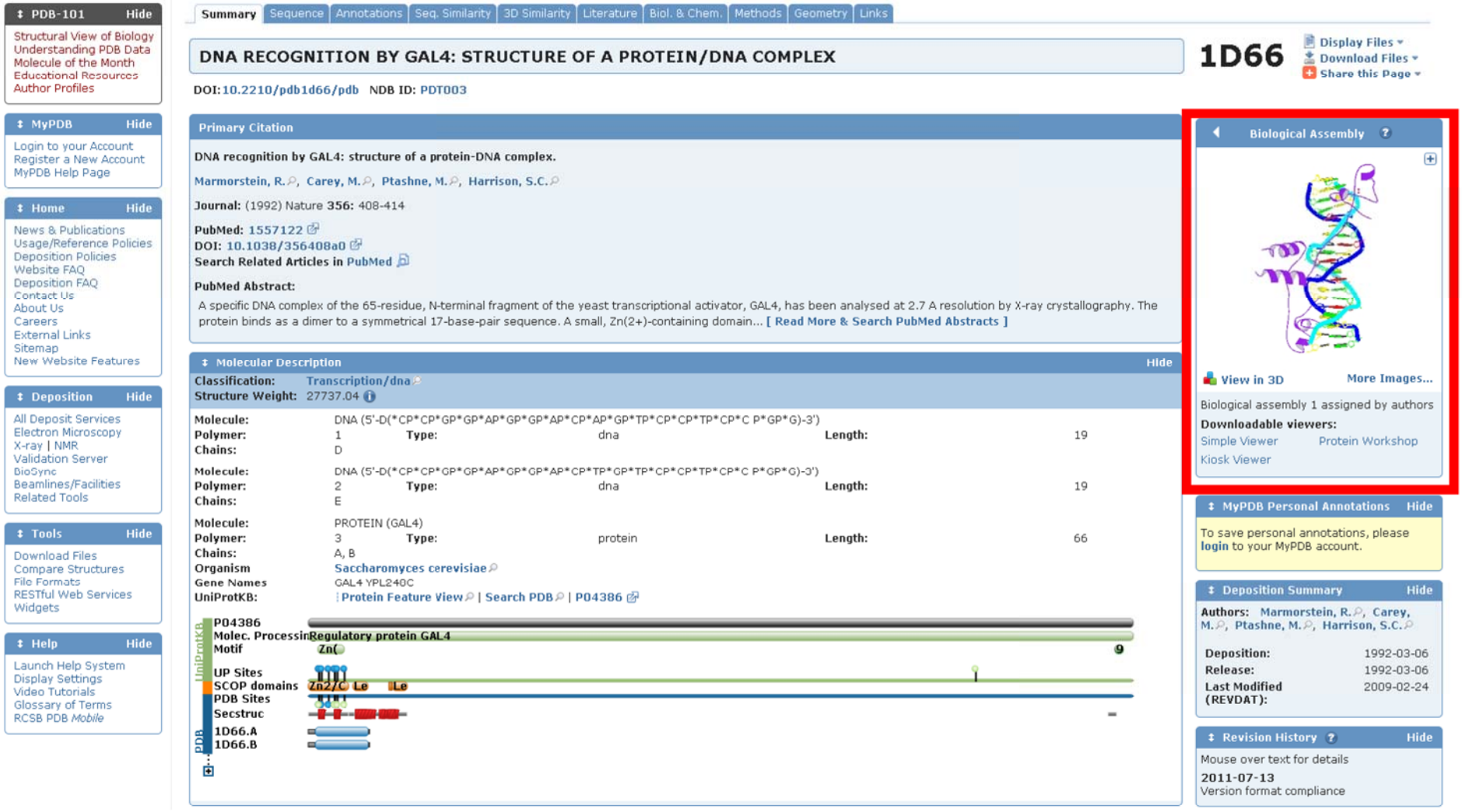
Functions have been assigned to various parts of the 881-amino-acid GAL4 protein (Fig. 1*a*), including DNA binding (1–65) is a monomer in the absence of DNA. The open features of the complex, in which a long stretch of DNA at the centre of the 17-bp site is accessible in the major groove, suggest that another protein may be able to bind coordinately with GAL4.

Structure determination

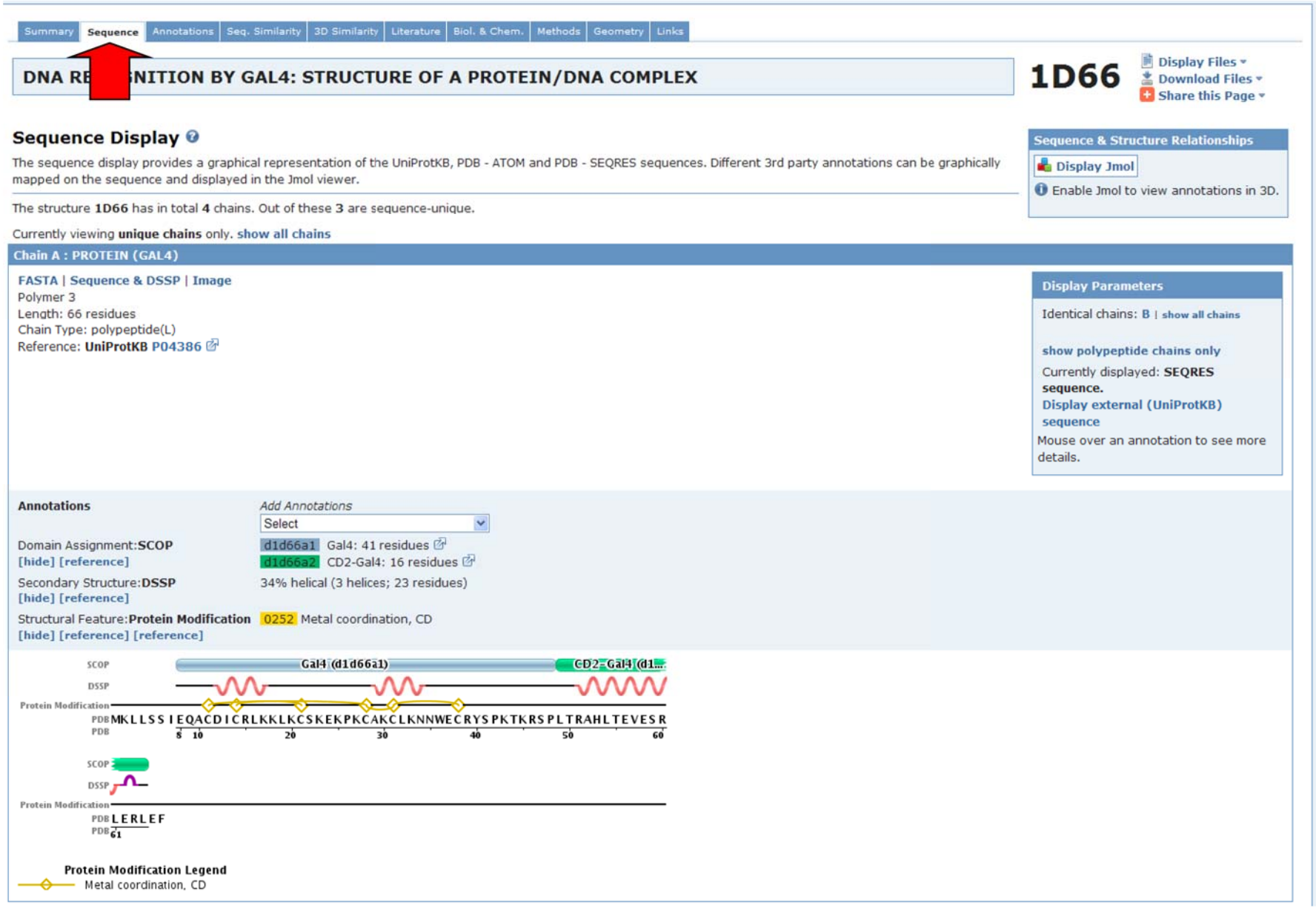
Crystals in space group $P4_32_12$ were prepared as described in the legend to Table 1. The structure of a Cd^{2+}-containing complex was determined and refined, because the crystals were of better quality than the isomorphous crystals containing Zn^{2+}. Isomorphous derivatives were obtained either by replacing Cd^{2+} with Zn^{2+} or Hg^{2+}, or by preparing duplex DNA in which 5-iodo-uridine was substituted for thymidine in selected positions (Fig. 1; Table 1).

