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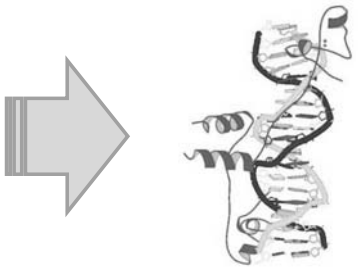
MKLLSSIEQACDICRLKKLKCSKEKPKCAKCLKN
NWECRYSPKTKRSPLTRAHLTEVESRLERLEF
>1D66:B|PDBID|CHAIN|SEQUENCE
MKLLSSIEQACDICRLKKLKCSKEKPKCAKCLKN
NWECRYSPKTKRSPLTRAHLTEVESRLERLEF
>1D66:D|PDBID|CHAIN|SEQUENCE
CCGGAGGACAGTCCTCCGG
>1D66:E|PDBID|CHAIN|SEQUENCE
CCGGAGGACTGTCCTCCGG



Databases for Protein Structure

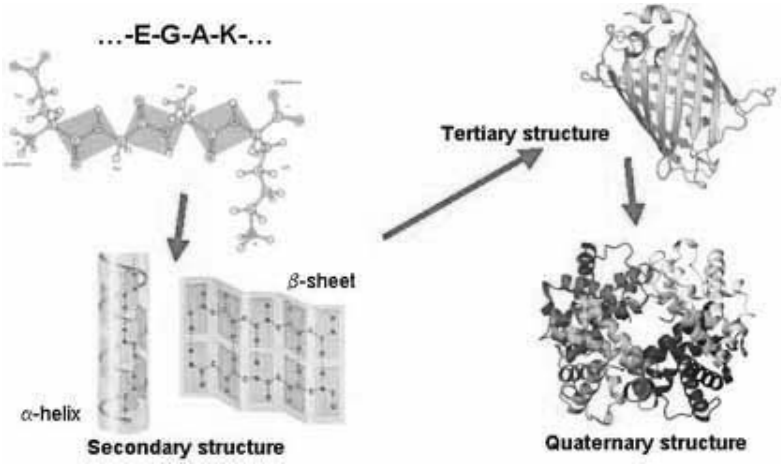
呂平江

國立清華大學

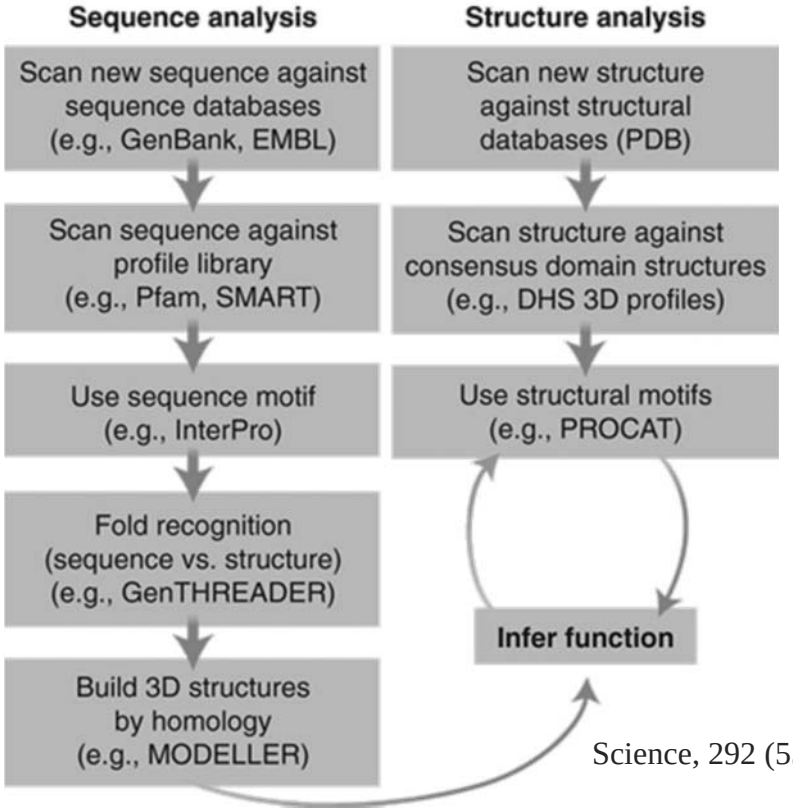
生命科學系/生物資訊與結構生物研究所

2012/06/27

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

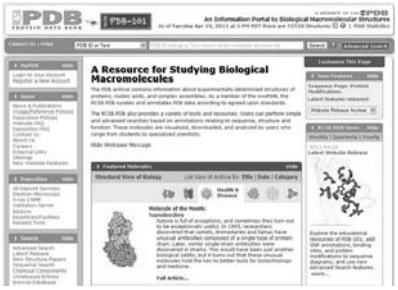
- **Structure Databases**
  - Nucleic acid structure
    - Greglist
    - GRSDB
    - ITS2
    - MeRNA
    - NCIR - Non-Canonical Interactions in RNA
    - NDB
    - NTDB
    - QuadBase
    - Rfam
    - RNA FRABASE
    - RNA SSTRAND
    - RNABase
    - RNAJunction
    - SARS-CoV RNA SSS
    - SCOR - 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

