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PROTEIN DATA BANK

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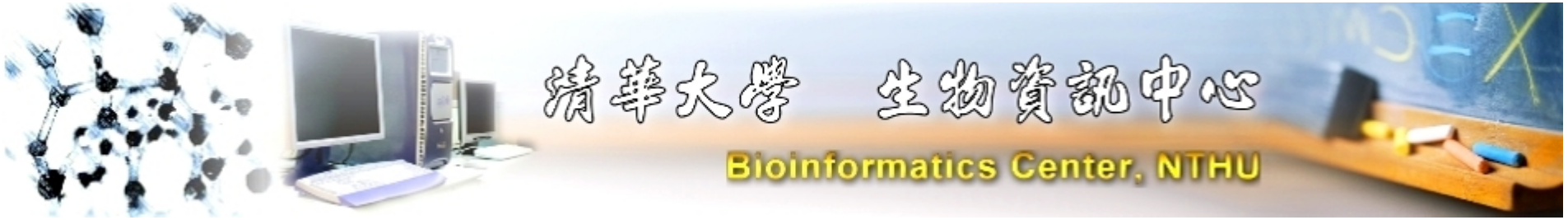

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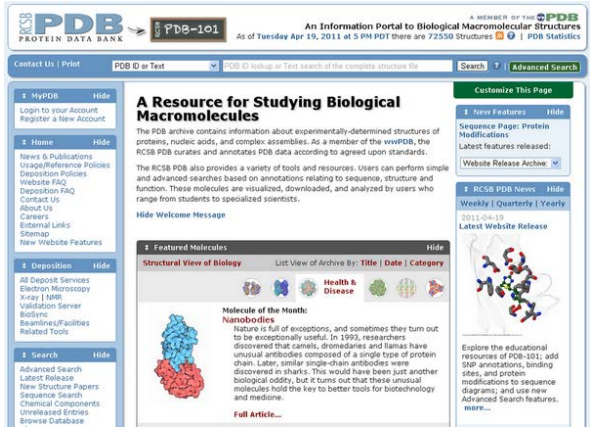
- http://**www.pdb.org/**
- Structure data determined by X-ray crystallography and NMR
- The data include the atom coordinate, reference, sequence, secondary structure, disulfide bond ……etc.



The number of protein structure and the last update date

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Biological Macromolecular Resource

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Featured Molecules

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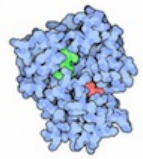
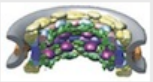


Molecule of the Month
Aminoglycoside Antibiotics
The discovery of streptomycin in 1944 provided the first effecti
Ever since then, we have fought an escalating battle with bact
other aminoglycoside antibiotics. Researchers have discovered
made by bacteria, and chemists have created entirely new anti
effective natural defenses.

Full Article



Protein Structure Initiative Featured System
Revealing the Nuclear Pore Complex
Researchers at NYSGRC are helping to build a detailed map of the nuclear pore complex, defining its modular architecture piece by piece.

Full Article | Archive | PSI Structural Biology Knowledgebase

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Organism | Taxonomy | Exp. Method | X-Ray Resolution | Release Date | Polymer Type | Enzyme Classificatio | SCOP Classification

Show all

Organism

- Homo sapiens (19507)
- Escherichia coli (4536)
- Mus musculus (3462)
- Saccharomyces cerevisiae (2129)
- Bos taurus (2030)
- Rattus norvegicus (1692)
- Escherichia coli K-12 (1291)
- Other (42678)