The structure of the cadmium-containing complex was initially determined to 3.2 Å by multiple isomorphous replacement (MIR) using phase information from one Hg^{2+} and four 5-iodo-uridine derivatives (Table 1). Locations of the heavy atom derivations confirmed that there was one complete protein–DNA complex per asymmetric unit, and that the protein bound the consensus DNA site as a homodimer. The initial MIR map showed clear density for B-form DNA, and the highest peaks in the map confirmed earlier spectroscopic experiments indicating that each protein monomer bound two closely spaced metal ions[16]. But the protein chain could not be traced. The map was improved by non-crystallographic averaging about a dyad relating the two protein–DNA half-sites[19]. The initial dyad was calculated using heavy-atom positions. Base pairs with ideal B-DNA geometry were built into the twofold averaged map using the model-building program FRODO[20]. The DNA model

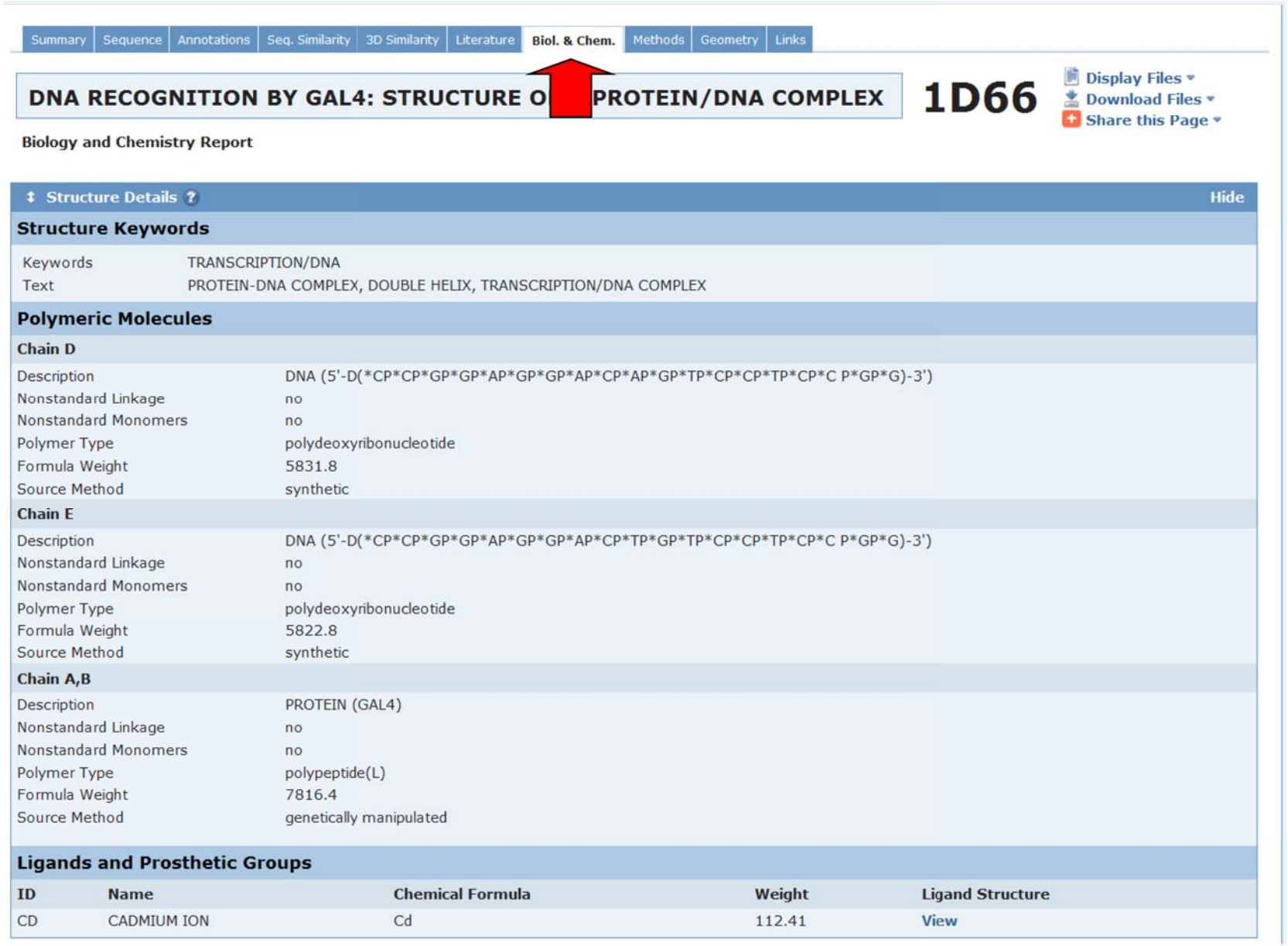
View Structure : 1D66



Sequence / Structure Details



Biology and Chemistry Report



Summary | Sequence | Annotations | Seq. Similarity | 3D Similarity | Literature | **Biol. & Chem.** | Methods | Geometry | Links

DNA RECOGNITION BY GAL4: STRUCTURE O PROTEIN/DNA COMPLEX **1D66**

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Biology and Chemistry Report

Structure Details Hide

Structure Keywords

Keywords	TRANSCRIPTION/DNA
Text	PROTEIN-DNA COMPLEX, DOUBLE HELIX, TRANSCRIPTION/DNA COMPLEX

Polymeric Molecules

Chain D

Description	DNA (5'-D(*CP*CP*GP*GP*AP*GP*GP*AP*CP*AP*GP*TP*CP*CP*TP*CP*C P*GP*G)-3')
Nonstandard Linkage	no
Nonstandard Monomers	no
Polymer Type	polydeoxyribonucleotide
Formula Weight	5831.8
Source Method	synthetic

Chain E

Description	DNA (5'-D(*CP*CP*GP*GP*AP*GP*GP*AP*CP*TP*GP*TP*CP*CP*TP*CP*C P*GP*G)-3')
Nonstandard Linkage	no
Nonstandard Monomers	no
Polymer Type	polydeoxyribonucleotide
Formula Weight	5822.8
Source Method	synthetic

Chain A,B

Description	PROTEIN (GAL4)
Nonstandard Linkage	no
Nonstandard Monomers	no
Polymer Type	polypeptide(L)
Formula Weight	7816.4
Source Method	genetically manipulated

Ligands and Prosthetic Groups

ID	Name	Chemical Formula	Weight	Ligand Structure
CD	CADMIUM ION	Cd	112.41	View

Geometry

Summary | Sequence | Annotations

DNA RECOGNITION E

Geometry: Structure Variance An

RCSB Graphics

Chain Id	B factor
C	Plot |
D	Plot |

*Note: FDS (fold deviation score) is

MolProbity Ramachandran Plot

Click here to download the Mol

- Click on specific 'Bond Type' to ge
- Click on 'Tot Num' to get table of
- Click on 'Minimum' and 'Maximum'
- The color code is based on FDS (

