# PROTEIN DATE BANK

高宏博
冯华朋
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RCSB Research Collaboratory for Structural Bioinformatics

RCSB PDB PROTEIN DATA BANK

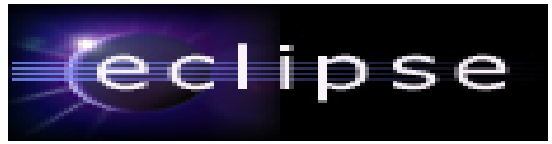
PDB于1971年建于位于美国长岛的Brookhaven国家实验室，于1988年转移到结构生物信息学研究合作组织，是全世界最完整的包括蛋白质，核酸，蛋白质核酸复合物及病毒等生物大分子的三维结构资料库。库中类型包括生物大分子的原子座标、注释、一级结构、二级结构、晶体结构描述和NMR实验资料等。PDB通过评估模型质量和它们与实验数据的吻合程度来证实结构。

# 资金支持


- NSF美国国家科学基金会
- NIGMS国家普通医学科学研究所
- DOE美国能源部
- NLM国家医学图书馆
- NCI国立癌症研究中心
- NCRR国家资源研究中心
- NIBIB国立生物医学影像和生物工程研究所
- NINDS国立神经疾病和卒中研究院
- NIDDK美国国家糖尿病、消化道与肾疾病研究院.

# Powered By


MySQL


eclipse


MOLECULAR
BIOLOGY TOOLKIT


The Jakarta Project
http://jakarta.apache.org


my
eclipse


HIBERNATE


lucene


APACHE ANT


redhat Linux


Struts


axis


ChemAxon


JChem


Java

**Are you missing data updates? The PDB archive has moved to ftp://ftp.wwpdb.org. For more information click here.**

- Home
- Getting Started
- Download Files
- Deposit and Validate
- Structural Genomics
- Dictionaries & File Formats
- Software Tools
- General Education
- Site Tutorials
- BioSync
- General Information
  - About the PDB
  - Citing the PDB
  - News & Publications
  - Related External Links
- Acknowledgements
- Frequently Asked Questions

# Welcome to the RCSB PDB

The RCSB PDB provides a variety of tools and resources for studying the structures of biological macromolecules and their relationships to sequence, function, and disease.

The RCSB is a member of the wwPDB whose mission is to ensure that the PDB archive remains an international resource with uniform data.

This site offers tools for browsing, searching, and reporting that utilize the data resulting from ongoing efforts to create a more consistent and comprehensive archive.

Information about compatible browsers can be found here.

A narrated tutorial illustrates how to search, navigate, browse, generate reports and visualize structures using this new site. [This requires the Macromedia Flash player download.]