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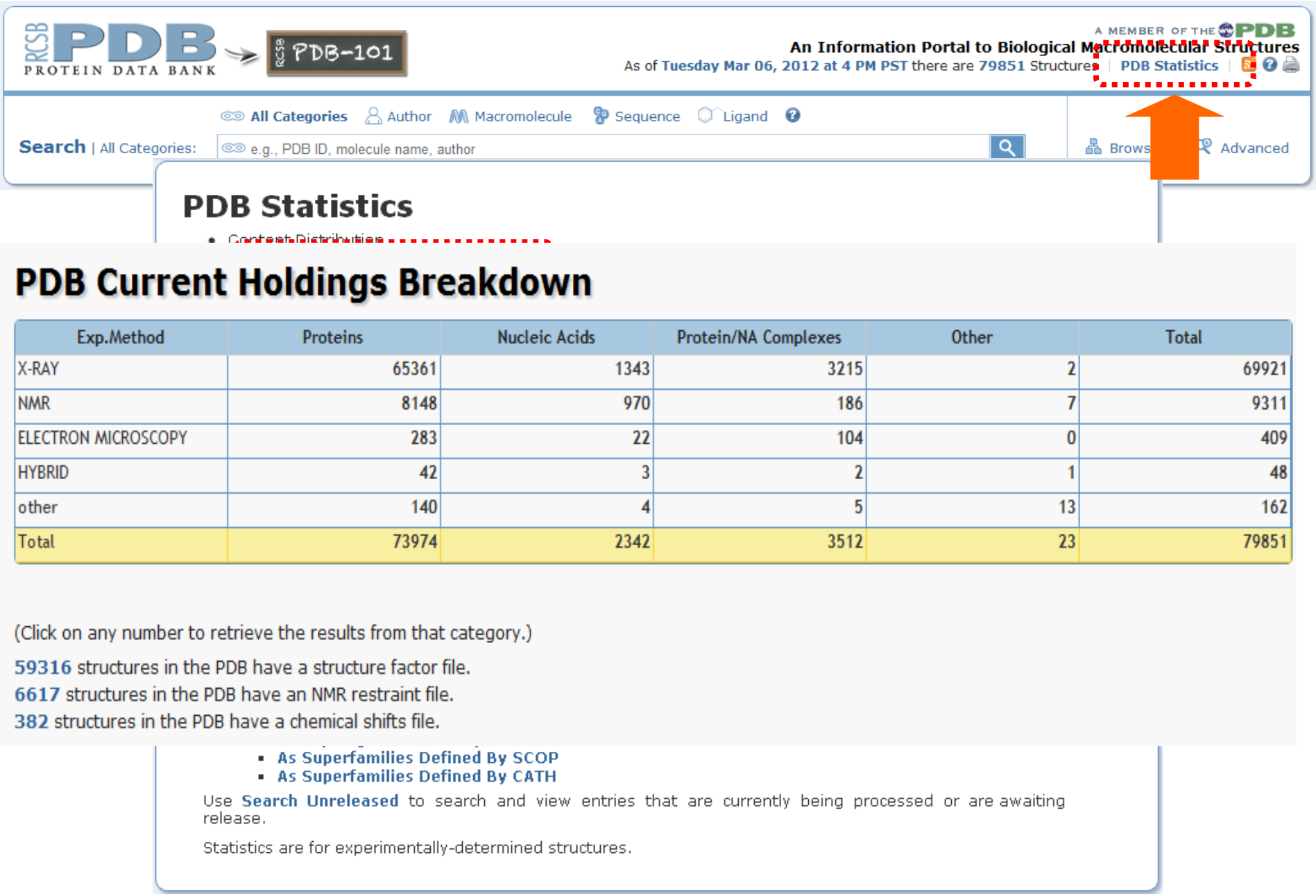
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X-RAY | 65361 | 1343 | 3215 | 2 | 69921
NMR | 8148 | 970 | 186 | 7 | 9311
ELECTRON MICROSCOPY | 283 | 22 | 104 | 0 | 409
HYBRID | 42 | 3 | 2 | 1 | 48
other | 140 | 4 | 5 | 13 | 162
Total | 73974 | 2342 | 3512 | 23 | 79851
(Click on any number to retrieve the results from that category.)
59316 structures in the PDB have a structure factor file.
6617 structures in the PDB have an NMR restraint file.
382 structures in the PDB have a chemical shifts file.
As Superfamilies Defined By SCOP
As Superfamilies Defined By CATH
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RCSB PDB PROTEIN DATA BANK | PDB-101

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All Categories | Author | Macromolecule | Seque

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  - By Structure Molecular Weight
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    - 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

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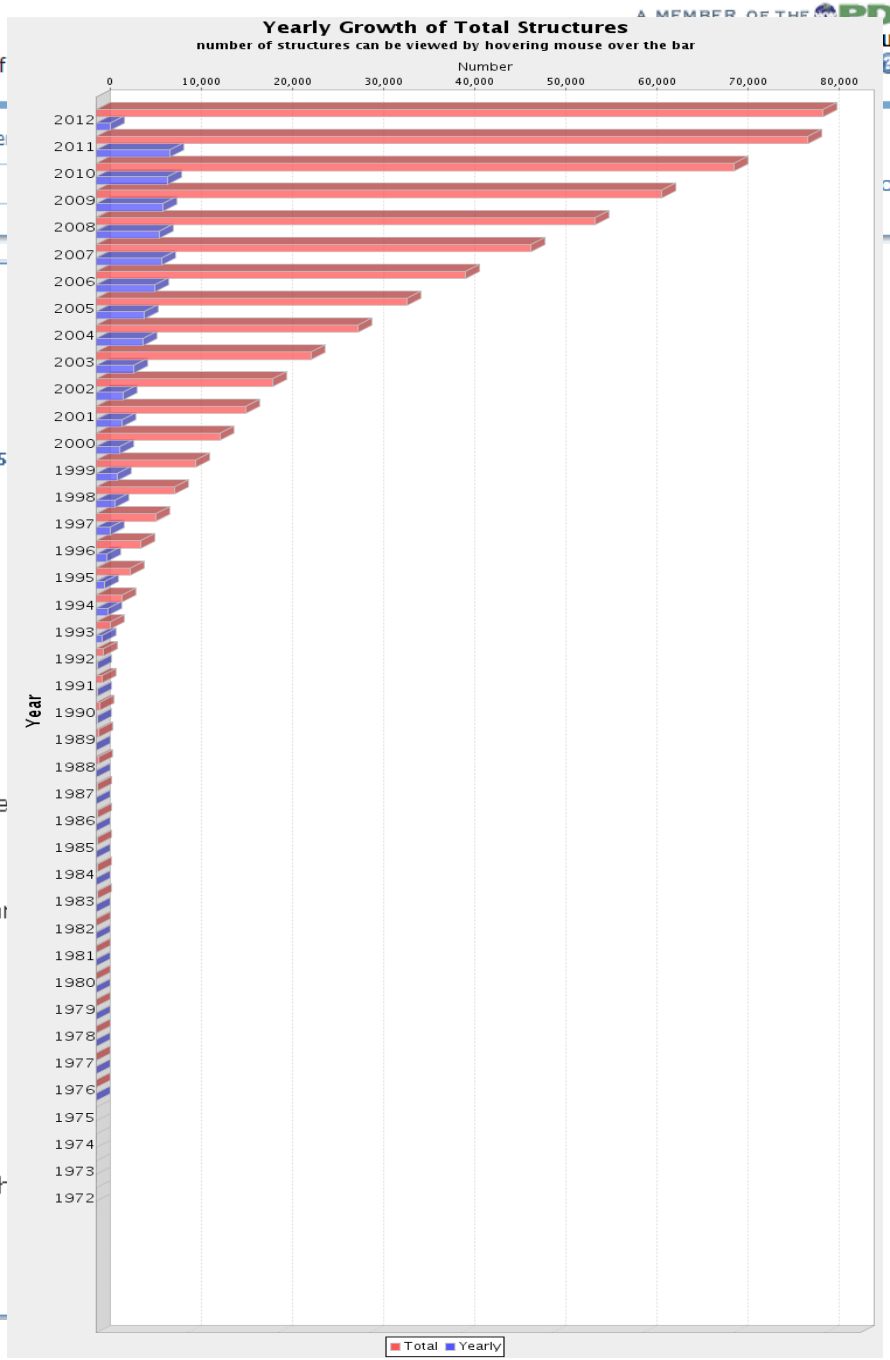