<0.5

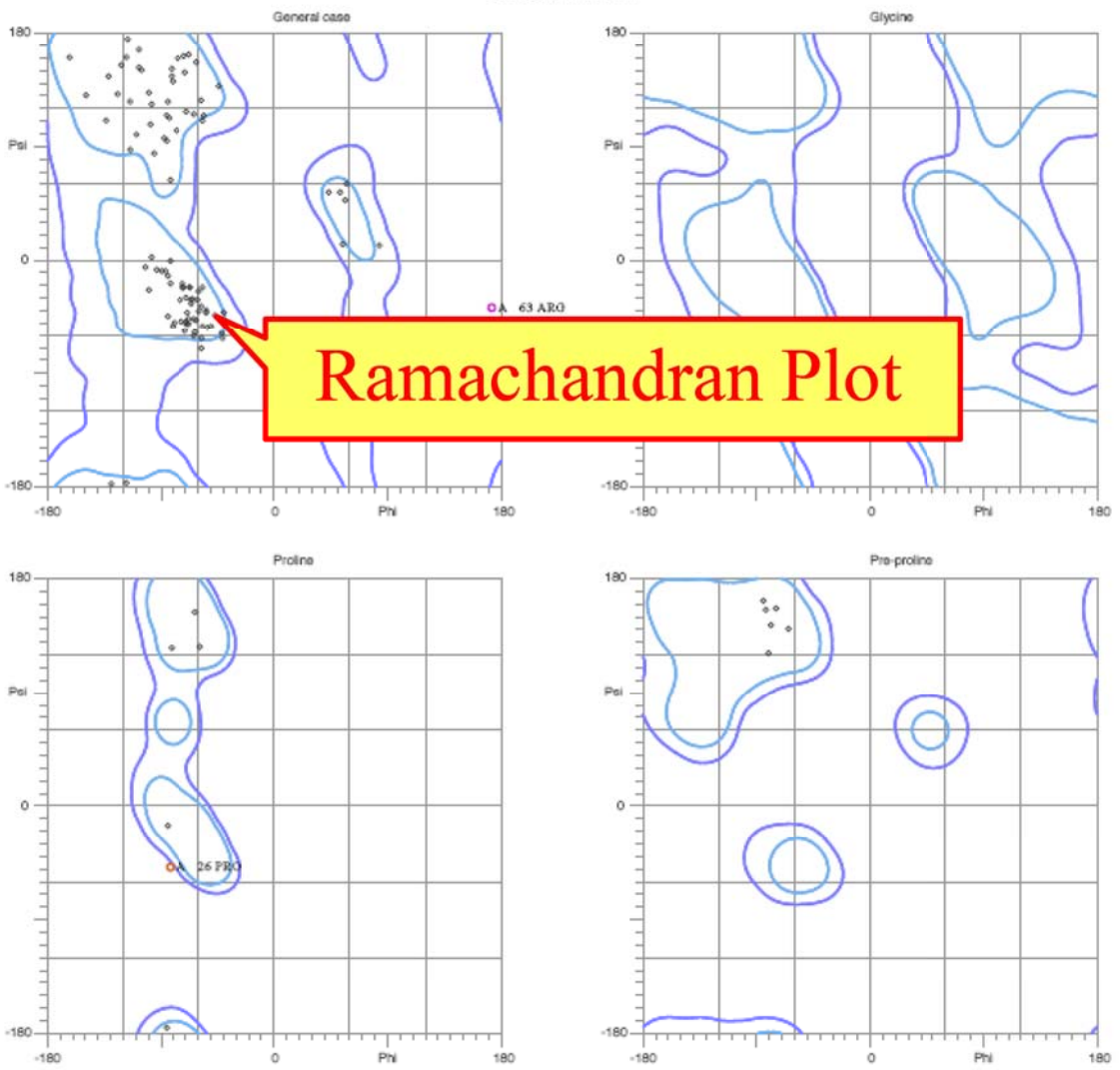
Bond Length

Bond Type	Ch
C-N	A
C-N(P)	A
C-O	A
CA-C	A
CA-CB	A
CA-CB(A)	A
CA-CB(I,T,V)	A
N-CA	A
N-CA(P)	A
C-N	B
C-N(P)	B
C-O	B
CA-C	B
CA-CB	B
CA-CB(A)	B
CA-CB(I,T,V)	B
N-CA	B
N-CA(P)	B

Save Bond Length Summary in:

MolProbity Ramachandran analysis

1D66, model 1



Ramachandran Plot

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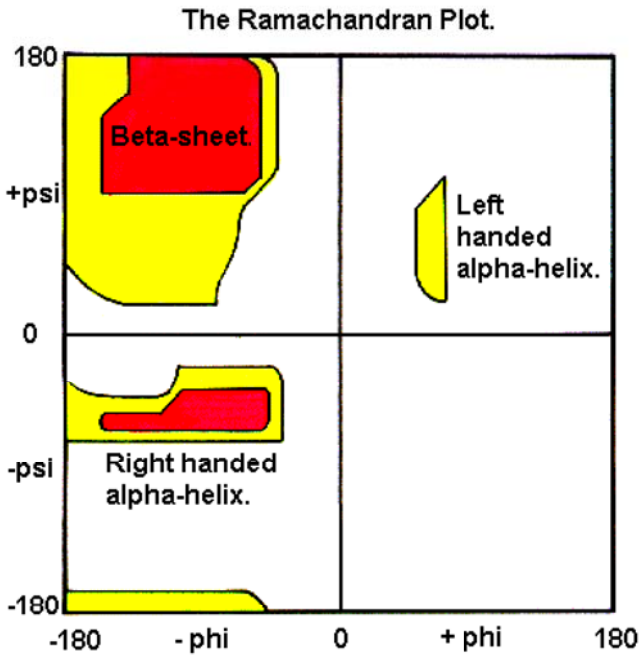
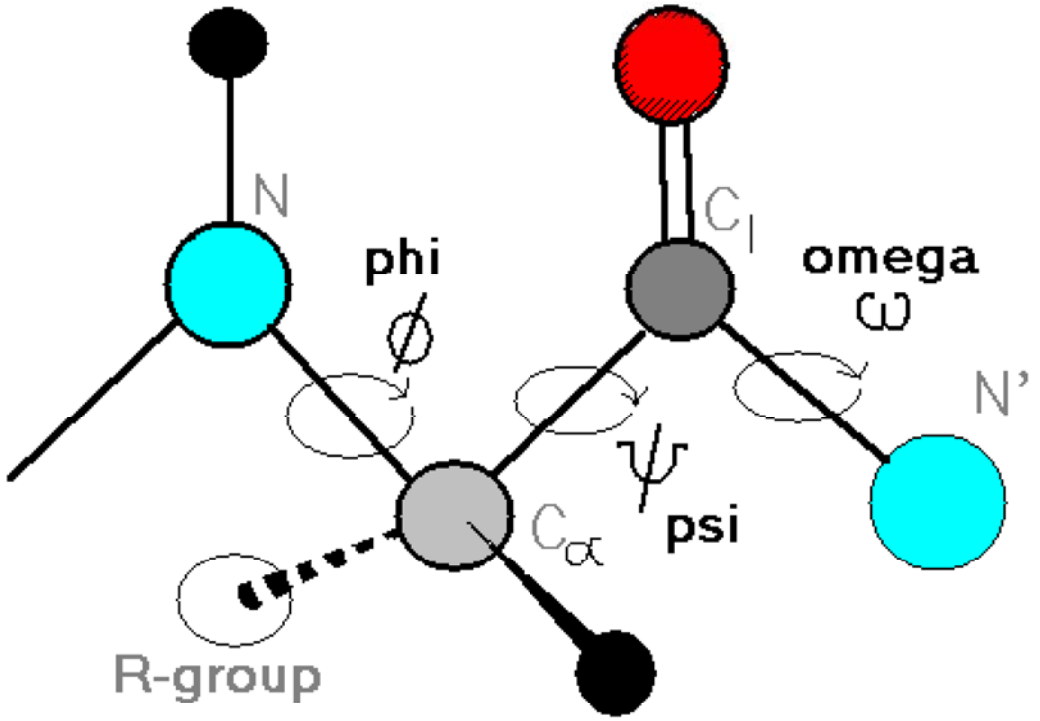
Maximum
1.36
1.36
1.26
1.55
1.58
1.52
1.63
1.48
1.46
1.36
1.36
1.25
1.54
1.57
1.53
1.61
1.48
1.46

Ramachandran plot





β-strand:

$-180 < \phi < -60$

$180 > \varphi > 60$

α-helix:

φ: ~ -60

Φ (phi, Cα–N bond) vs. Ψ (psi, Cα–C(O) bond)