Comments? info@rcsb.org

## Molecule of the Month: Circadian Clock Proteins

## News

- Complete News
- Newsletter
- Discussion Foru
- Job Listings

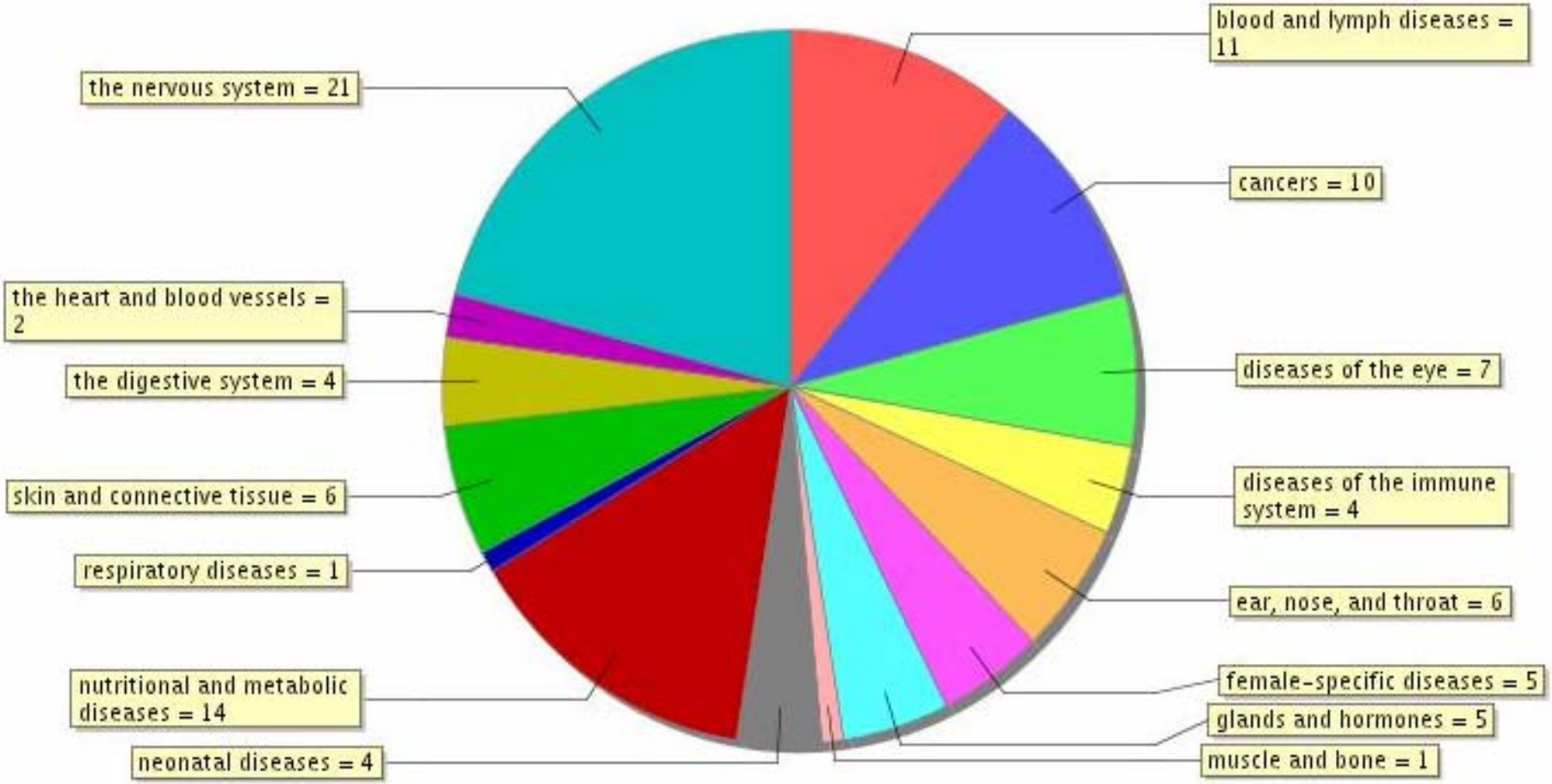
08-January-2008

**sf-convert: A Form Conversion Tool fo Structure Factor Fi**

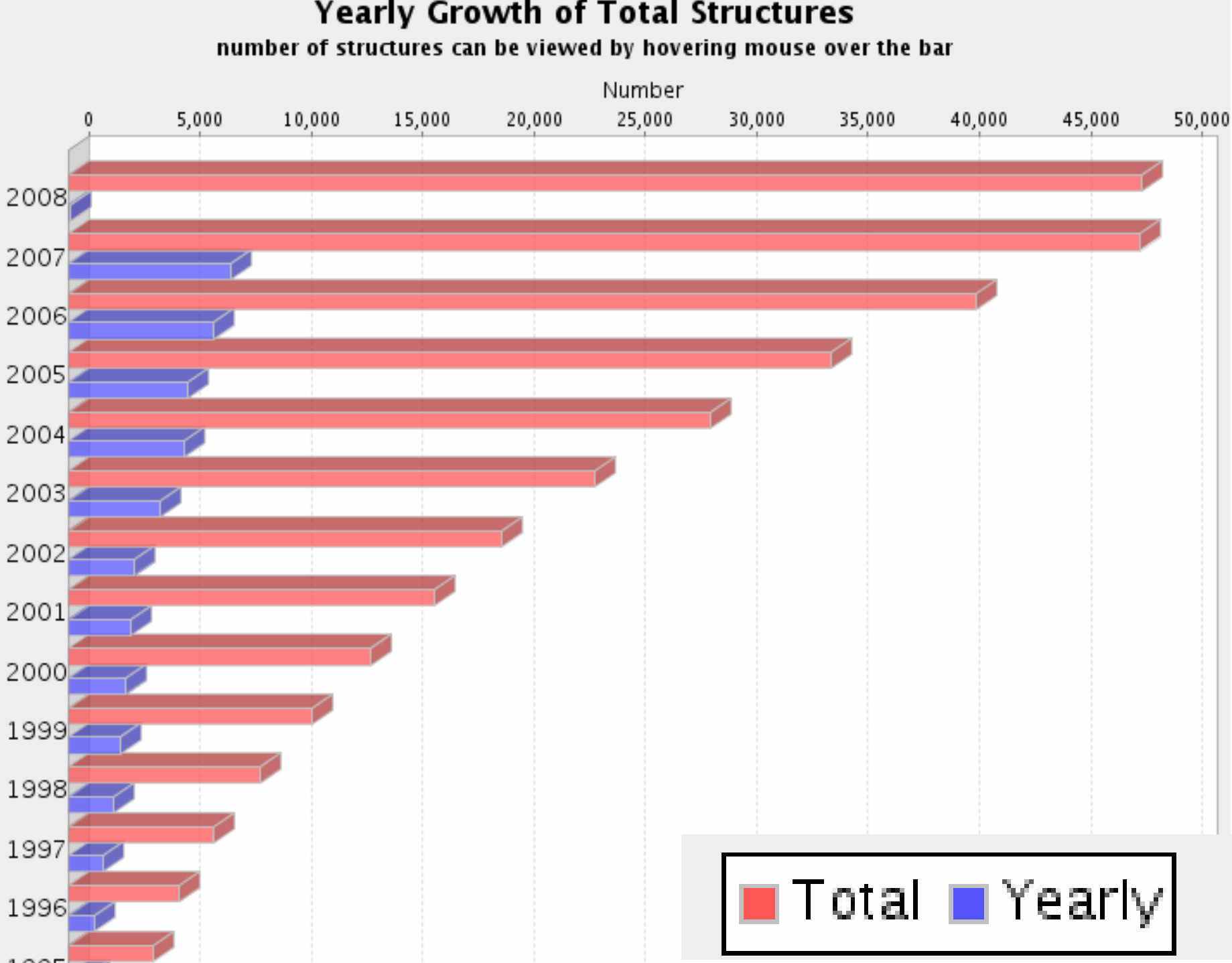
The command-line program sf-convert easily translate data various formats to th mmCIF format for us ADIT validation and deposition software. sf_convert can also translate structure f already released in t PDB from mm different formats.

# 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 Function
  - By Resolution
  - By Space Group
  - By Nature Source Organism
  - By Engineered Source Organism
  - By Top 100 Journals
  - By Structural Genomics Centers
  - By Structure Molecular Weight
  - By Enzyme Classification

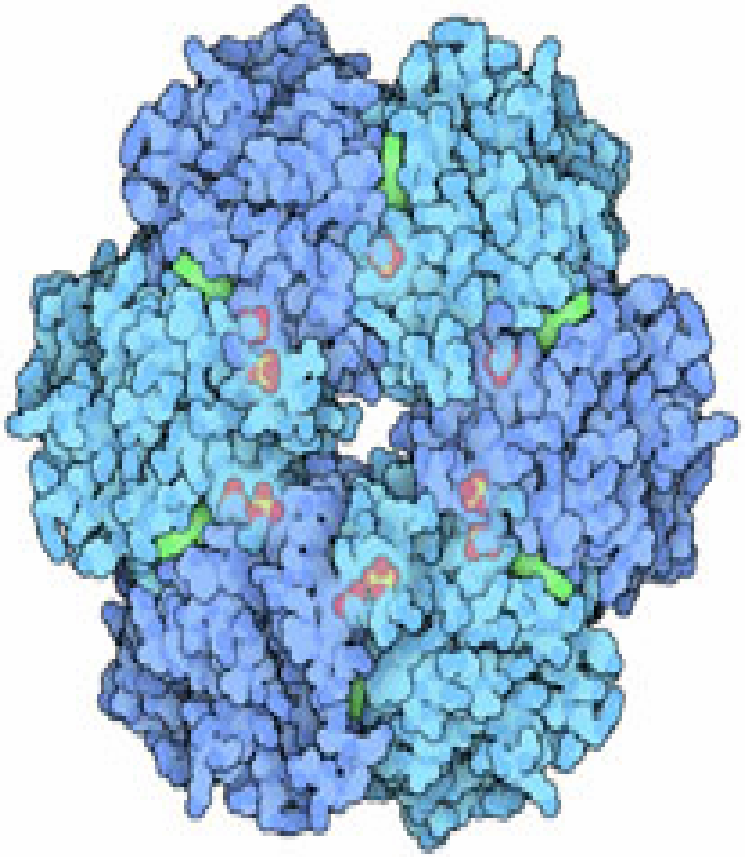

blood and lymph diseases = 11
cancers = 10
diseases of the eye = 7
diseases of the immune system = 4
ear, nose, and throat = 6
female-specific diseases = 5
glands and hormones = 5
muscle and bone = 1
neonatal diseases = 4
nutritional and metabolic diseases = 14
respiratory diseases = 1
skin and connective tissue = 6
the digestive system = 4
the heart and blood vessels = 2
the nervous system = 21