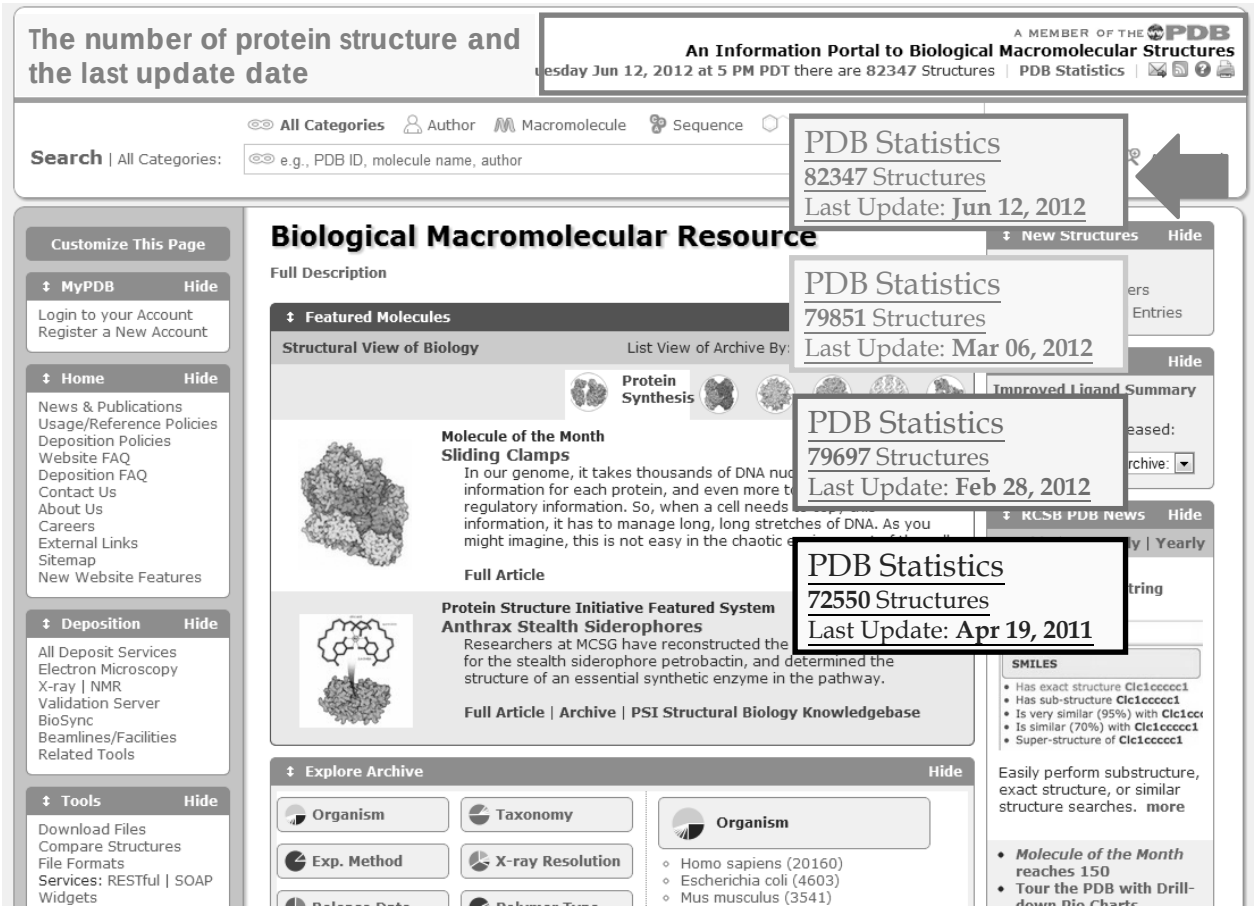
- **Structure Databases**
  - Protein structure
    - Columba
    - CSA - Catalytic Site Atlas
    - Dali database
    - DBAli
    - Decoys-R-Us
    - DisProt - Database of Protein Disorder
    - DMAPS
    - Dockground
    - DomIns - Database of Domain Insertions
    - DSDBASE - Disulfide Database
    - 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

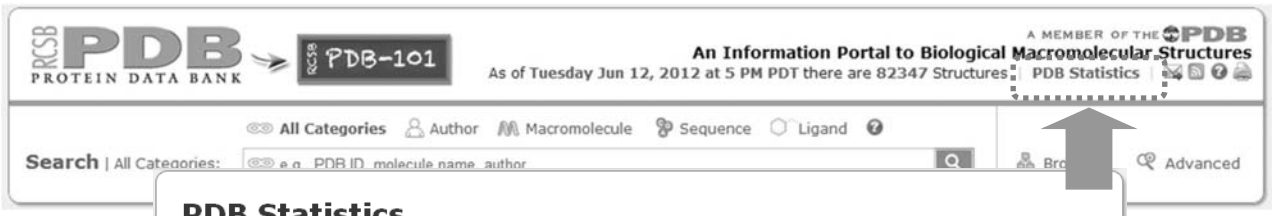
- **Structure Databases**
  - Protein structure
    - PDB
    - PDB-REPRDB
    - PDBselect
    - PDBsum
    - PDB_TM
    - PepConfDB
    - PFD - Protein Folding Database
    - Phospho3D
    - PIDD
    - PMDB - Protein Model Database
    - Structure Superposition Database
    - ProSAS
    - PROTCOM
    - 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)

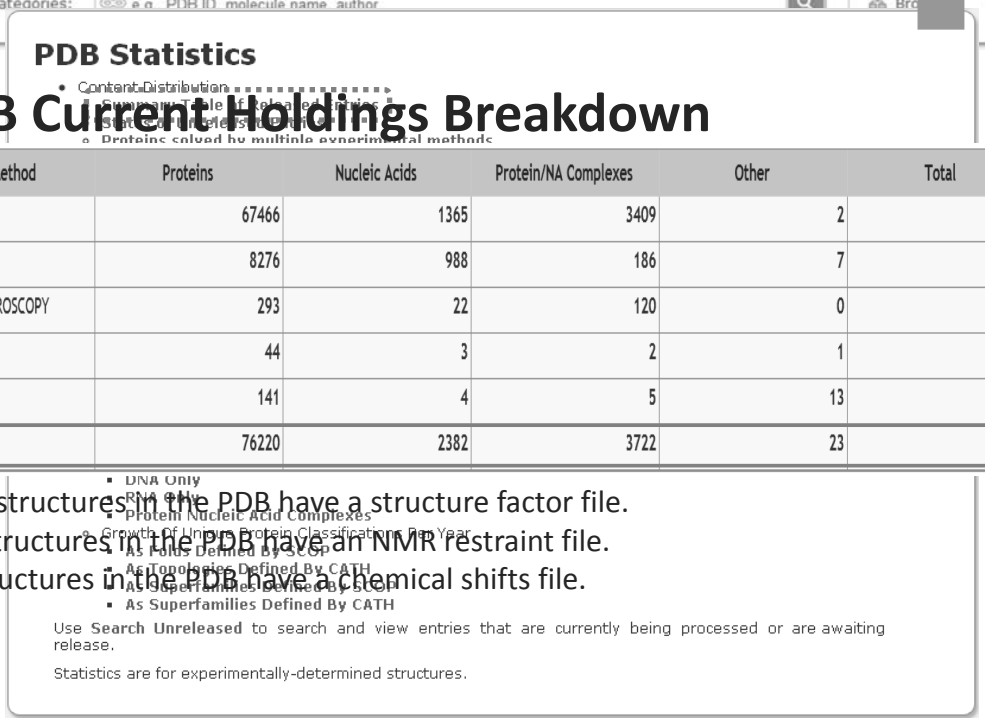
- http://**www.pdb.org/**
- Structure data determined by X-ray crystallography and NMR
- The data include the atom coordinate, reference, sequence, secondary structure, disulfide bond ……etc.