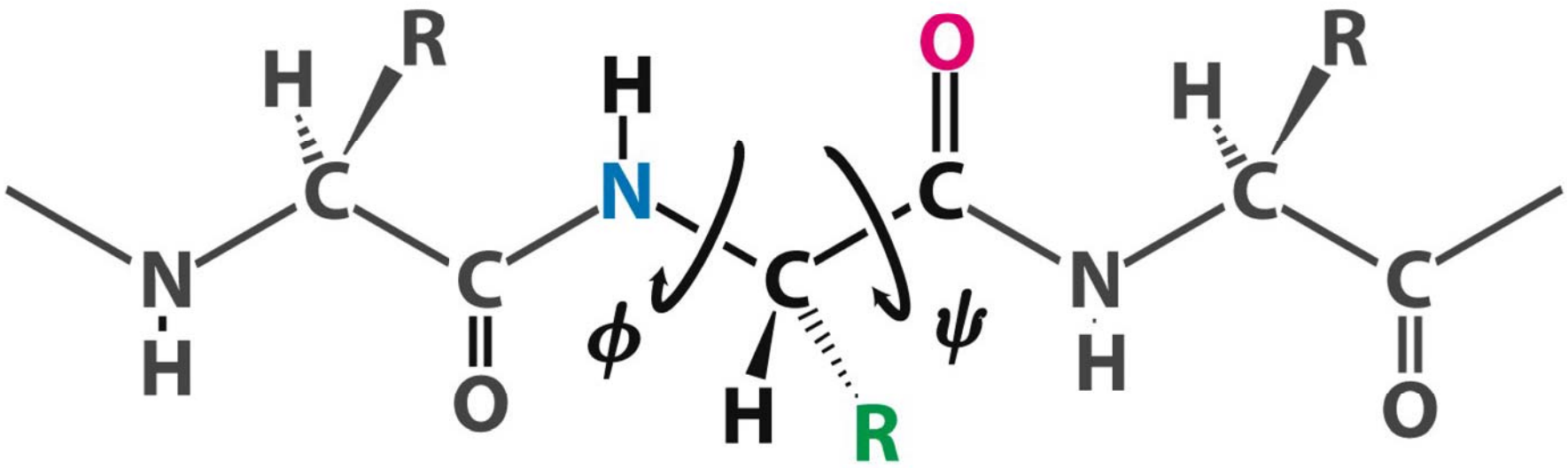
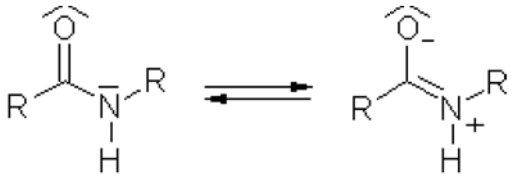
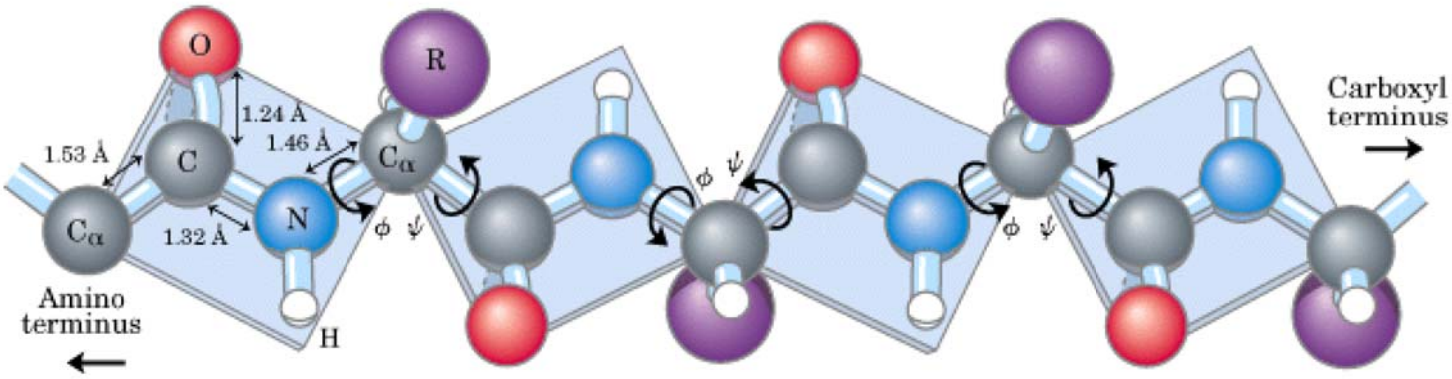


Figure 2.22a
***Biochemistry,* Seventh Edition**



"partial" **double bond character**

- Peptide bond **N–C–O** atoms and atoms attached to them lie all in the same plane
  - Peptide bond is planar !
- Only 2 bonds can freely rotate
  - Cα–N bond and Cα–C(O) bond



Limit amount of free rotations possible (high torsion barriers)

Specified by the **torsion angles Φ** (phi, C_α–N bond) and **Ψ** (psi, C_α–C(O) bond)

Possible Φ and Ψ values are **constrained** by the structure of adjacent amino acid residues

繞N-Cα鍵旋轉的角度稱為phi(ψ)，而繞Cα-C'鍵旋轉的角度則稱為psi(Ψ)。因此，每一胺基酸的phi(ψ) & psi(Ψ)兩個角度決定主鏈原子的型態。