- 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


Yearly Growth of Total Structures
number of structures can be viewed by hovering mouse over the bar
Number
0
5,000
10,000
15,000
20,000
25,000
30,000
35,000
40,000
45,000
50,000
2008
2007
2006
2005
2004
2003
2002
2001
2000
1999
1998
1997
1996
Total
Yearly

# 每月之星-生物钟蛋白

## Molecule of the Month: Circadian Clock Proteins



Our cells contain tiny molecular clocks that measure out a 24-hour circadian rhythm. This clock decides when we get hungry and when we get sleepy. This clock can sense when the days are getting longer and shorter, and then trigger seasonal changes. Our major clock is housed in a small region of the brain, called the suprachiasmic nuclei. It acts as our central pacemaker, checking the cycles of light and dark outside, and then sending signals to synchronize clocks throughout the rest of the body.

- More ...
- Previous Features

## News

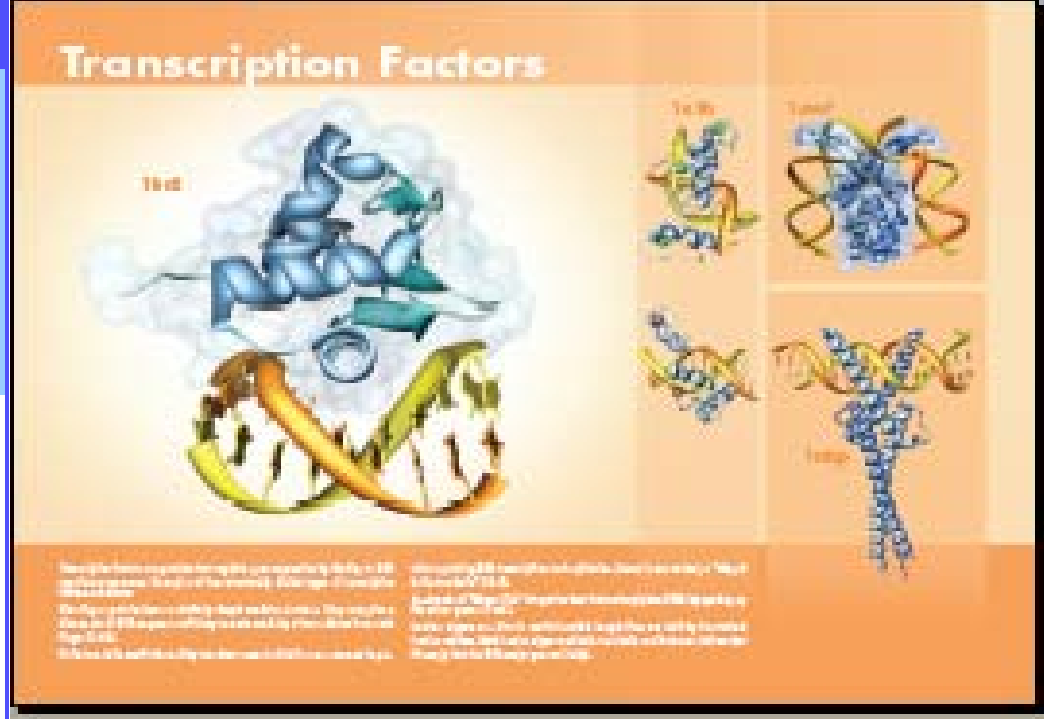
- Complete News
- Newsletter
- Discussion Forum
- Job Listings

08-January-2008

### sf-convert: A Format Conversion Tool for Structure Factor Files

The command-line program sf-convert can easily translate data in various formats to the mmCIF format for use with ADIT validation and deposition software. sf_convert can also translate structure factors already released in the PDB from mmCIF to different formats.

- Full article ...