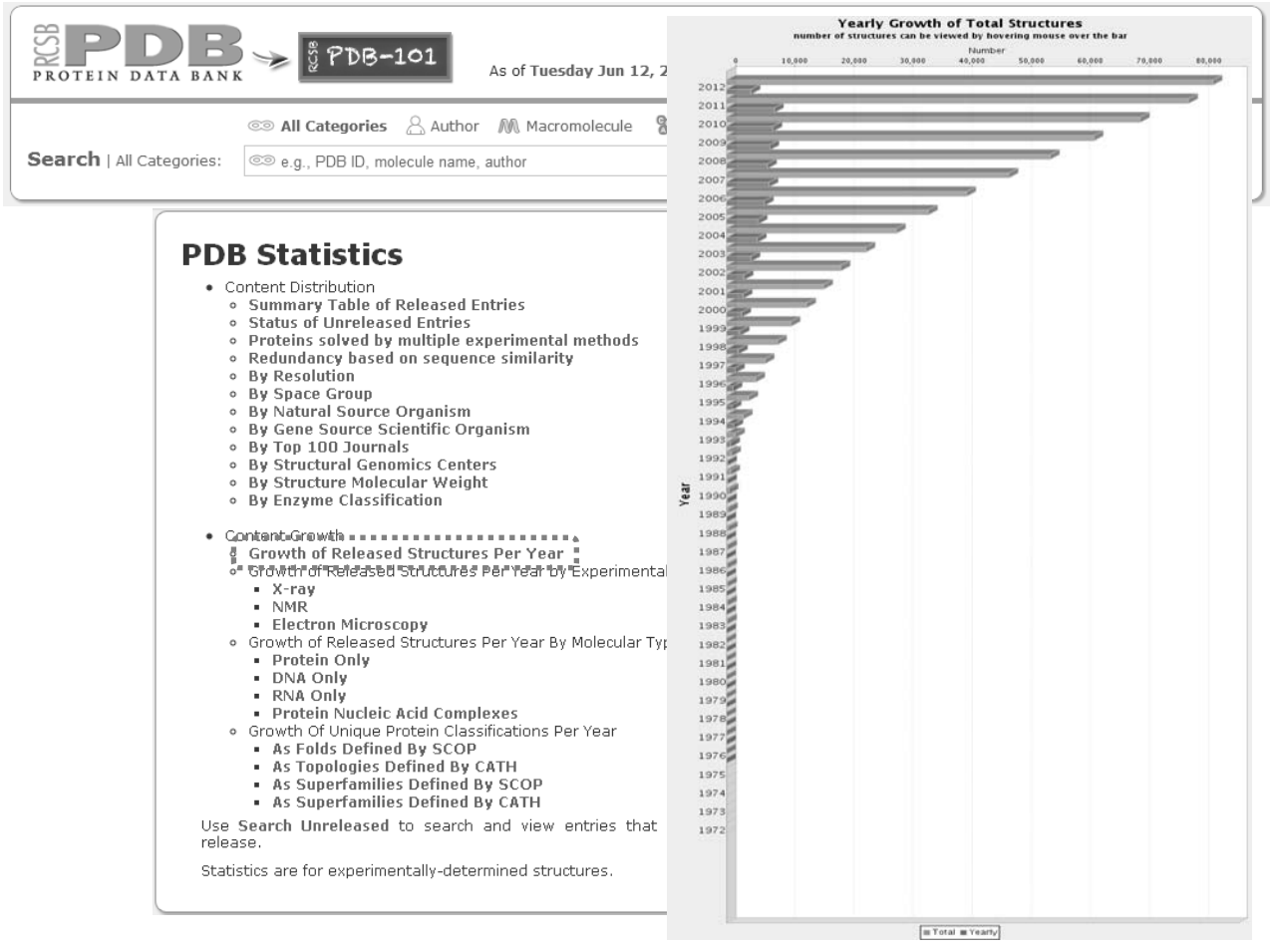


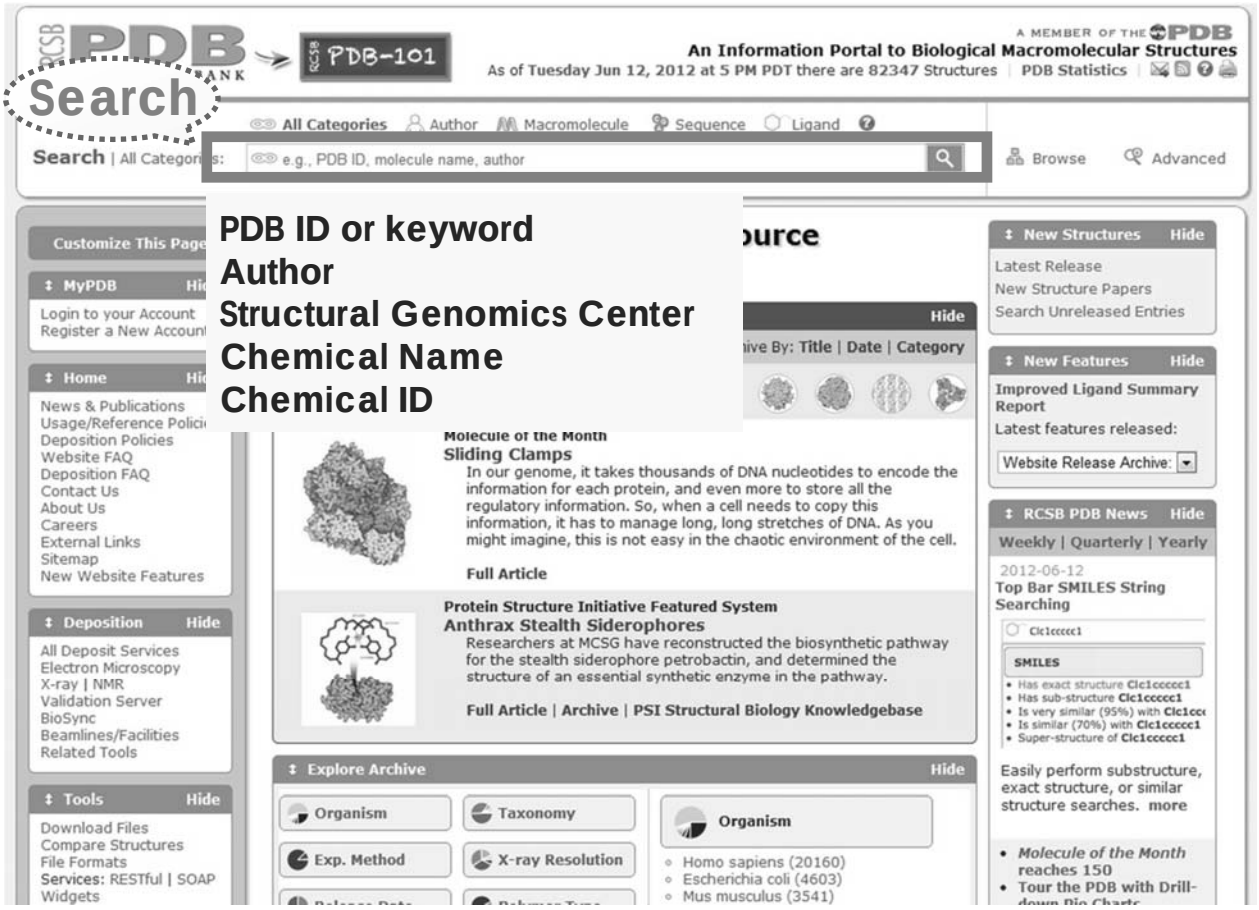
PDB Current Holdings Breakdown



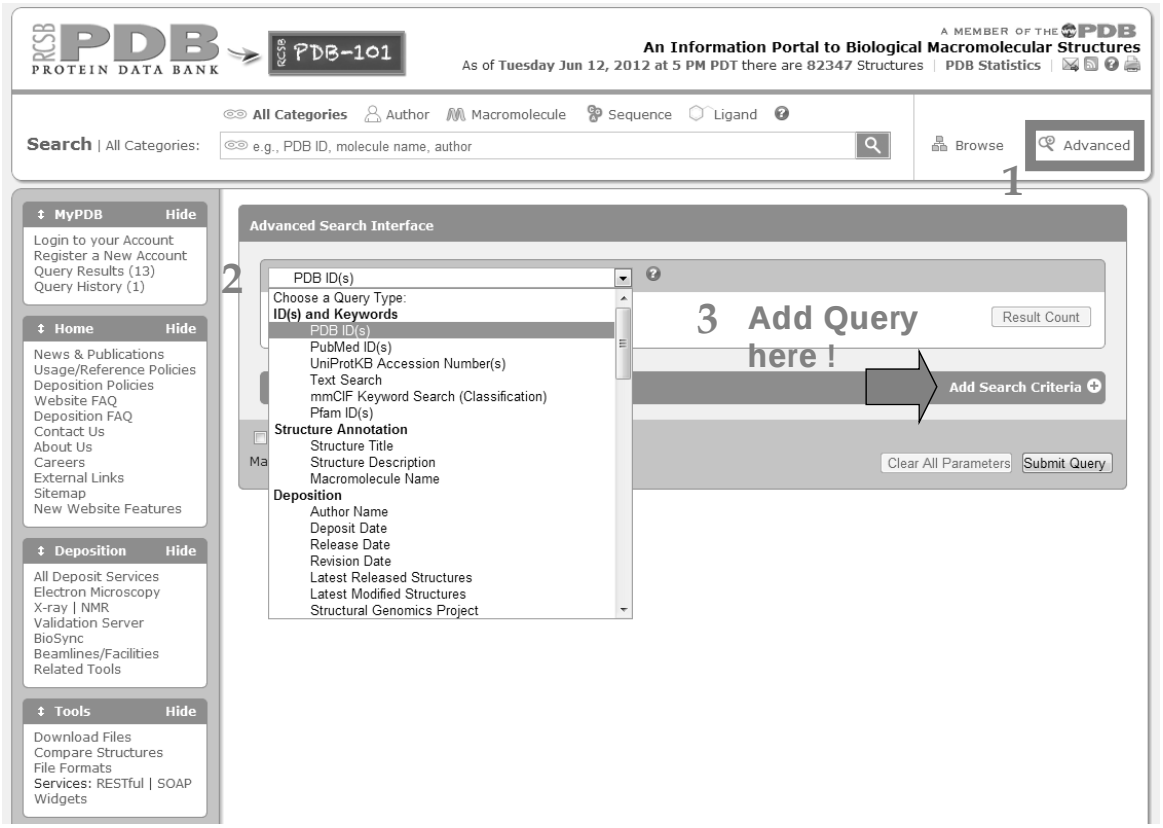
Exp.Method	Proteins	Nucleic Acids	Protein/NA Complexes	Other	Total
X-RAY	67466	1365	3409	2	72242
NMR	8276	988	186	7	9457
ELECTRON MICROSCOPY	293	22	120	0	435
HYBRID	44	3	2	1	50
other	141	4	5	13	163
Total	76220	2382	3722	23	82347

61642 structures in the PDB have a structure factor file.
6764 structures in the PDB have an NMR restraint file.
526 structures in the PDB have a chemical shifts file.