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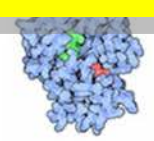
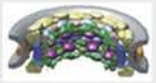


The discovery of streptomycin in 1944 provided the first effective treatment for tuberculosis. Ever since then, we have fought an escalating battle with bacteria using streptomycin and other aminoglycoside antibiotics. Researchers have discovered many natural aminoglycosides made by bacteria, and chemists have created entirely new antibiotics based on these effective natural defenses.

Full Article



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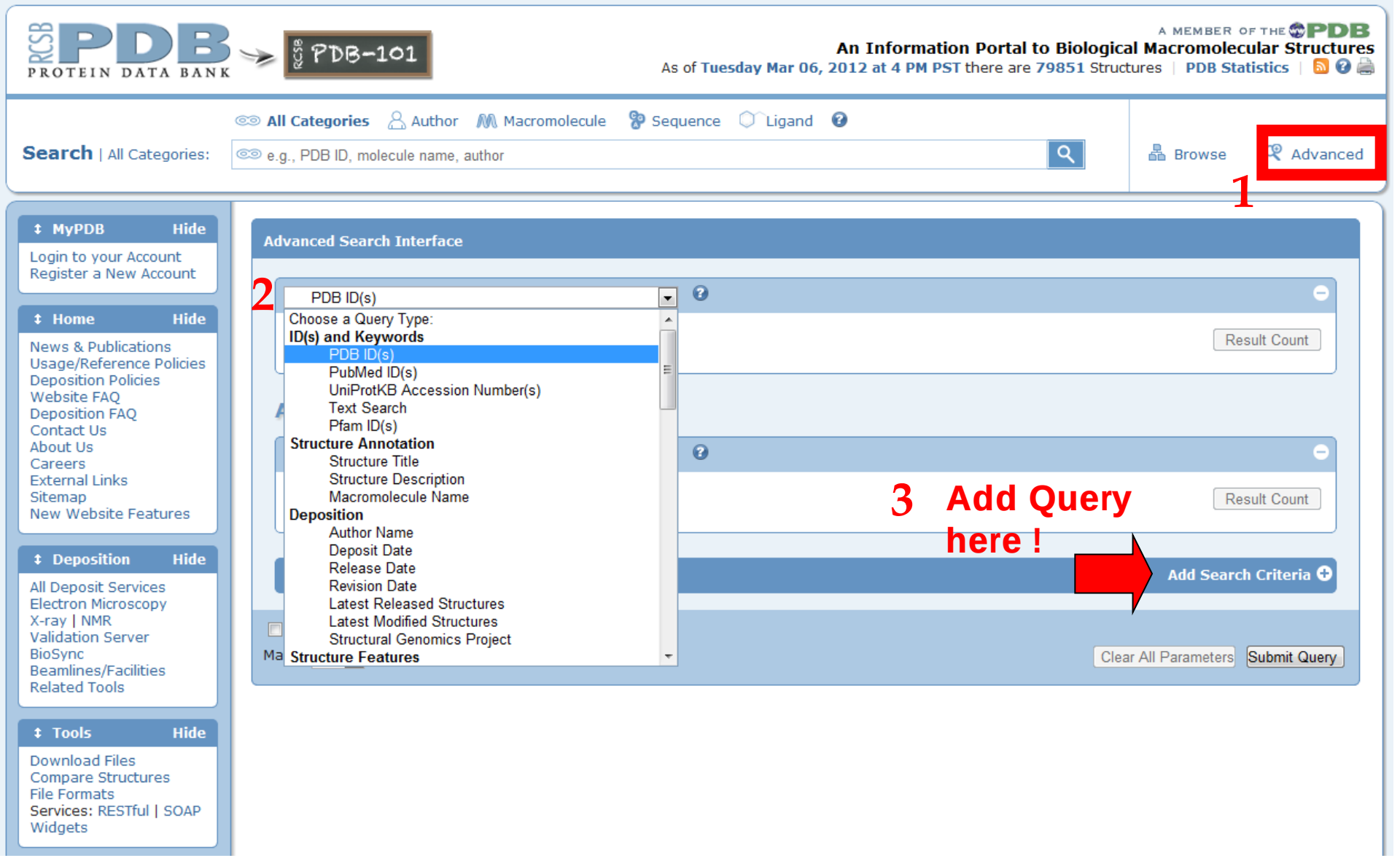

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DNA RECOGNITION BY GAL4: STRUCTURE OF A PROTEIN/DNA COMPLEX

PDB ID → 1D66

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DOI:10.2210/pdb1d66/pdb NDB ID: PDT003

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

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				
UniProtKB:	P04386				

Source

Polymer: 1
Scientific Name: Synthetic construct — Taxonomy

Polymer: 2
Scientific Name: Synthetic construct — Taxonomy

Polymer: 3
Scientific Name: Saccharomyces cerevisiae — Taxonomy — **Common Name:** Baker's yeast — **Expression System:** Escherichia coli

Ligand Chemical Component

Identifier	Formula	Name	Interactions
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External Domain Annotations

- SCOP Classification v1.75: **4 Domains** - data from SCOP
- CATH Classification v3.4.0: **3 Domains** - data from CATH
- PFAM Classification: **4 Domains** - data from PFAM

Structural Biology Knowledgebase Data

Information from the Structural Biology Knowledgebase

- Models from the Protein Model Portal: **40 models**
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Data in orange boxes are gathered from external resources (when available).