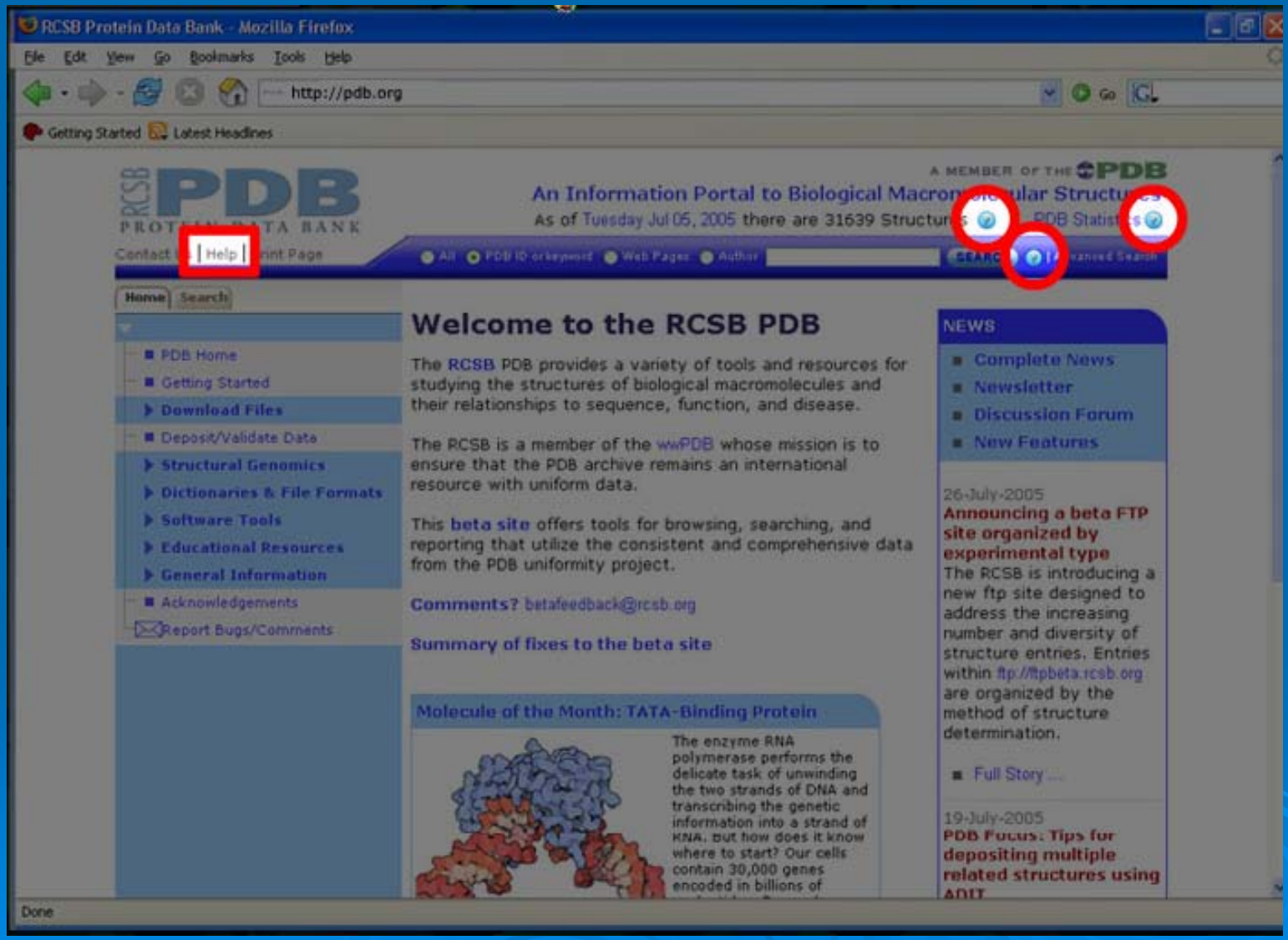

# Getting Started

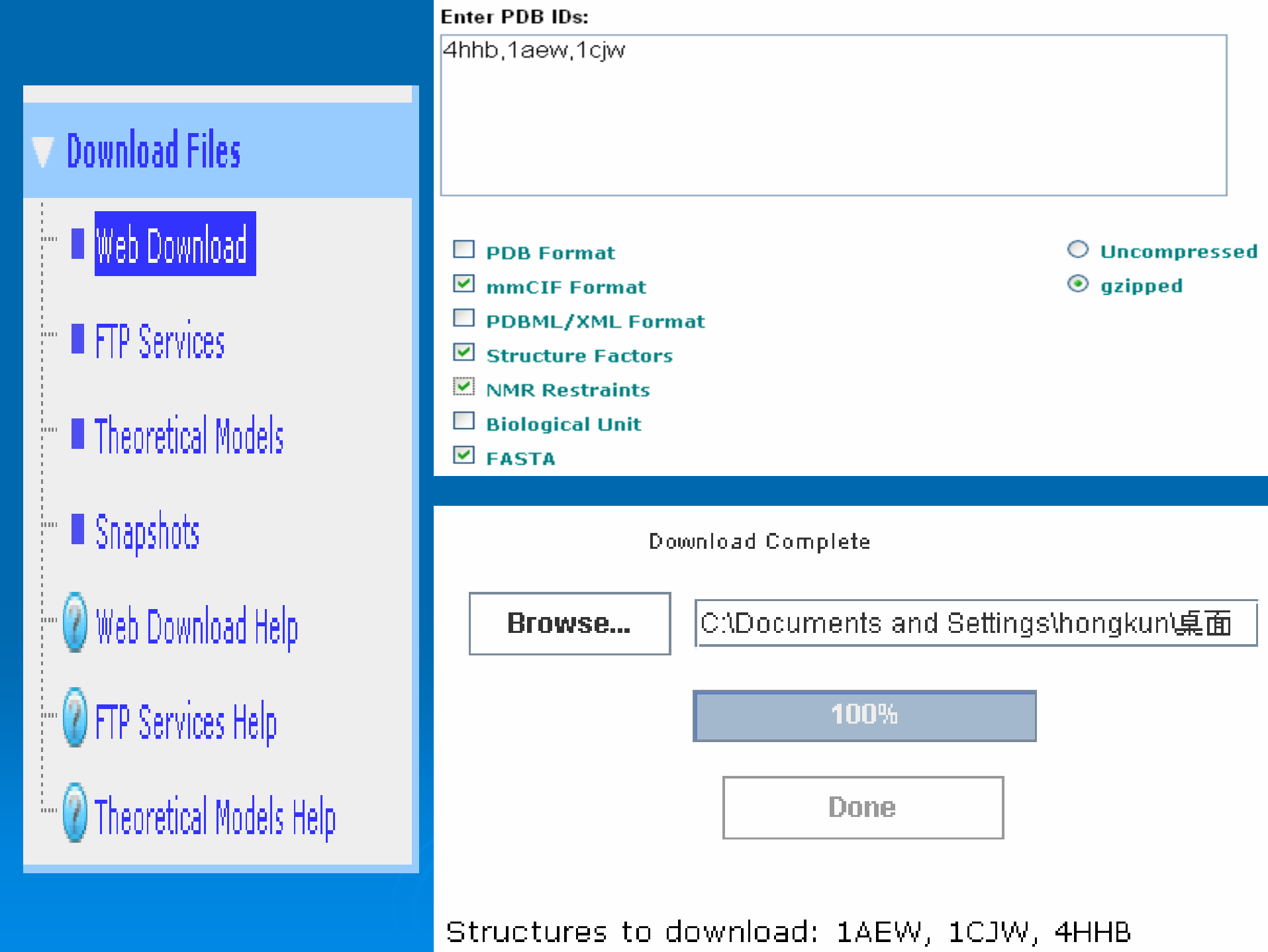
- What do I need to begin?
- How do I navigate the site?
- Where can I get help?