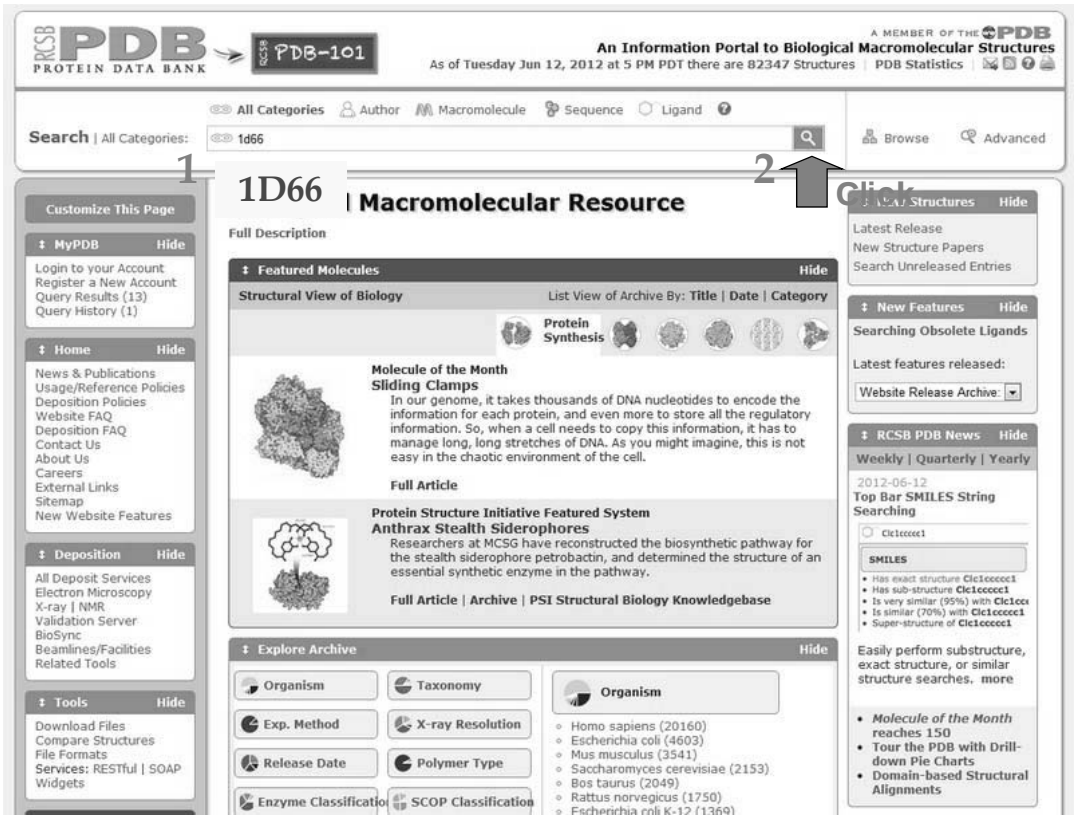




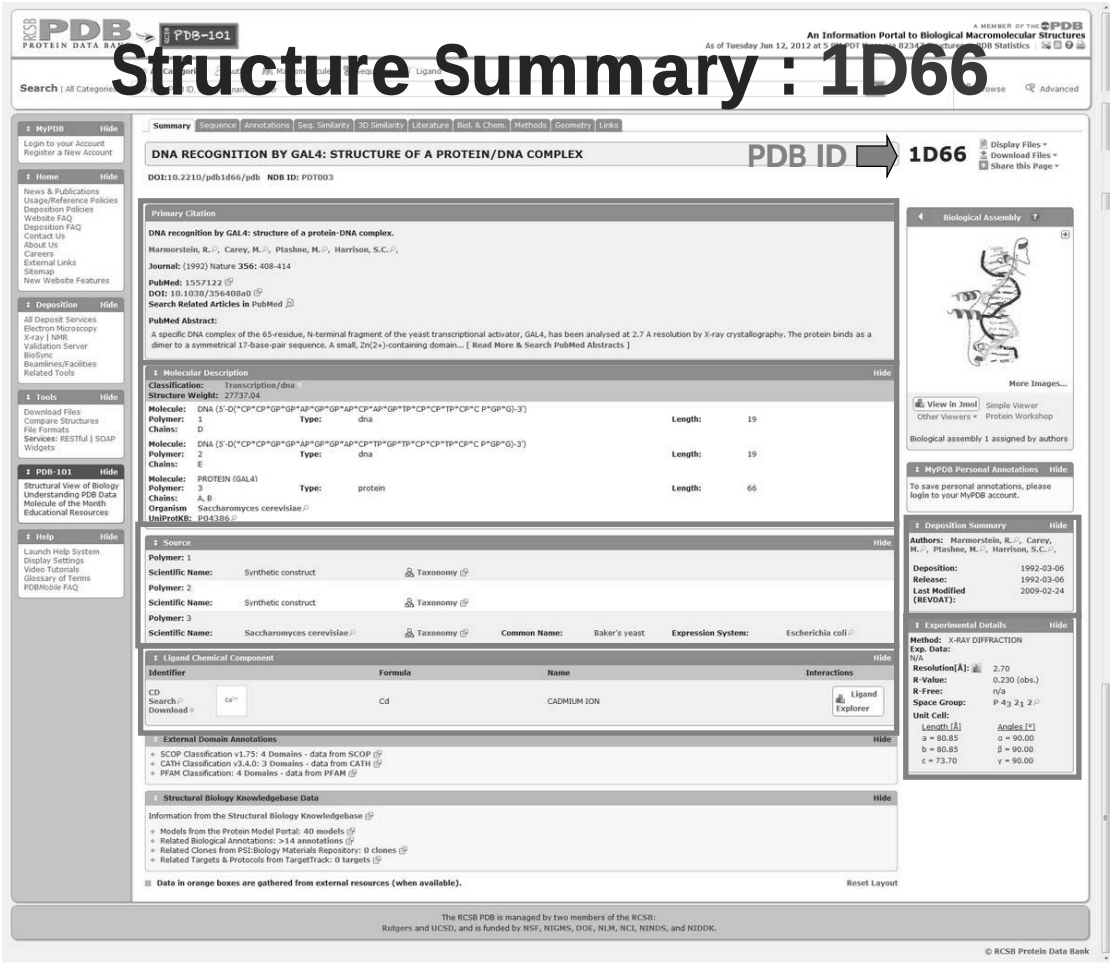
Advanced Search Interface



Search PDB ID: 1D66



Structure Summary : 1D66



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

RCSB PDB PROTEIN DATA BANK — PDB-101

A MEMBER OF THE PDB
An Information Portal to Biological Macromolecular Structures
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DNA RECOGNITION BY GAL4: STRUCTURE OF A PROTEIN/DNA COMPLEX

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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 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

More Images...

View in Jmol | Simple Viewer | Other Viewers | Protein Workshop

Biological assembly 1 assigned by authors

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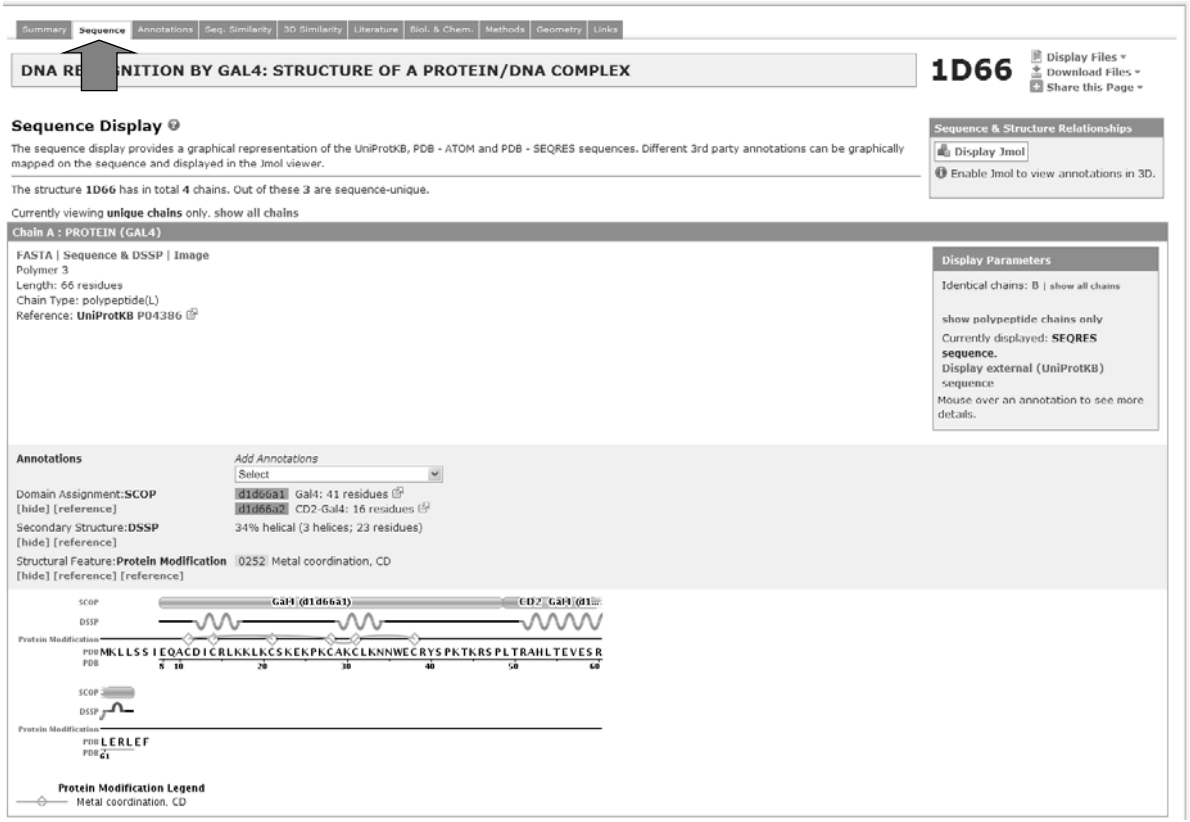
Deposition Summary Hide