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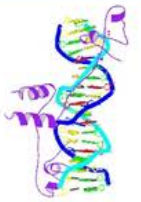
Biological Assembly



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Deposition Summary

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

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

Experimental Details

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

Resolution[Å]:	2.70
R-Value:	0.230 (obs.)
R-Free:	n/a
Space Group:	$P\,4_3\,2_1\,2$

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

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

1D66

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DOI:10.2210/pdb1d66/pdb NDB ID: PDT003

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

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

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Molecular Description Hide

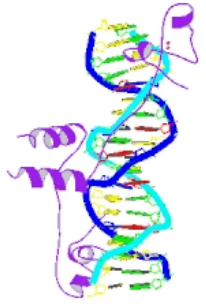
Classification: Transcription/dna
Structure Weight: 27737.04

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
UniProtKB: P04386

Biological Assembly



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Authors: Marmorstein, R., Carey,

Sequence / Structure Details

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DNA RE GNITION BY GAL4: STRUCTURE OF A PROTEIN/DNA COMPLEX

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Sequence Display

The sequence display provides a graphical representation of the UniProtKB, PDB - ATOM and PDB - SEQRES sequences. Different 3rd party annotations can be graphically mapped on the sequence and displayed in the Jmol viewer.

The structure **1D66** has in total **4** chains. Out of these **3** are sequence-unique.

Currently viewing **unique chains** only. **show all chains**

Sequence & Structure Relationships

Display Jmol

Enable Jmol to view annotations in 3D.

Chain A : PROTEIN (GAL4)

FASTA | **Sequence & DSSP** | **Image**
Polymer 3
Length: 66 residues
Chain Type: polypeptide(L)
Reference: **UniProtKB** P04386

Display Parameters

Identical chains: B | show all chains

show polypeptide chains only

Currently displayed: **SEQRES sequence.**
Display external (UniProtKB) sequence

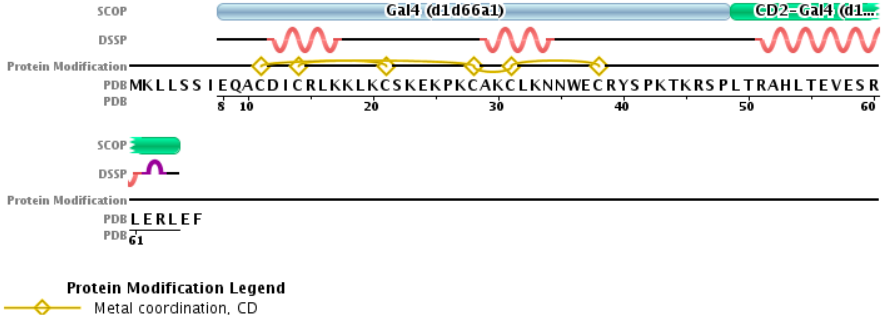
Mouse over an annotation to see more details.