Ramachandran plot

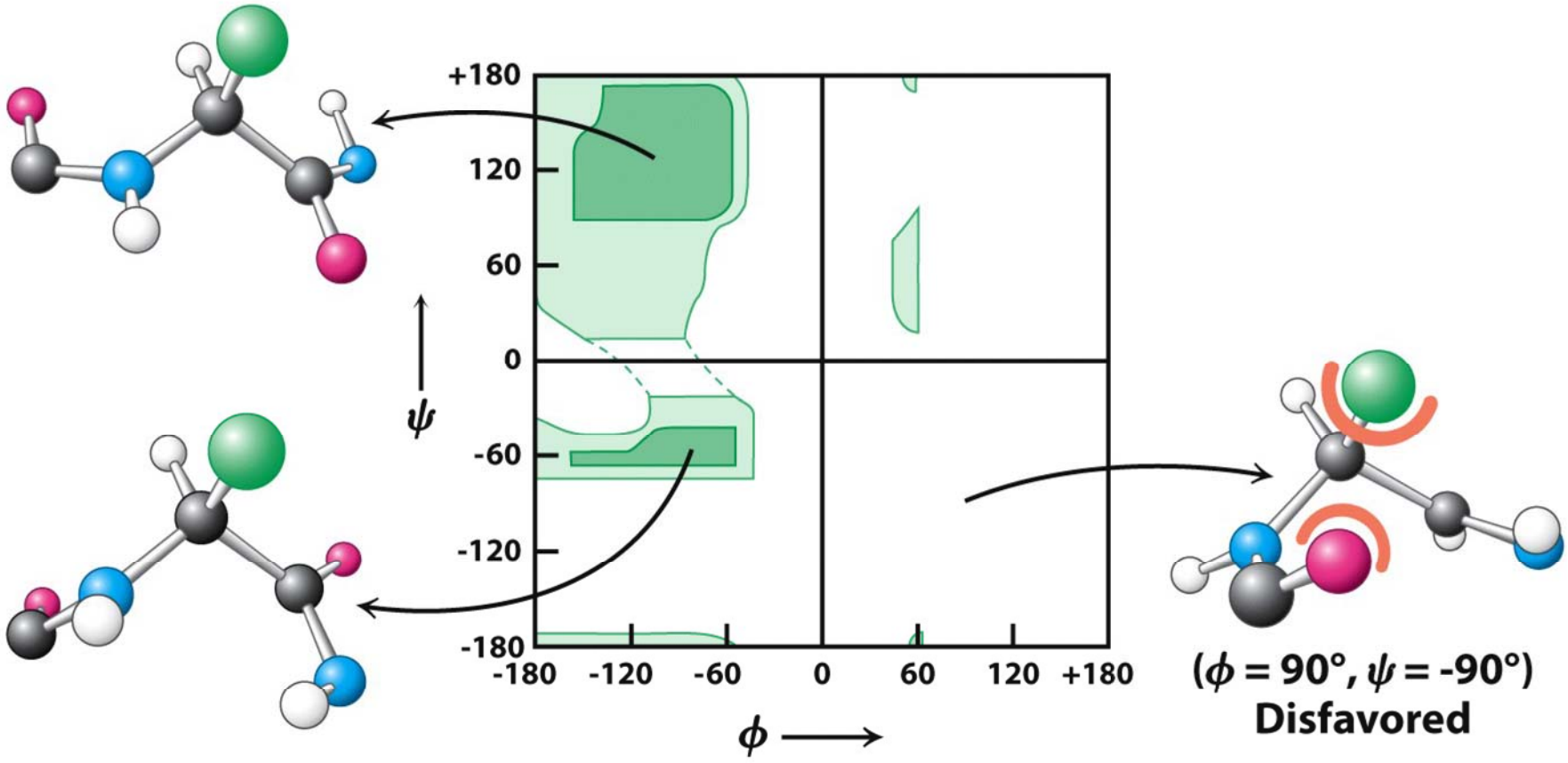
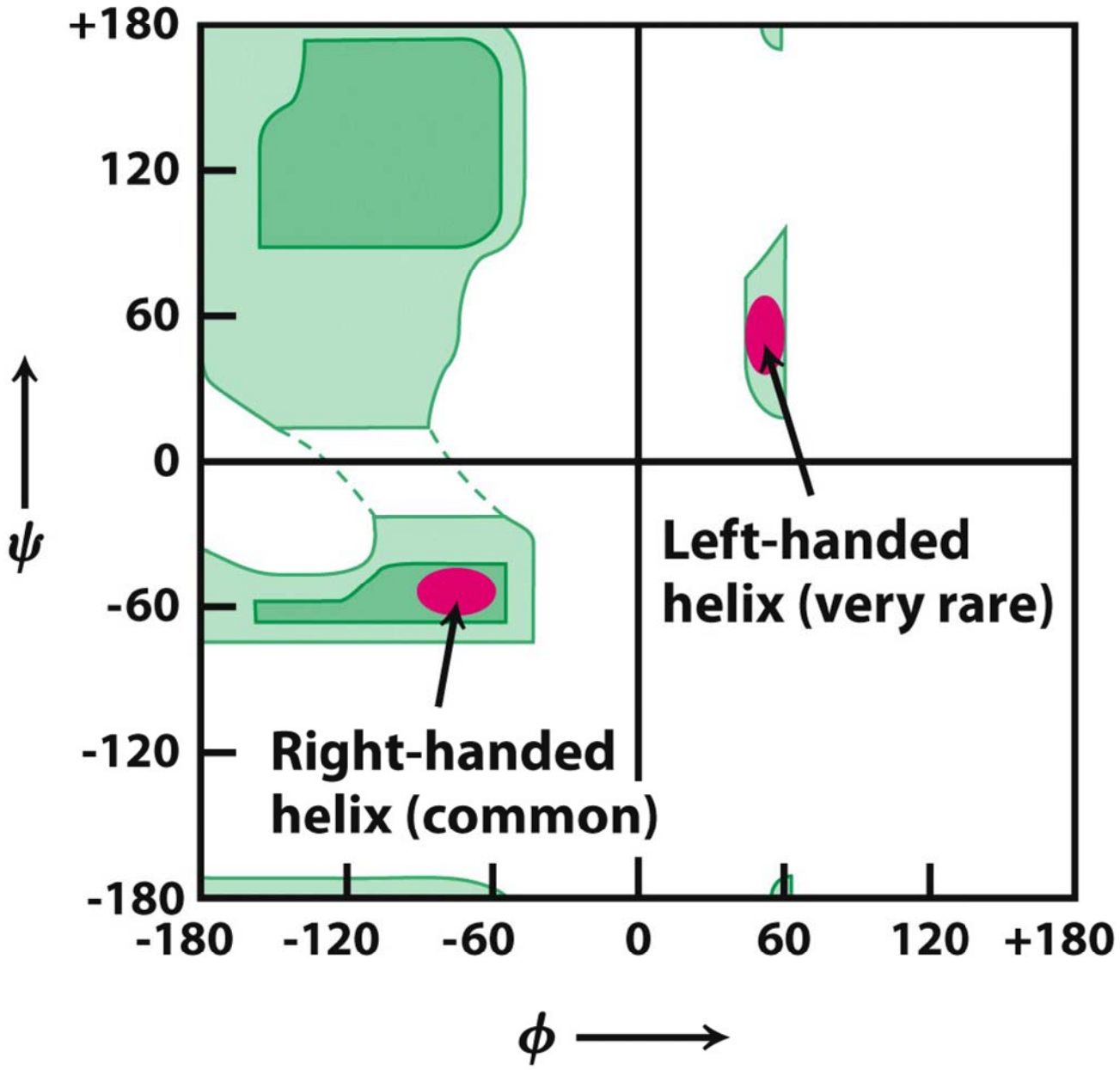


Figure 2.23
***Biochemistry*, Seventh Edition**

- Shows **allowed Φ and Ψ angles**
- **White areas** = **sterically disallowed** conformations
- Protein structures all fall within allowed regions



β-strand:

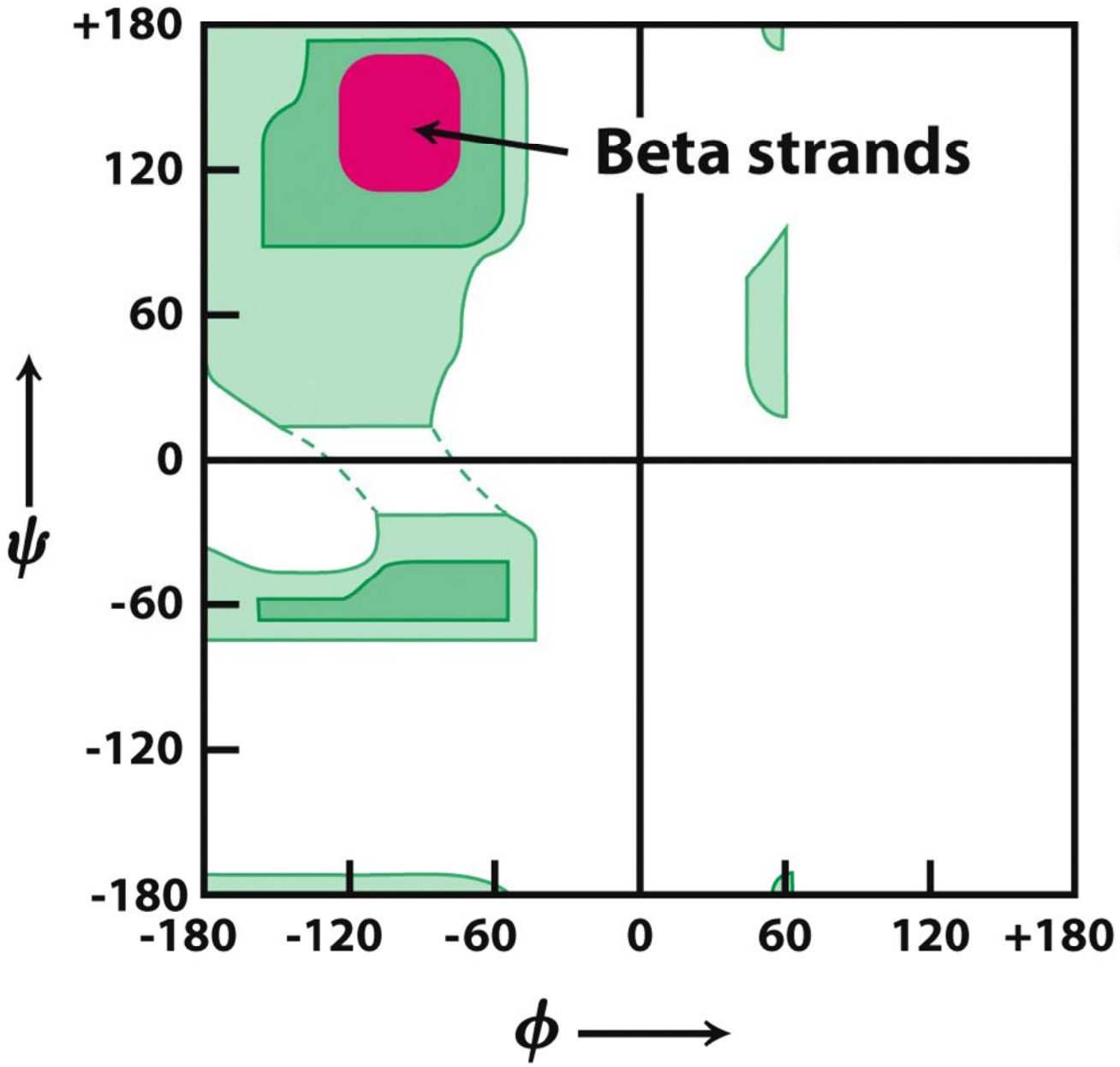
$-180 < \phi < -60$

$180 > \varphi > 60$

α-helix:

φ: ~ -60

Figure 2.26
***Biochemistry*, Seventh Edition**



β-strand:

-180 < ϕ < -60

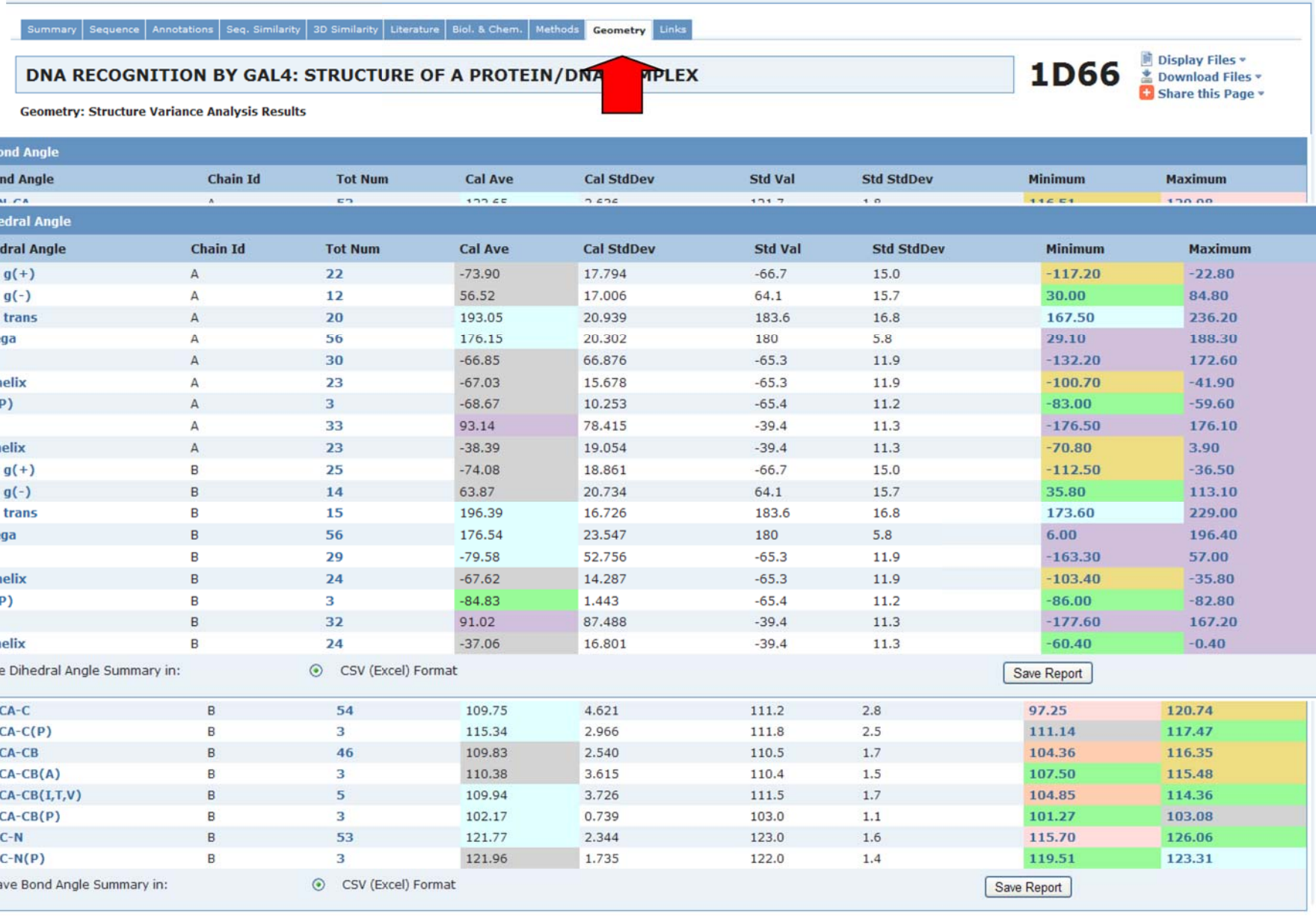
180 > φ > 60

α-helix:

φ: ~ -60

Figure 2.29
***Biochemistry*, Seventh Edition**

Geometry



Summary | Sequence | Annotations | Seq. Similarity | 3D Similarity | Literature | Biol. & Chem. | Methods | Geometry | Links

DNA RECOGNITION BY GAL4: STRUCTURE OF A PROTEIN/DNA [illegible]MPLEX

1D66

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Geometry: Structure Variance Analysis Results

Bond Angle

Bond Angle	Chain Id	Tot Num	Cal Ave	Cal StdDev	Std Val	Std StdDev	Minimum	Maximum
C-N-CA	A	53	122.65	2.626	121.7	1.9	116.51	129.08
N-CA-C	B	54	109.75	4.621	111.2	2.8	97.25	120.74
N-CA-C(P)	B	3	115.34	2.966	111.8	2.5	111.14	117.47
N-CA-CB	B	46	109.83	2.540	110.5	1.7	104.36	116.35
N-CA-CB(A)	B	3	110.38	3.615	110.4	1.5	107.50	115.48
N-CA-CB(I,T,V)	B	5	109.94	3.726	111.5	1.7	104.85	114.36
N-CA-CB(P)	B	3	102.17	0.739	103.0	1.1	101.27	103.08
O-C-N	B	53	121.77	2.344	123.0	1.6	115.70	126.06
O-C-N(P)	B	3	121.96	1.735	122.0	1.4	119.51	123.31

Save Bond Angle Summary in: CSV (Excel) Format Save Report

Dihedral Angle

Dihedral Angle	Chain Id	Tot Num	Cal Ave	Cal StdDev	Std Val	Std StdDev	Minimum	Maximum
Chi1 g(+)	A	22	-73.90	17.794	-66.7	15.0	-117.20	-22.80
Chi1 g(-)	A	12	56.52	17.006	64.1	15.7	30.00	84.80
Chi1 trans	A	20	193.05	20.939	183.6	16.8	167.50	236.20
Omega	A	56	176.15	20.302	180	5.8	29.10	188.30
Phi	A	30	-66.85	66.876	-65.3	11.9	-132.20	172.60
Phi helix	A	23	-67.03	15.678	-65.3	11.9	-100.70	-41.90
Phi(P)	A	3	-68.67	10.253	-65.4	11.2	-83.00	-59.60
Psi	A	33	93.14	78.415	-39.4	11.3	-176.50	176.10
Psi helix	A	23	-38.39	19.054	-39.4	11.3	-70.80	3.90
Chi1 g(+)	B	25	-74.08	18.861	-66.7	15.0	-112.50	-36.50
Chi1 g(-)	B	14	63.87	20.734	64.1	15.7	35.80	113.10
Chi1 trans	B	15	196.39	16.726	183.6	16.8	173.60	229.00
Omega	B	56	176.54	23.547	180	5.8	6.00	196.40
Phi	B	29	-79.58	52.756	-65.3	11.9	-163.30	57.00
Phi helix	B	24	-67.62	14.287	-65.3	11.9	-103.40	-35.80
Phi(P)	B	3	-84.83	1.443	-65.4	11.2	-86.00	-82.80
Psi	B	32	91.02	87.488	-39.4	11.3	-177.60	167.20
Psi helix	B	24	-37.06	16.801	-39.4	11.3	-60.40	-0.40