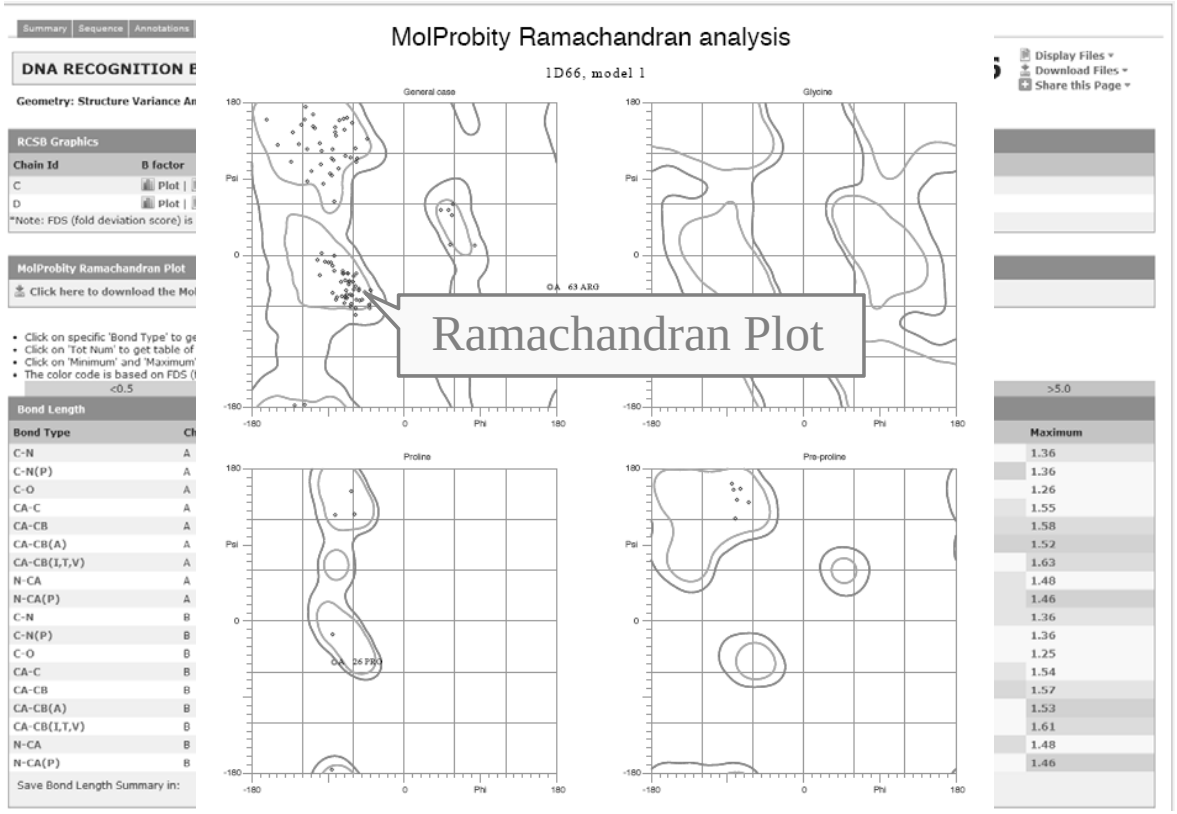
Authors: Marmorstein, R., Carey,

Sequence / Structure Details

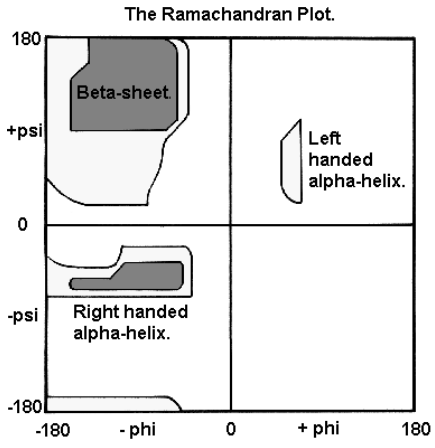


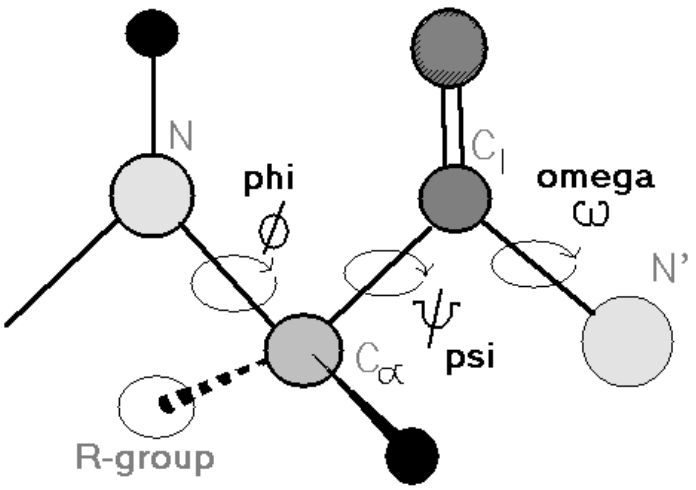
Biology and Chemistry Report

Geometry



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)

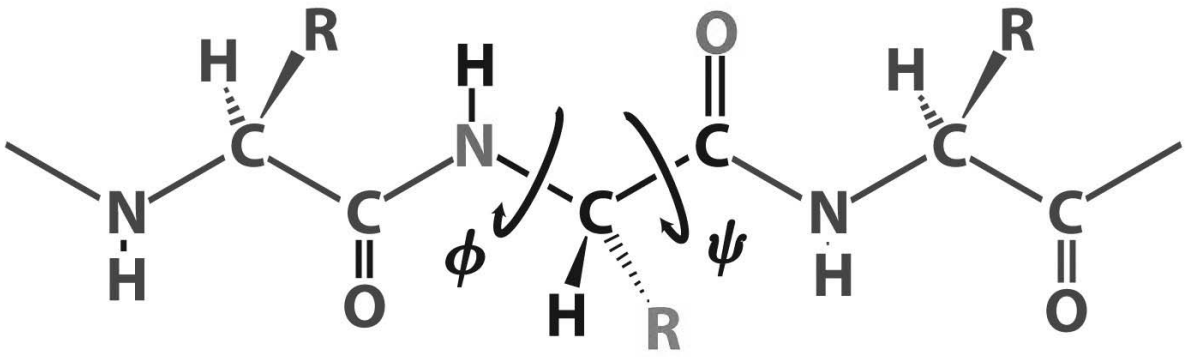
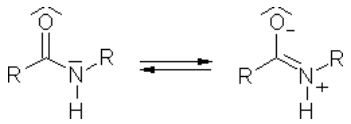
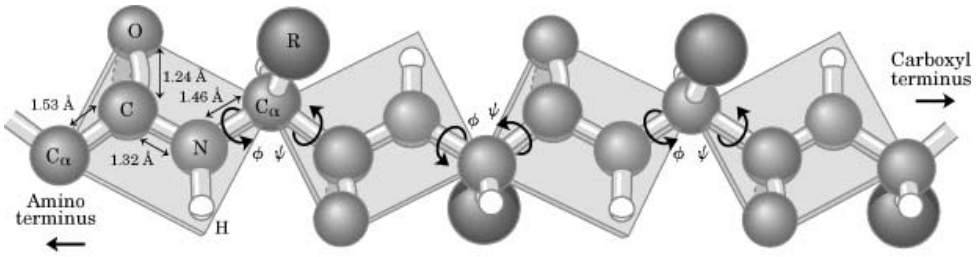