The following topics may also help you to get started:

- Introduction to RoboHelp
- How to Java Enable your Browser
- How to Search the Archive
- How to Deposit a Structure
- How to Browse the Archive
- PDB Frequently Asked Questions

# narrated tutorial illustrates




Download Files
Web Download
FTP Services
Theoretical Models
Snapshots
Web Download Help
FTP Services Help
Theoretical Models Help
Enter PDB IDs:
4hhb,1aew,1cjw
PDB Format
mmCIF Format
PDBML/XML Format
Structure Factors
NMR Restraints
Biological Unit
FASTA
Uncompressed
gzipped
Download Complete
Browse...
C:\Documents and Settings\hongkun\桌面
100%
Done
Structures to download: 1AEW, 1CJW, 4HHB


data deposition tools

- Prepare: pdb_cxtract1 desktop version of ADIT Crystallographic Data Validation
- Validate:Validation Server at PDB or PDBj
- Deposit:beta-ADIT at PDB or ADIT at PDBj or AutoDep at MSD-EBI.

# Validation Server

Validation Tutorial | File Format Information | Possible Format Problems
Validation Server at PDBj

The ADIT Validation Server allows the user to check the format consistency of coordinates (PRECHECK) and to create validation reports about a stru
before deposition (VALIDATION). These checks can be done independently by the user.

To **start a new** validation session, select the experimental method (X-ray or NMR) from the pull-down menus below, and press the **BEGIN** button.

| **Method:** | X-ray | BEGIN |
|---|---|---|

Questions, comments, and suggestions should be sent to help@deposit.rcsb.org.

Enter coordinate file name: [浏览...] Compress (.gz or.Z files) first.
Select file type: ○PDB ○mmCIF

Enter structure factor file name: [浏览...] Compress (.gz or.Z files) first.
Select file type: ○mmCIF ○mtz ○Other ASCII

Choose Operation: ○Precheck ○Validate BEGIN

# Structural Genomics

## Worldwide Initiatives and TargetDB Summary Reports

| PSI Protein Structure Initiative Centers |
| --- |
| **Accelerated Technologies Center for Gene to 3D Structure (ATCG3D) – PSI-2** |
| **The Berkeley Structural Genomics Center (BSGC) – PSI-1**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **The Center for Eukaryotic Structural Genomics (CESG) – PSI-2**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **Center for High-Throughput Structural Biology (CHTSB) – PSI-2**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **Center for Structure of Membrane Proteins (CSMP) – PSI-2**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **The Joint Center for Structural Genomics (JCSG) – PSI-2**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **The Integrated Center for Structure and Function Innovation(ISFI) – PSI-2**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **The Midwest Center for Structural Genomics (MCSG) – PSI-2**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **The NorthEast Structural Genomics Consortium (NESG) – PSI-2**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **New York Consortium on Membrane Protein Structure (NYCOMPS)– PSI-2** |
| **The New York Structural Genomics Research Consortium (NYSGXRC) – PSI-2**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **The Southeast Collaboratory for Structural Genomics (SECSG) – PSI-1**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **Structural Genomics of Pathogenic Protozoa Consortium (SGPP) – PSI-1**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |
| **Mycobacterium tuberculosis Structural Genomics Consortium (TBSGC) – PSI-1**<br>**Reports:** Targets \| Status \| Organisms \| PDB \| Redundancy |

## Protein Structure Initiative Centers

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**Reports:** Targets | Status | Organisms | PDB | Redundancy

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**Reports:** Targets | Status | Organisms | PDB | Redundancy

**Center for High-Throughput Structural Biology (CHTSB) – PSI-2**
**Reports:** Targets | Status | Organisms | PDB | Redundancy

**Center for Structure of Membrane Proteins (CSMP) – PSI-2**
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**Reports:** Targets | Status | Organisms | PDB | Redundancy

## Structural Genomics projects in North America

**Montreal-Kingston Bacterial Structural Genomics Initiative, Canada (BSGI)**
**Reports:** Targets | Status | Organisms | PDB | Redundancy

**Structure 2 Function Project, USA (S2F)**
**Reports:** Targets | Status | Organisms | PDB | Redundancy

## Structural Genomics projects in Asia

**RIKEN Structural Genomics Initiative, Japan (RSGI)**
**Reports:** Targets | Status | Organisms | PDB | Redundancy

# Dictionaries & Files Formats

PDB文件格式为我们提供了一种表示那些由X射线衍射和核磁共振得到的生物大分子结构数据的标准方法。自上世纪70年代创立以来，大量的软件都在使用这种表示方法。

# Software Tools

- **Data Extraction and Deposition Preparation Tools**
- **Data Format Conversion Tools**
- **Data Validation Tools**
- **Data Parsing Tools**
- **Dictionary and Data Management Tools**

# General Education

## What are Proteins and Nucleic Acids?

- **What is a Gene?**
  A basic introduction to genes
  *Audience: Elementary students*

- **How Do Proteins Fold?**
  Methods being applied to crack the protein folding mystery. Requires **RealPlayer**
  *Audience: Undergraduate*

- **Biology as Literature: Learning to Read the Molecular Book of Life**
  Reading the blueprint for living systems that is built on the molecular language contained within cells. Requires **RealPlayer**
  *Audience: Undergraduate*

- **Beginner's Guide to Molecular Biology**
  Introductory course material on molecular biology
  *Audience: Undergraduate*

- **An Introduction to Nucleic Acids**
  Introduction to the chemistry and structure of nucleic acids
  *Audience: Undergraduate*

- **Molecule of the Month**
  A series of short articles by **David Goodsell** on selected molecules
  *Audience: General*

- **The Structures of Life (also available as a PDF)**
  General information from NIGMS on structural biology's insights into health and disease, including brief descriptions of proteins, X-ray crystallography, NMR, and structure-based drug design
  *Audience: High School/Undergraduate*