Save Dihedral Angle Summary in: CSV (Excel) Format Save Report

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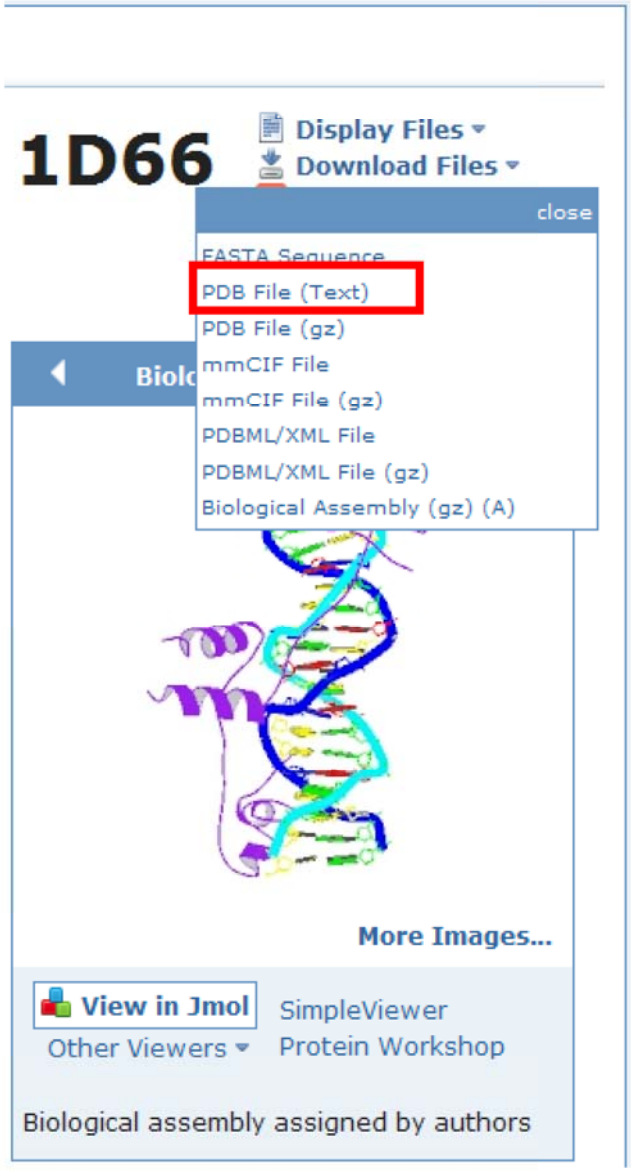


```
HEADER    TRANSCRIPTION REGULATION           06-MAR-92   1D66     1D66   2
COMPND    GAL4 (RESIDUES 1 - 65) COMPLEX WITH 19MER DNA                1D66   3
SOURCE    (SACCHAROMYCES $CEREVISIAE) OVEREXPRESSED IN (ESCHERICHIA     1D66   4
SOURCE    2 $COLI)                                                     1D66   5
AUTHOR    R.MARMORSTEIN,S.HARRISON                                     1D66   6
REVDAT
JRNL                                                                   1D66   8
JRNL                                                                   6  9
JRNL
JRNL
JRNL
REMARK
REMARK
REMARK
REMARK
REMARK
REMARK
REMARK                                                                 66 19
REMARK
REMARK                                                                 21
REMARK
REMARK
REMARK    4 THERE ARE TWO DNA CHAINS WHICH HAVE BEEN ASSIGNED CHAIN    1D66  24
REMARK    4 INDICATORS *D* AND *E*.  THERE ARE TWO PROTEIN CHAINS      1D66  25
REMARK    4 WHICH HAVE BEEN ASSIGNED CHAIN INDICATORS *A* AND *B*.     1D66  26
REMARK    4 EACH PROTEIN - DNA COMPLEX CONTAINS FOUR BOUND CD IONS.    1D66  27
REMARK    5                                                            1D66  28
REMARK    5 THE PROTEIN CONTAINS THE N-TERMINAL 65 RESIDUES OF GAL4    1D66  29
REMARK    5 PLUS A C-TERMINAL PHE DERIVED FROM THE CLONING CONSTRUCT.  1D66  30
REMARK    6                                                            1D66  31
REMARK    6 RESIDUES LEU A 19 - LYS A 27 AND LEU B 19 - LYS B 27 FORM  1D66  32
REMARK    6 TIGHT TURNS WHICH CONNECT HELICES.  RESIDUES TRP A 39 -    1D66  33
REMARK    6 LEU A 49 AND TRP B 39 - LEU B 49 FORM EXTENDED CHAINS      1D66  34
REMARK    6 WHICH CONNECT HELICES.                                     1D66  35
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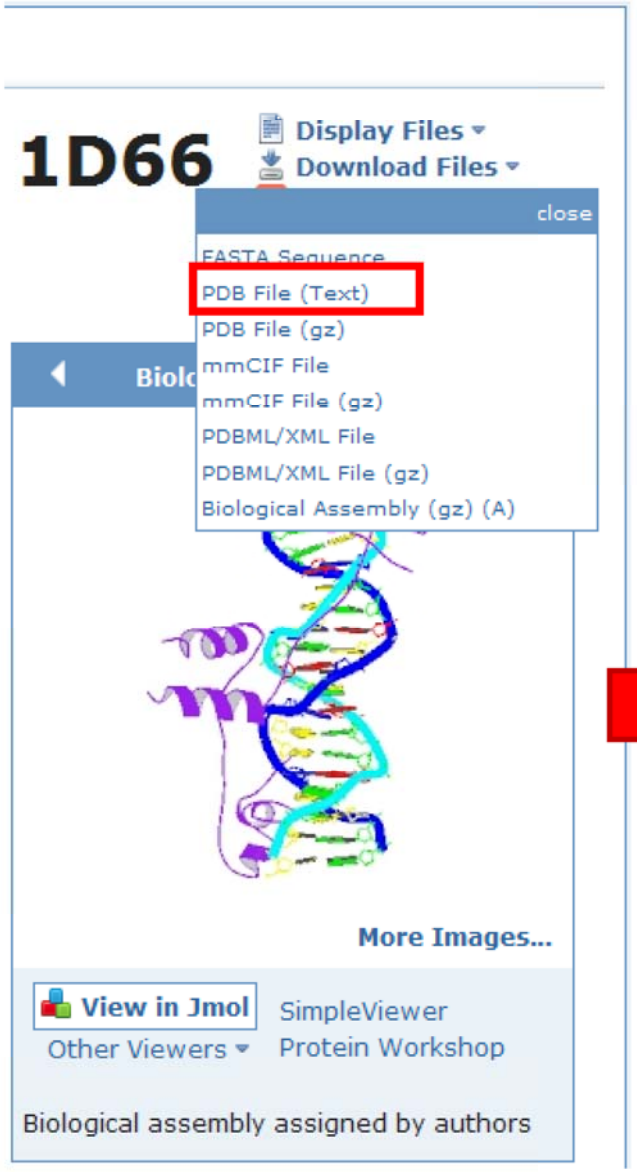


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HET    CD   41     1   CADMIUM                          1D66  68
HET    CD   42     1   CADMIUM                          1D66  69
FORMUL  5  CD   4(CD1)                                 1D66  70
FORMUL  6  HOH  *51(H2 O1)                            1D66  71
HELIX   1 H1A CYS A  11  LYS A  18  1 RESIDUE 18 HAS POSITIVE PHI   1D66  72
HELIX   2 H2A CYS A  28  ASN A  35  1 RESIDUE 35 HAS POSITIVE PHI   1D66  73
HELIX   3 H3A THR A  50  LEU A  64  1                               1D66  74
HELIX   4 H1B CYS B  11  LYS B  18  1 RESIDUE 18 HAS POSITIVE PHI   1D66  75
HELIX   5 H2B CYS B  28  ASN B  35  1 RESIDUE 35 HAS POSITIVE PHI   1D66  76
HELIX   6 H3B THR B  50  LEU B  64  1                               1D66  77
CRYST1  80.850  80.850  73.700  90.00  90.00  90.00 P 43 21 2    8  1D66  78
ORIGX1      1.000000  0.000000  0.000000        0.00000           1D66  79
ORIGX2      0.000000  1.000000  0.000000        0.00000           1D66  80
ORIGX3      0.000000  0.000000  1.000000        0.00000           1D66  81
SCALE1      0.012369  0.000000  0.000000        0.00000           1D66  82
SCALE2      0.000000  0.012369  0.000000        0.00000           1D66  83
SCALE3      0.000000  0.000000  0.013569        0.00000           1D66  84
MTRIX1  1  0.969990  0.014680 -0.242700      7.19246    1         1D66  85
MTRIX2  1  0.014290 -0.999900 -0.003900     83.38941    1         1D66  86
MTRIX3  1 -0.242710 -0.000190 -0.970100     42.87497    1         1D66  87
ATOM    1  O5*  C D   1      23.081  73.401  36.511  1.00 44.77    1D66  88
ATOM    2  C5*  C D   1      24.340  73.259  35.792  1.00 46.46    1D66  89
ATOM    3  C4*  C D   1      24.267  72.789  34.262  1.00 42.04    1D66  90
ATOM    4  O4*  C D   1      25.550  72.957  33.595  1.00 41.08    1D66  91
ATOM    5  C3*  C D   1      23.957  71.289  34.142  1.00 38.19    1D66  92
ATOM    6  O3*  C D   1      23.249  71.081  32.947  1.00 33.45    1D66  93
ATOM    7  C2*  C D   1      25.339  70.690  33.983  1.00 35.90    1D66  94
ATOM    8  C1*  C D   1      26.031  71.694  33.078  1.00 39.17    1D66  95
ATOM    9  N1   C D   1      27.530  71.609  33.190  1.00 38.42    1D66  96
ATOM   10  C2   C D   1      28.318  71.429  32.033  1.00 32.78    1D66  97
ATOM   11  O2   C D   1      27.833  71.357  30.908  1.00 30.98    1D66  98
ATOM   12  N3   C D   1      29.661  71.362  32.174  1.00 28.51    1D66  99
ATOM   13  C4   C D   1      30.215  71.469  33.389  1.00 30.53    1D66 100
ATOM   14  N4   C D   1      31.535  71.390  33.519  1.00 28.65    1D66 101
```