Annotations *Add Annotations* Select

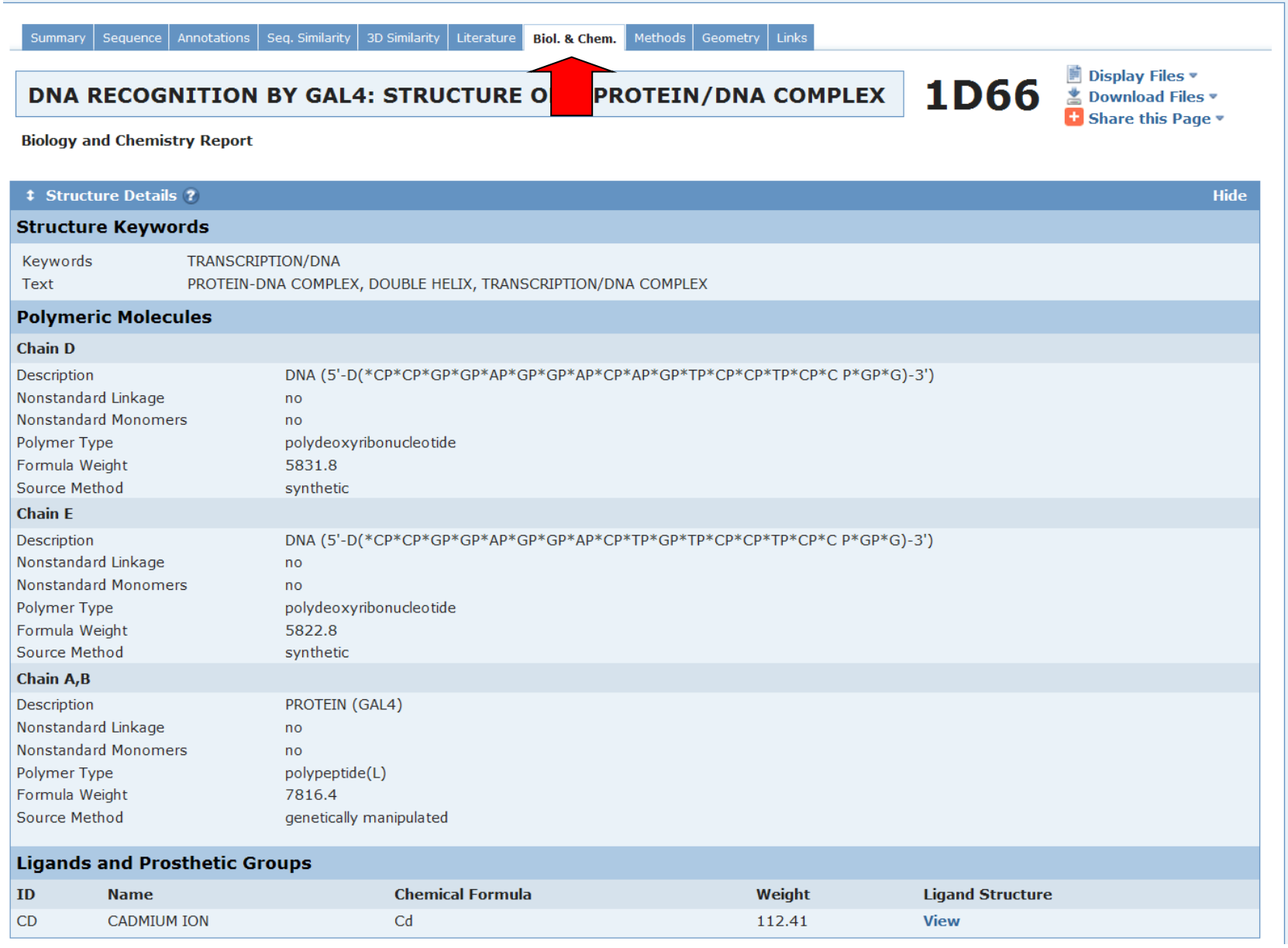
Domain Assignment:**SCOP** [hide] [reference]
d1d66a1 Gal4: 41 residues
d1d66a2 CD2-Gal4: 16 residues

Secondary Structure:**DSSP** [hide] [reference]
34% helical (3 helices; 23 residues)

Structural Feature:**Protein Modification** [hide] [reference] [reference]
0252 Metal coordination, CD