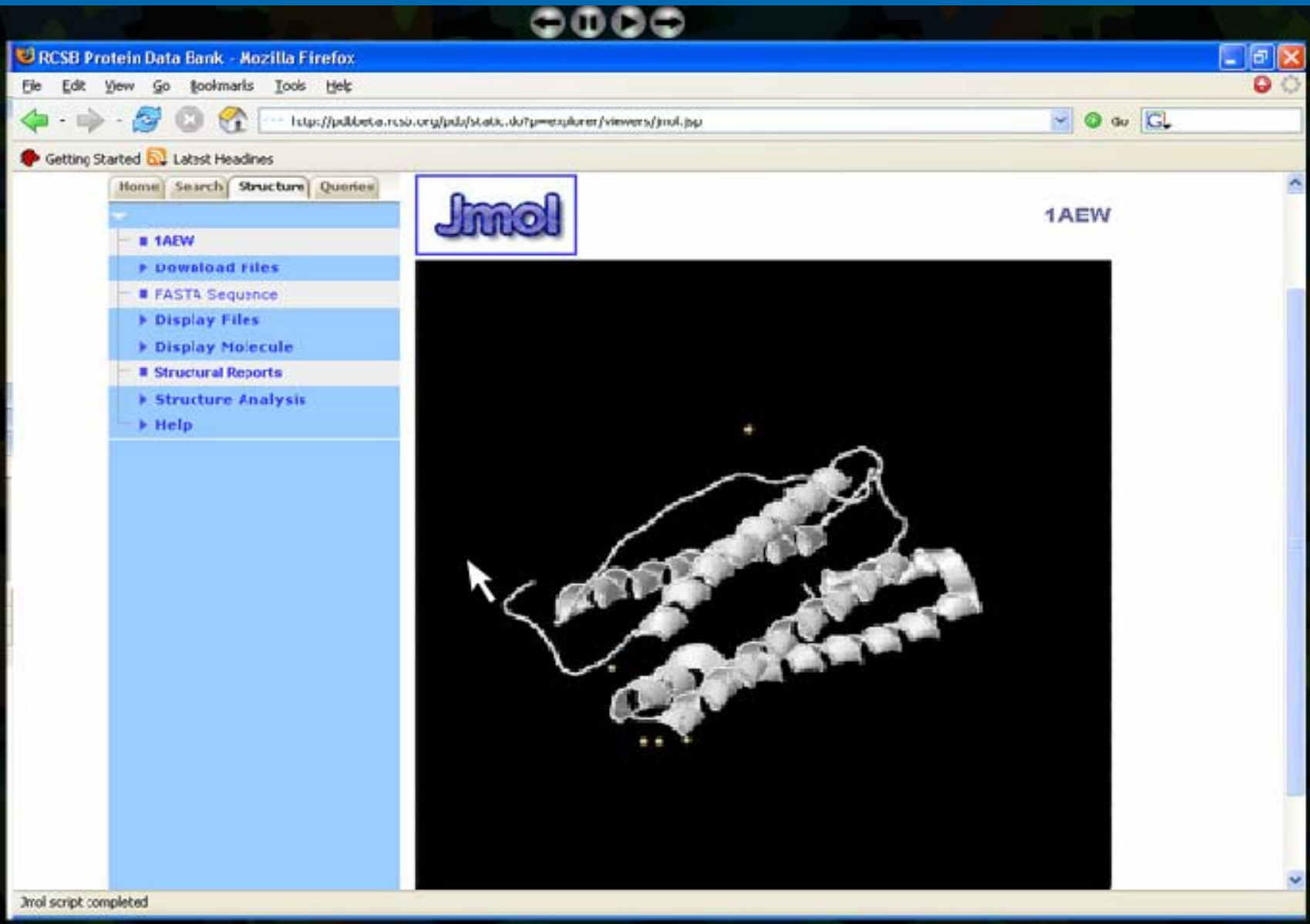
- **S-Star Consortium**
  Bioinformatics courses and lectures by the S-Star consortium
  *Audience: Undergraduate*

- **Nucleic Acid Structure and Recognition**
  Interactive site to compliment the **book** by the same name; uses the free **Chime** plug-in to visualize and examine structure concepts
  *Audience: Graduate*

# How PDB structures are determined

- Origins and limitations of 3D structural data
- X-Ray crystallography
- Solution nuclear magnetic resonance