x y z

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AUTHOR	List of contributors.	**SCALEn**	Transformation from orthogonal coordinates to fractional crystallographic coordinates (n = 1, 2, or 3).由直角座標系，轉換到晶圖(crystallographic)座標系，座標系之間的轉換值。
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DALI
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NO EXTERNAL LINK IN EXPERIMENTAL DATA
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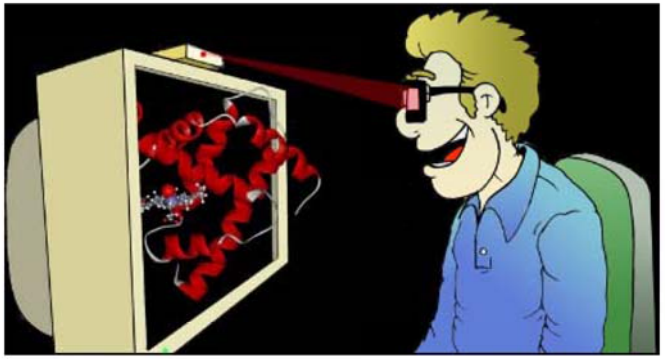
PROTEIN MOTIONS
Molecular Movements Database (MMD)
STEREOCHEMICAL QUALITY
WHAT_CHECK (WHAT IF)
PROCHECK

Molecular Graphics



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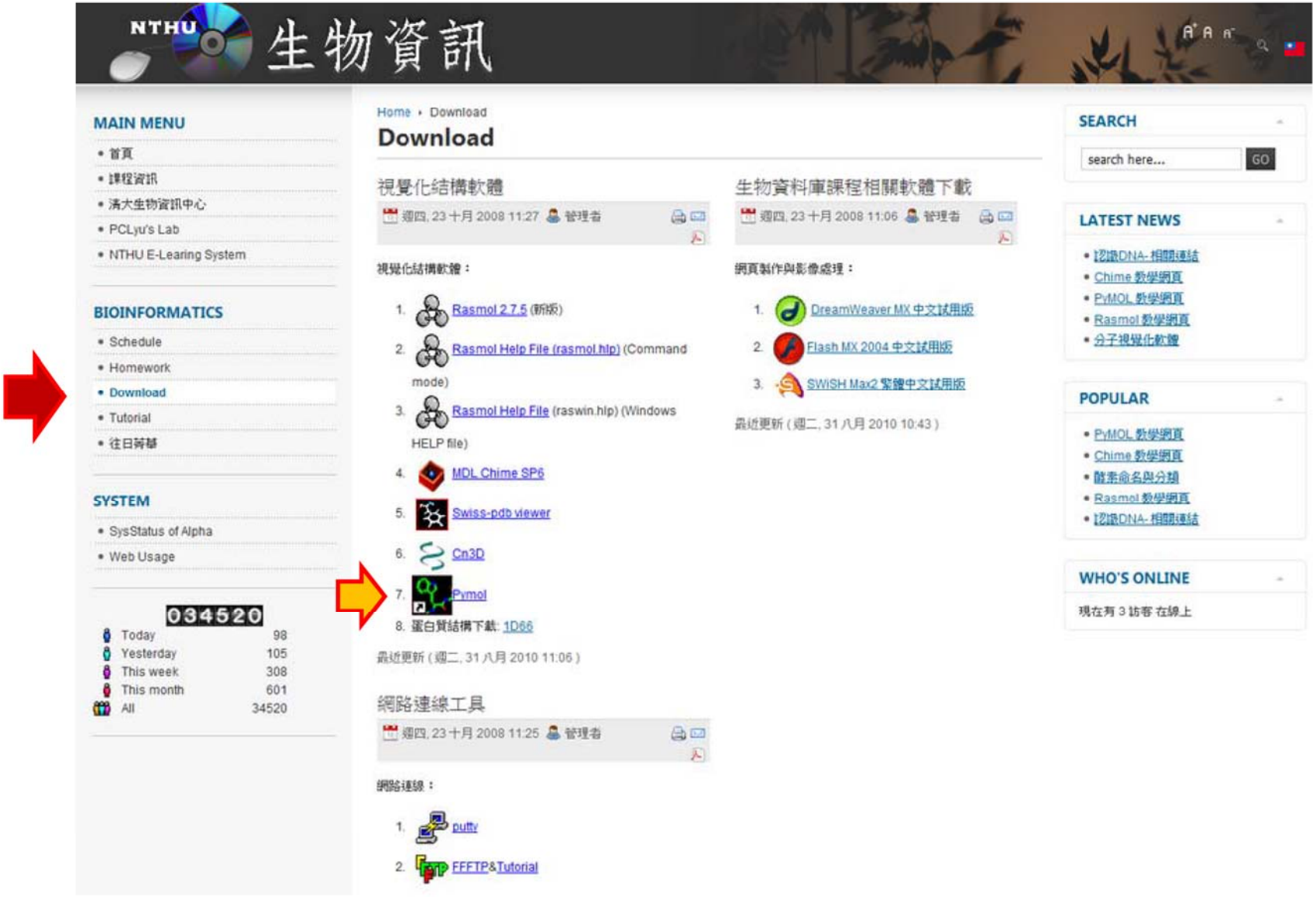

Thanks for your attentions.