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

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

<0.5

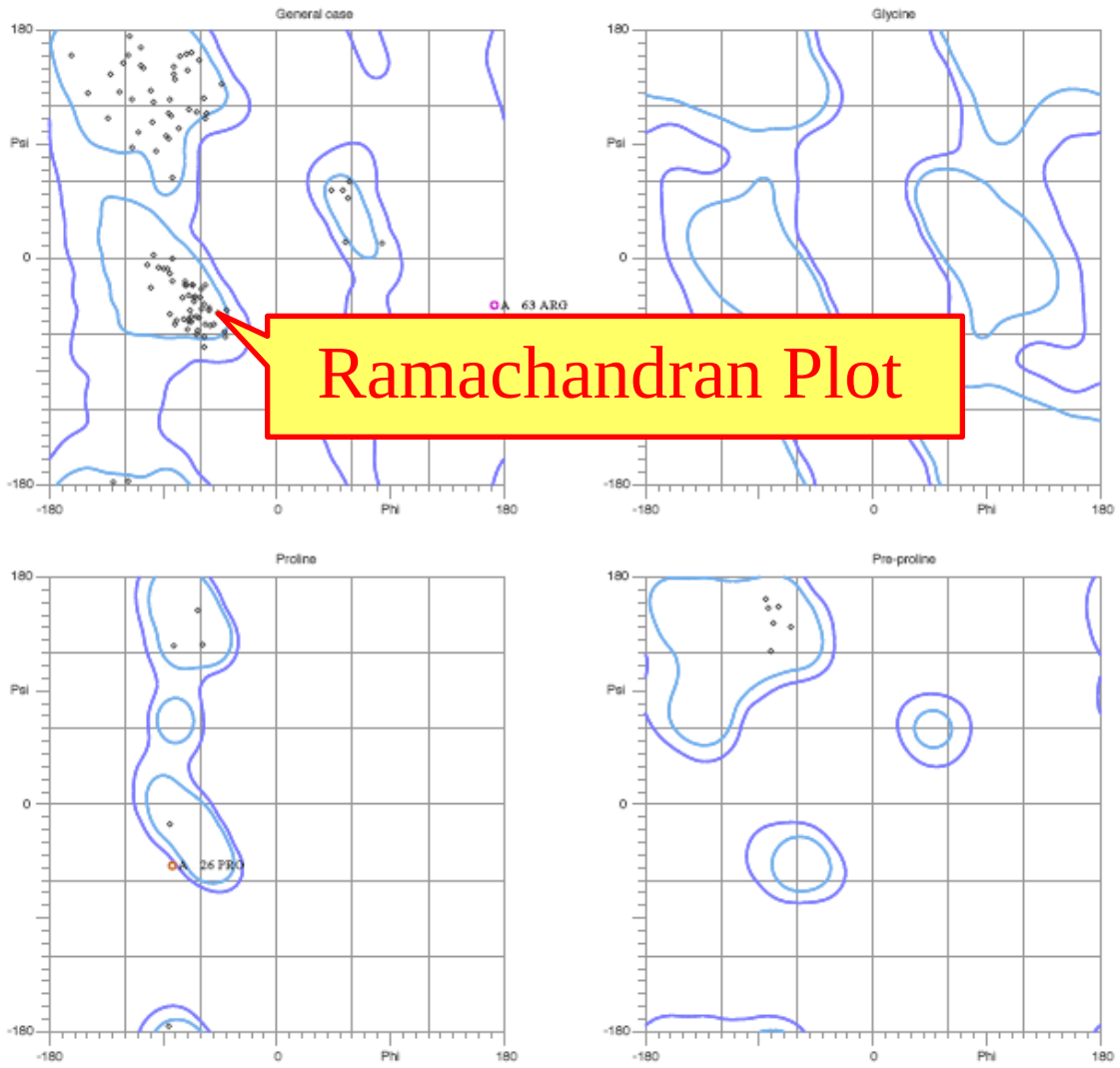
Bond Length

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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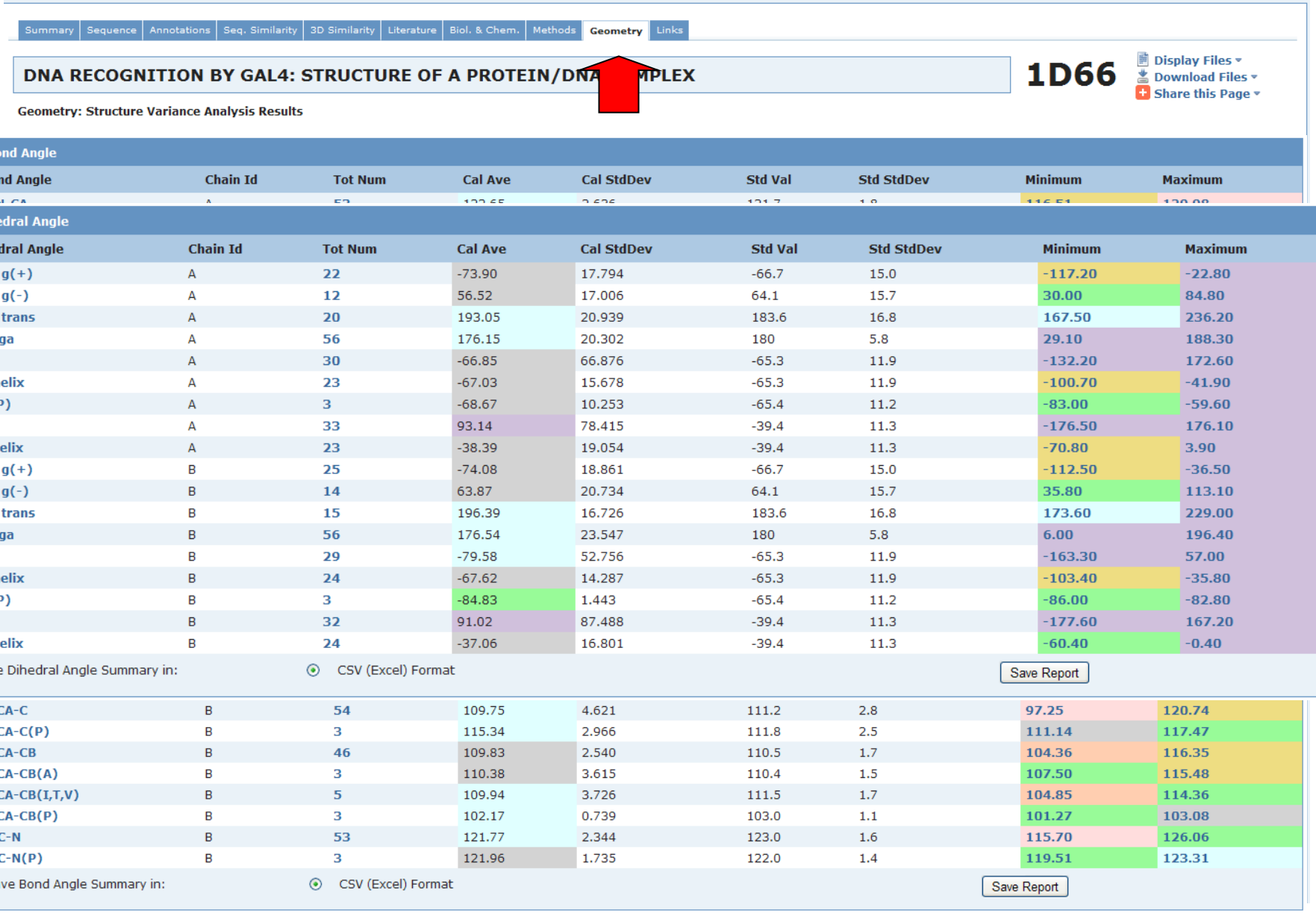
>5.0

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

Geometry



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

DNA RECOGNITION BY GAL4: STRUCTURE OF A PROTEIN/DNA 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	1.8	116.51	130.08