# Site Tutorials

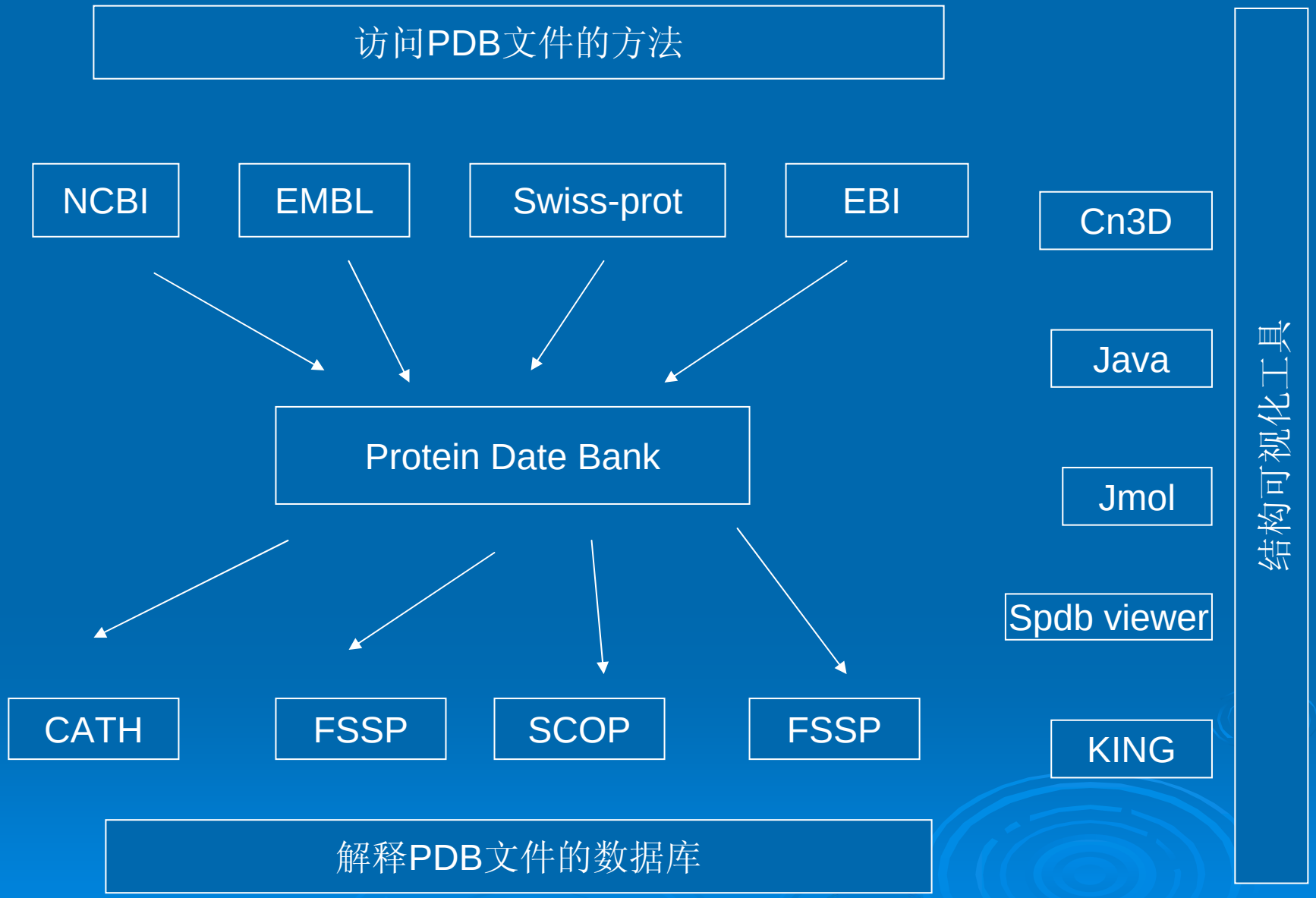



Click and drag structure to rotate. To zoom, hold the ALT button, click and drag up or down.

# General Information

## Databases

- **ABG: Directory of 3D structures of antibodies**
- **AfCS-Nature Signaling Gateway**
  Comprehensive resource for information on cell signaling, including facts about the proteins involved in that process
- **BIND**
  Biomolecular Interaction Network Database
- **BMCD**
  Biological Macromolecule Crystallization
- **BioImage**
  Multidimensional Biological Images (EM)
- **BMRB**
  BioMagResBank (NMR)
- **BRENDA**
  The Comprehensive Enzyme Information System
- **CAZy**
  Carbohydrate-Active enZYmes
- **CCDC**
  Cambridge Crystallographic Data Centre (small molecules)
- **Database of Macromolecular Movements**
- **ENZYME**
  Enzyme Nomenclature
- **Entrez**
  NCBI databases
- **ExPASy**
  Molecular Biology server
- **GeneCards**
  Database on human genes, proteins and diseases
- **GDB**
- **Lipid Data Bank**
  A convenient gateway to the world of lipids and related materials
- **Macromolecular Structure Database**
  MSD-EBI database and search tools
- **Membrane Protein Data Bank**
  A relational database with select structural and functional information on membrane proteins and peptides
- **MEROPS**
  Peptidase Database
- **Metalloprotein Database and Browser**
- **ModBase**
  A database of comparative protein structure models
- **NDB**
  Nucleic Acid Database
- **OCA**
  A browser-database for structure/function
- **PDB at a Glance**
  Classification of the structures in the PDB
- **PDBj**
  Protein Data Bank Japan database and search tools
- **PDBLite**
  Simple PDB search for students and educators
- **PDBOBS**
  Archive of obsolete PDB entries
- **PIR**
  Protein Information Resource
- **PROMISE**
  The Prosthetic groups and Metal Ions in Protein Active Sites Database


访问PDB文件的方法
NCBI
EMBL
Swiss-prot
EBI
Protein Date Bank
CATH
FSSP
SCOP
FSSP
解释PDB文件的数据库
结构可视化工具
Cn3D
Java
Jmol
Spdb viewer
KING

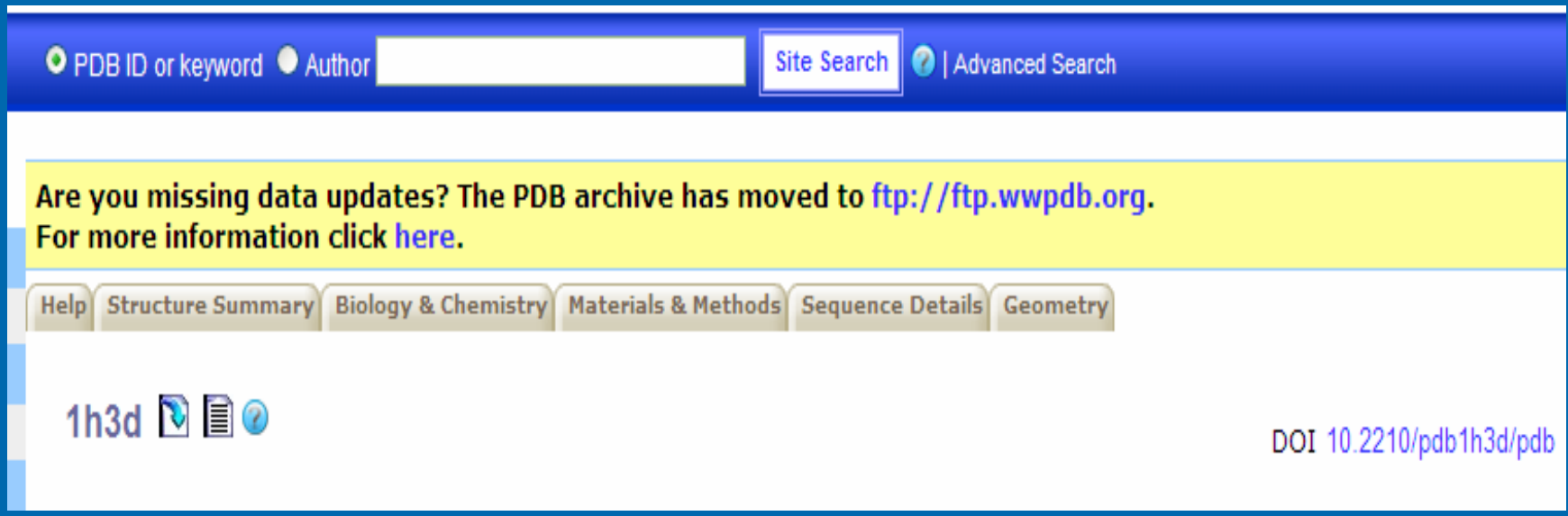
# 可链接到PDB的部分蛋白质结构数据库

| 数据库 | 备注 |
| --- | --- |
| 3dee | 结构域定义 |
| BMCD | 生物大分子晶体信息 |
| CATH | 蛋白质折叠分类 |
| CE | 完整与代表性的PDB结构对比 |
| DSSP | 二级结构分类 |
| Enzyme Structures | 酶的分类及术语 |
| FSSP | 结构相似家族 |
| GRASS | 图标描述与分析 |
| HSSP | 同源二级结构 |
| NDB | 核酸三维结构数据库 |
| SCOP | 结构分类 |
| VAST | NCBI的结构对比工具 |
| MMDB | 三维结构数据库 |