Figure 2.22a
***Biochemistry*, Seventh Edition**



"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

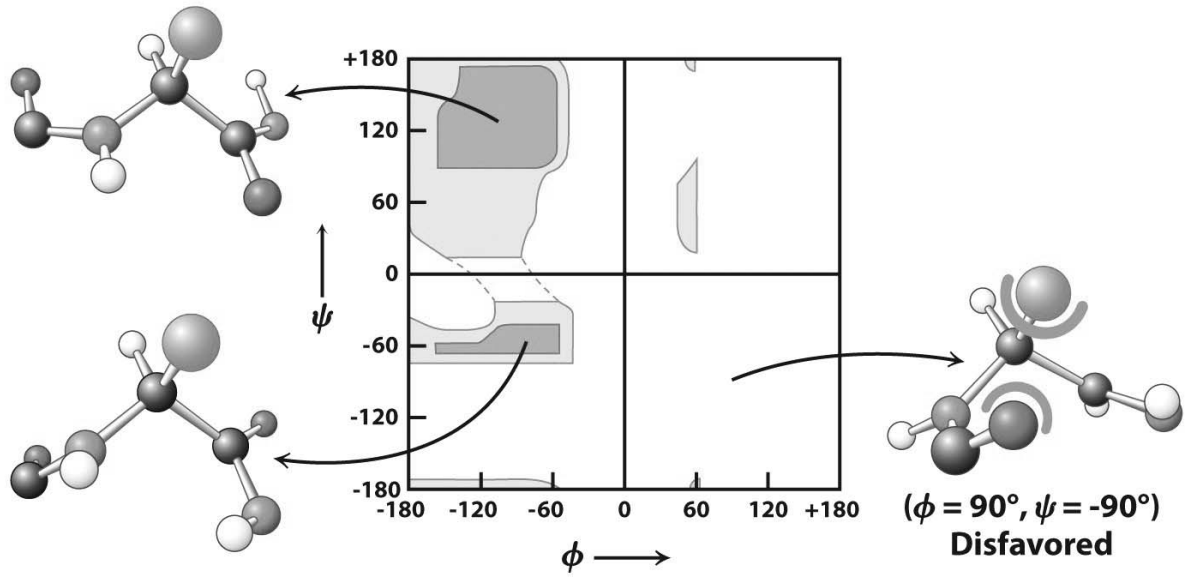
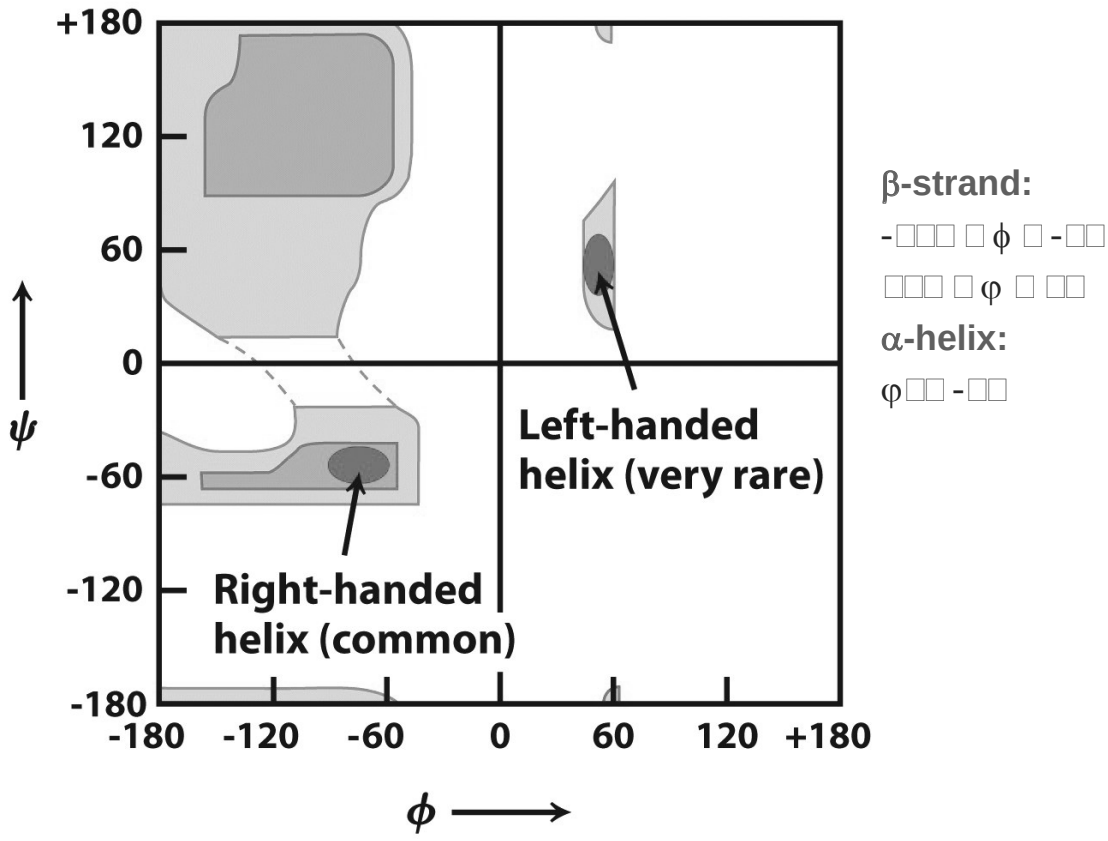


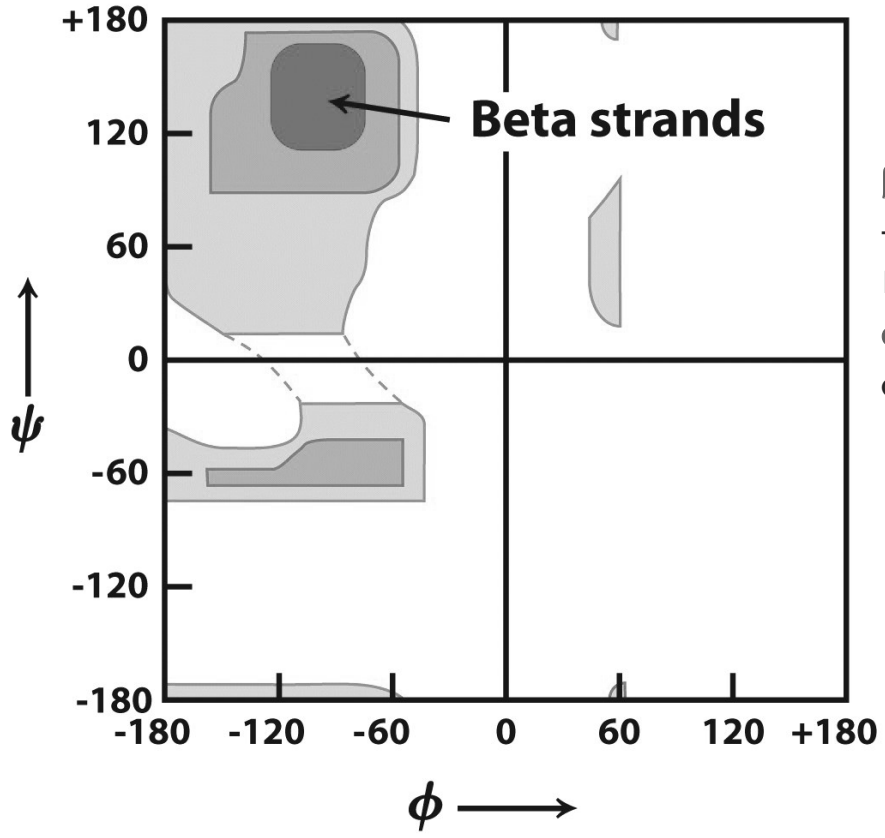
Figure 2.23
Biochemistry, Seventh Edition

- □ □h□□s **allowed Φ and Ψ angles**
- □ **White areas** □ **sterically disallowed** □□□□□□□ □i□□s
- □ □□□□i□ s□□□□□□□□s □□□□□□□□i□hi□ □□□□□ □□ □□□i□□s



β-strand:
-□□□ □ ϕ □ -□□
□□□ □ φ □ □□
α-helix:
φ□□ -□□

Figure 2.26
Biochemistry, Seventh Edition



β-strand:

-□□□ □ ϕ □ -□□

□□□ □ φ □ □□

α-helix:

φ□□ -□□

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 COMPLEX 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	57	122.65	2.626	121.7	1.8	116.51	129.08

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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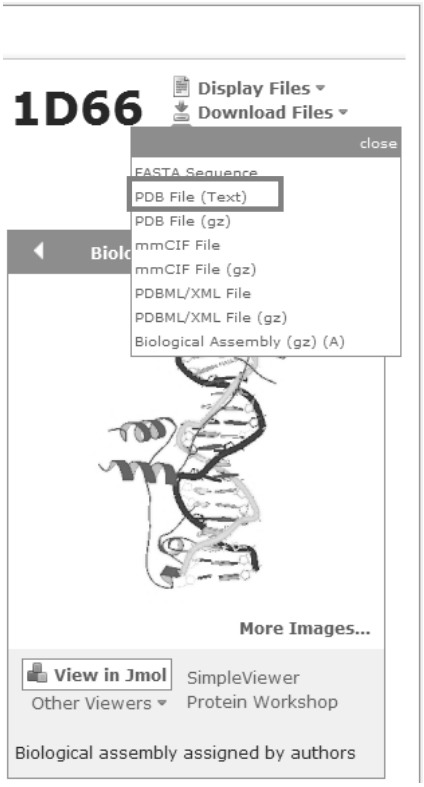


```
HEADER   TRANSCRIPTION REGULATION          06-MAR-92  1D66    1D66  2
COMPND   GAL4 (RESIDUES 1 - 65) COMPLEX WITH 19MER DNA             1D66  3
SOURCE   (SACCHAROMYCES $CEREVISIAE) OVEREXPRESSED IN (ESCHERICHIA   1D66  4
SOURCE  2 $COLI)                                                   1D66  5
AUTHOR   R.MARMORSTEIN,S.HARRISON                                  1D66  6
REVDAT
JRNL                                                               1D66  8
JRNL                                                               6  9
JRNL
JRNL
JRNL
REMARK
REMARK
REMARK
REMARK
REMARK
REMARK
REMARK                                                             56 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
```

檔案下載

是否要開啓或儲存這個檔案?

名稱: 1D66.pdb
類型: Brookhaven Protein Databank File
從: www.pdb.org

開啓舊檔(O) 儲存(S) 取消

雖然來自網際網路的檔案可能是有用的，但是某些檔案有可能會傷害您的電腦。如果您不信任其來源，請不要開啓或儲存這個檔案。有什麼樣的風險?

*Use **WordPad** to view the text file

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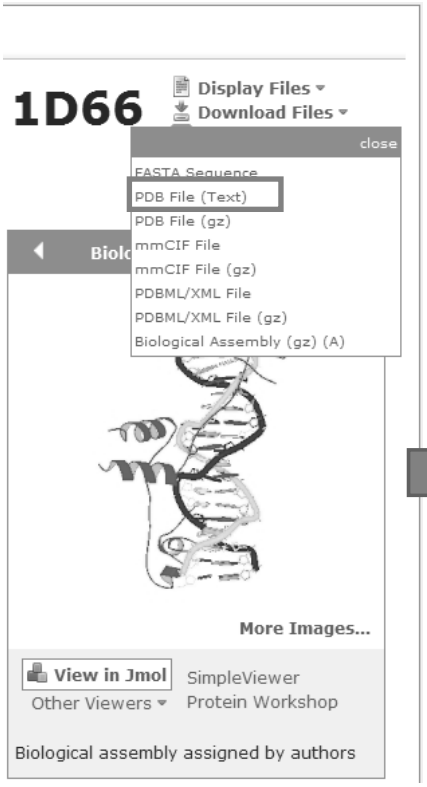


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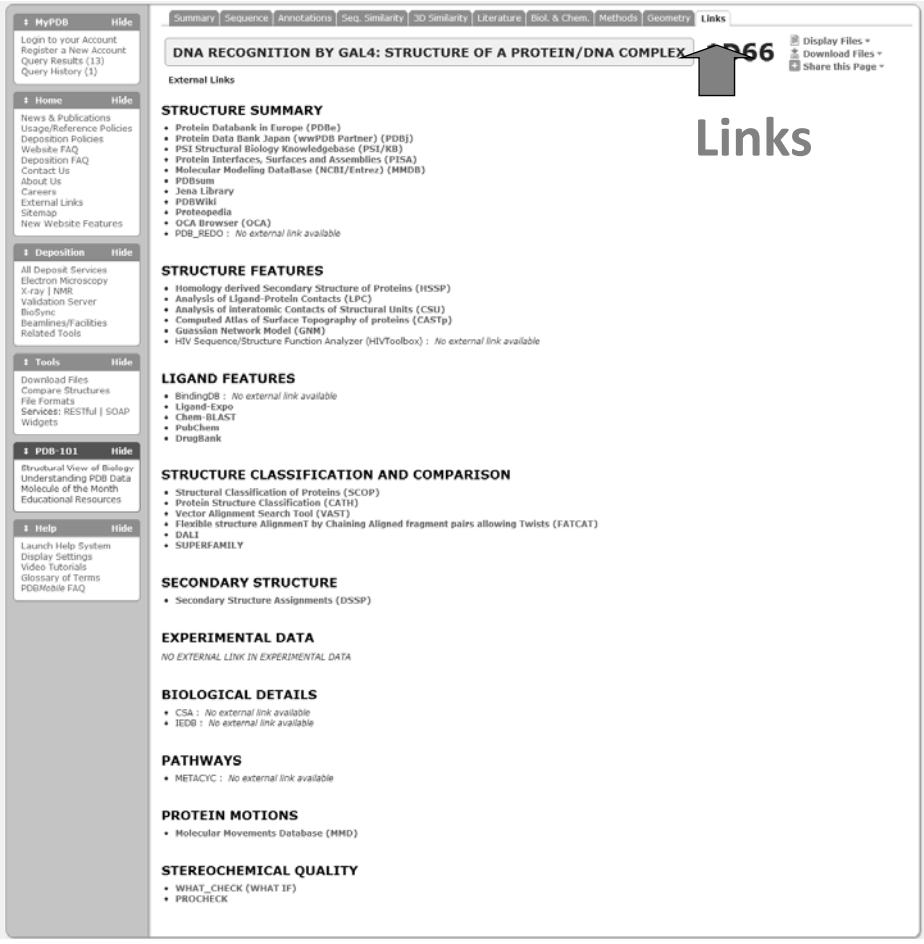
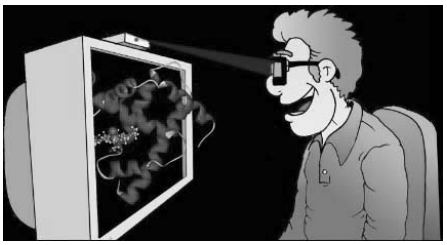
HET    CD   41     1   CADMIUM                          1D66  68
HET    CD   42     1   CADMIUM                          1D66  69
FORMUL  5  CD   4(CD1)                                  1D66  70
FORMUL  6  HOH   *51(H2 O1)                            1D66  71
HELIX   1 H1A CYS A  11  LYS A  18  1 RESIDUE 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
```

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(□□s□□□□□□phi□)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



- MDL Chime
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- Raster3D
- GRASP
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Thanks for your attentions.