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

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

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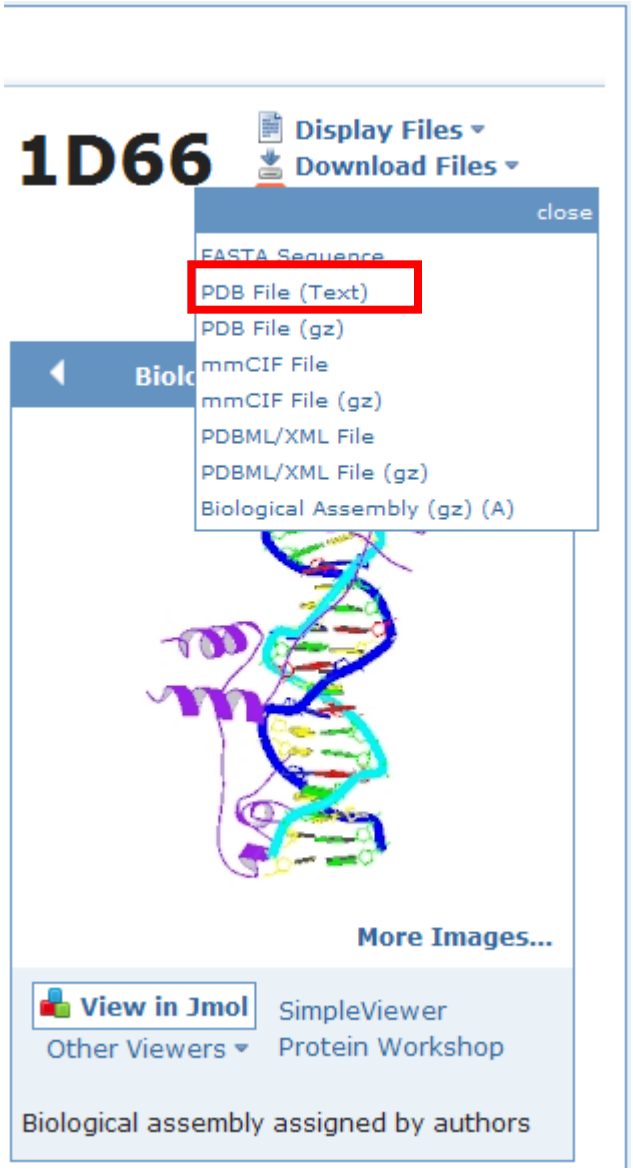


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HEADER    TRANSCRIPTION REGULATION          06-MAR-92   1D66    1D66  2
COMPND    GAL4 (RESIDUES 1 - 65) COMPLEX WITH 19MER DNA             1D66  3
SOURCE    (SACCHAROMYCES $CEREVISIAE) OVEREXPRESSED IN (ESCHERICHIA    1D66  4
SOURCE   2 $COLI)                                                   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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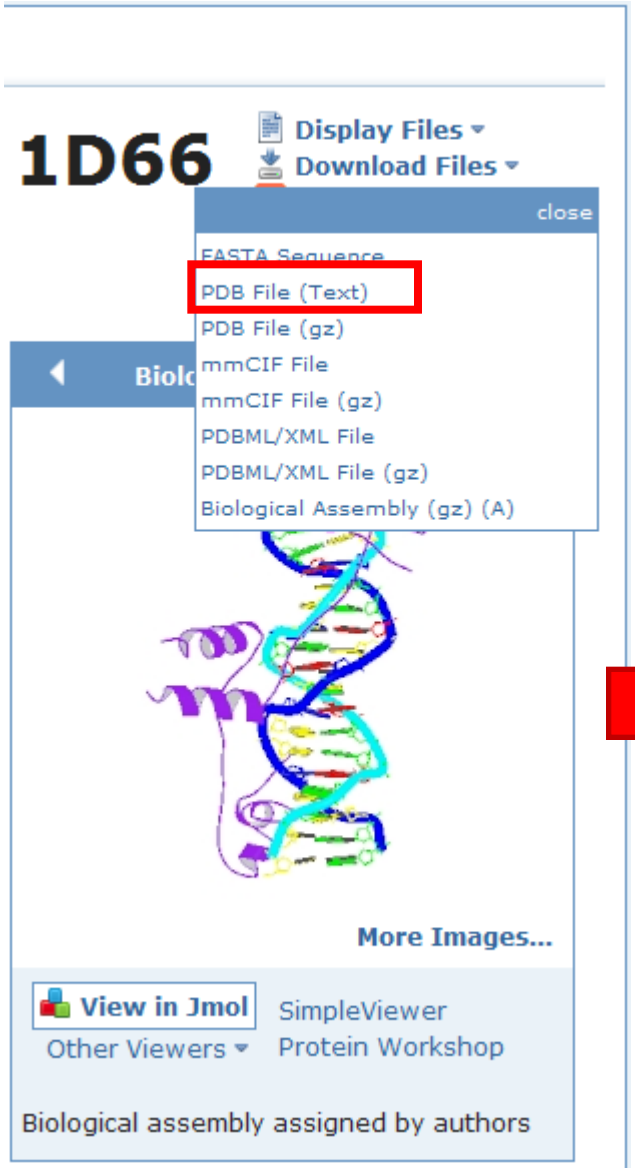


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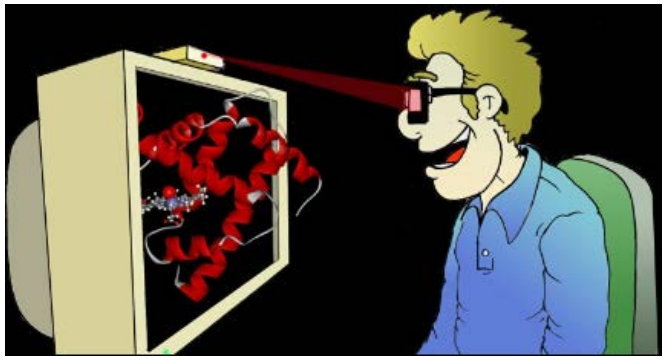
HET    CD   41     1   CADMIUM                                  1D66  68
HET    CD   42     1   CADMIUM                                  1D66  69
FORMUL  5  CD   4(CD1)                                         1D66  70
FORMUL  6  HOH  *51(H2 O1)                                     1D66  71
HELIX   1 H1A 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       22.87497    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

PDB File Title Section

HEAD	**First line of the entry, contains PDB ID code, classification, and date of deposition.**	**HELIX**	**Identification of helical substructures.**
COMPND	**Description of macromolecular contents of the entry.**	**CRYST1**	**Unit cell parameters, space group, and Z.**
SOURCE	**Biological source of macromolecules in the entry.**	**ORIGXn**	**Transformation from orthogonal coordinates to the submitted coordinates (n = 1, 2, or 3).** 由直角(orthogonal)座標系，轉換到submitted座標系，座標系之間的轉換
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。
REVDAT	**Revision date and related information.**	**MTRIXn**	**Transformations expressing non-crystallographic symmetry (n = 1, 2, or 3). There may be multiple sets of these records.** 非晶圖對稱的轉換
JRNL	**Literature citation that defines the coordinate set.**	**ATOM**	**Atomic coordinate records for standard groups.**
REMARK	**General remarks, some are structured and some are free form.**	**HETATM**	**Atomic coordinate records for heterogens.**
SEQRES	**Primary sequence of backbone residues.**	**TER**	**Chain terminator.**
FORMUL	**Chemical formula of non-standard groups.**	**END**	**Last record in the file.**

Molecular Graphics



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- MOLMOL
- MolScript
- Raster3D
- GRASP
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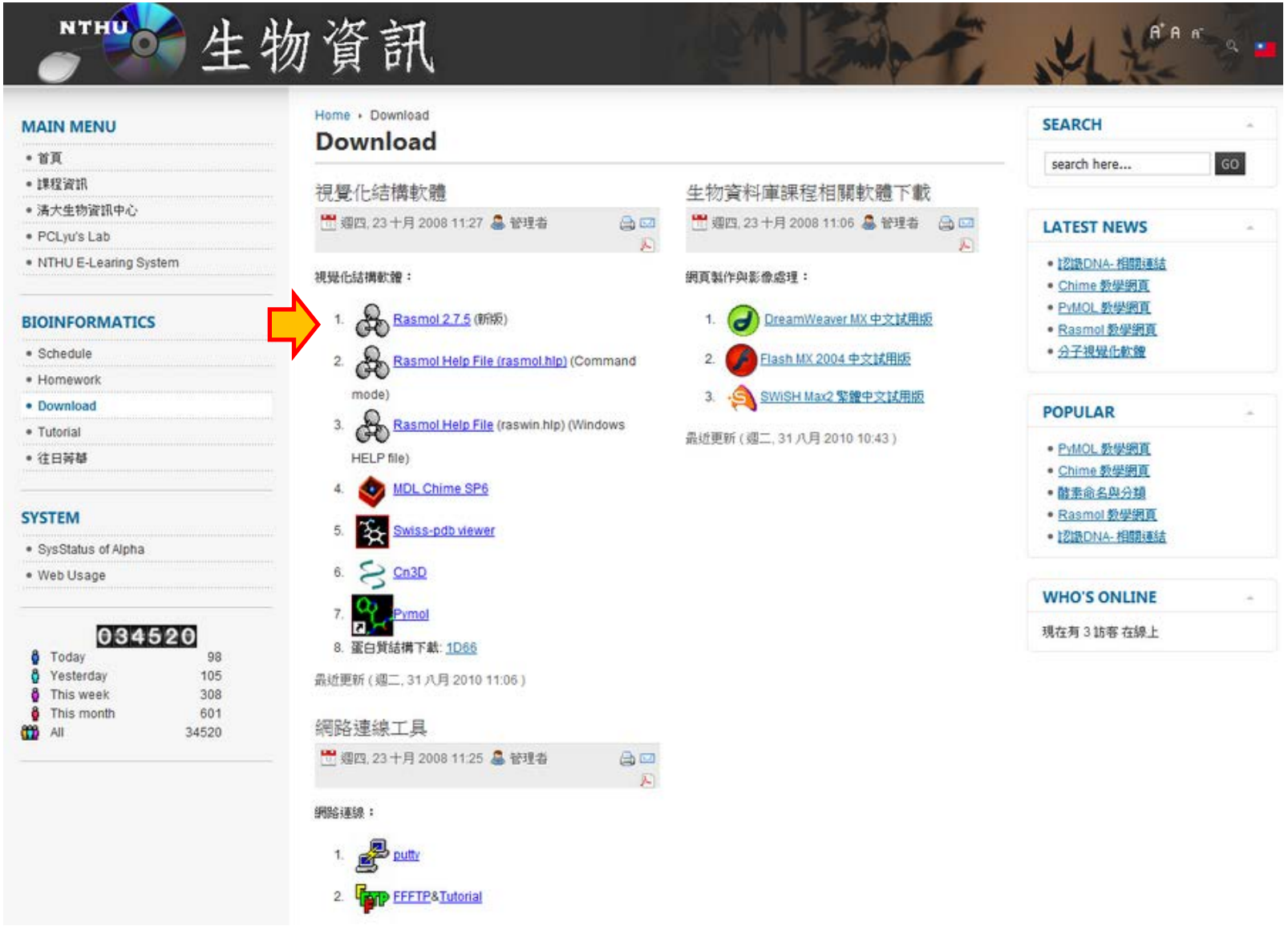

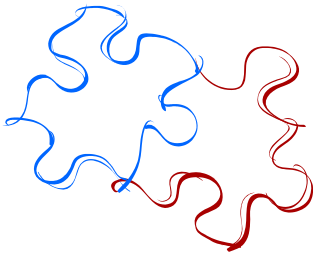

Thanks for your attentions.