# ATP-phosphoribosyltransferase

- 三磷酸腺苷磷酸核糖转移酶(ATP-PRT) 是组氨酸途径的第一个酶，存在于细胞质中，它是一个复杂的变构调控酶，通过组氨酸途径来控制媒介物的流通。
- 功能：催化ATP和磷酸核糖焦磷酸缩合形成N‘-5’-磷酸核糖ATP (PR-ATP).在组氨酸途径中起着关键的作用。

# ATP-PRT的PDB ID是1H3D

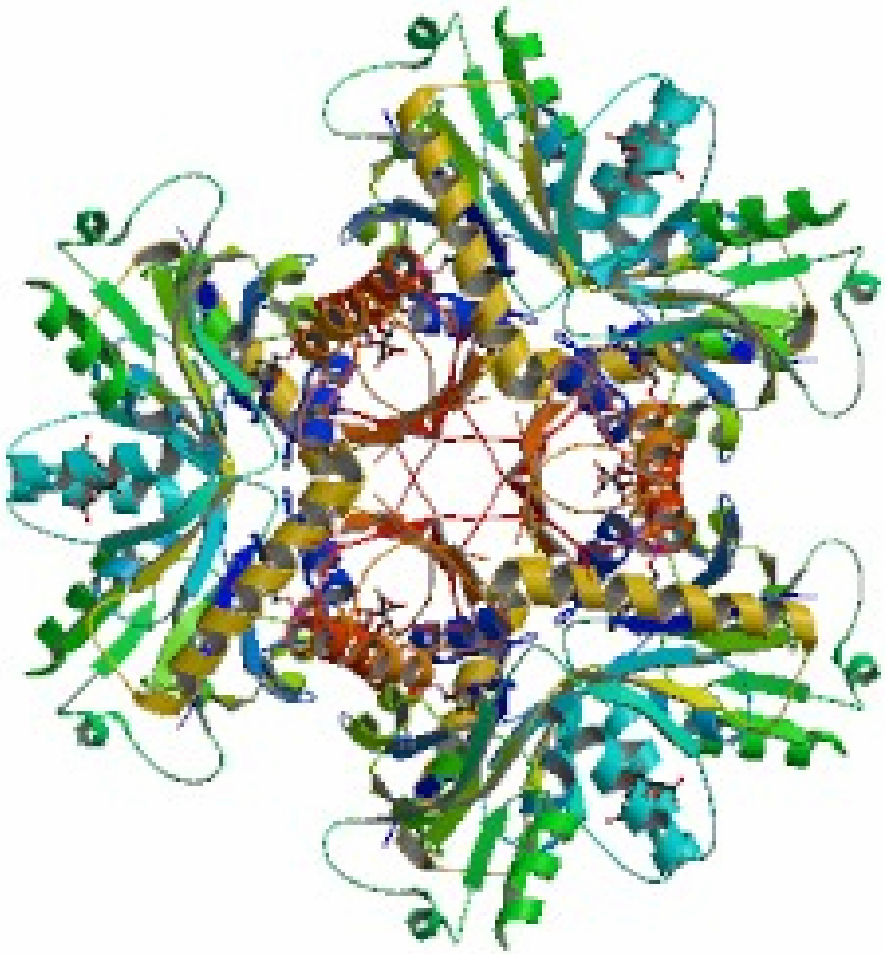



- 通过点击箭头可以下载1H3D的pdb格式的序列信息，从而可以在swiss-pdbviewer中对其立体结构进行研究。

- Structure summary
- Biology & Chemistry
- Materials $ Methods
- Sequence Details
- Geometry
- Images and Visualization

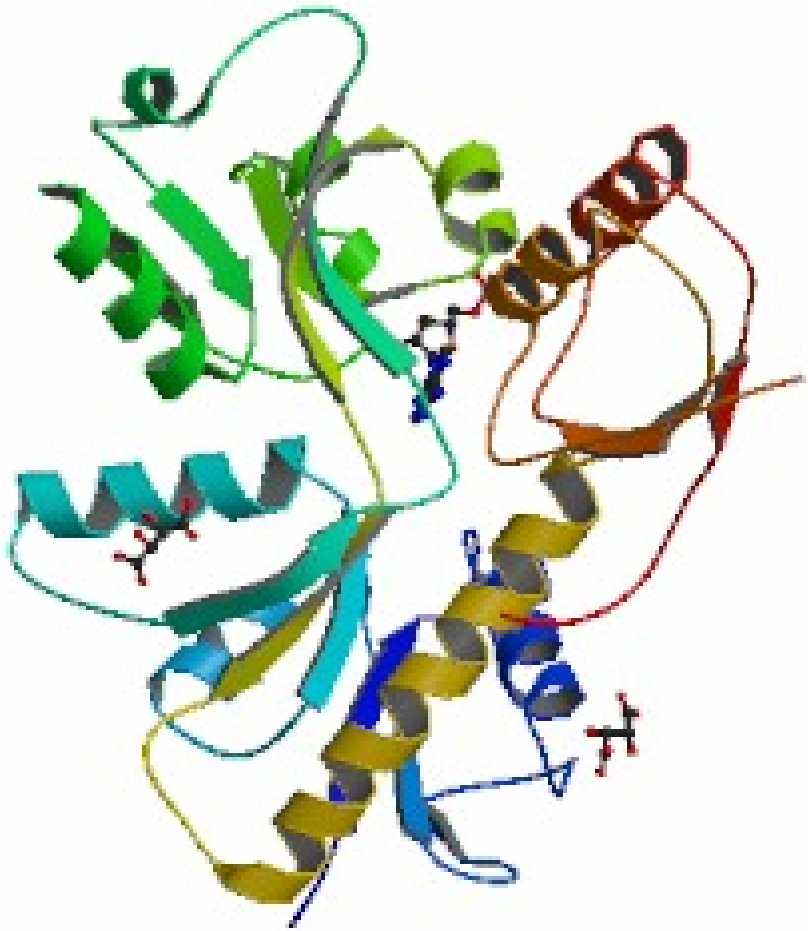
## Images and Visualization

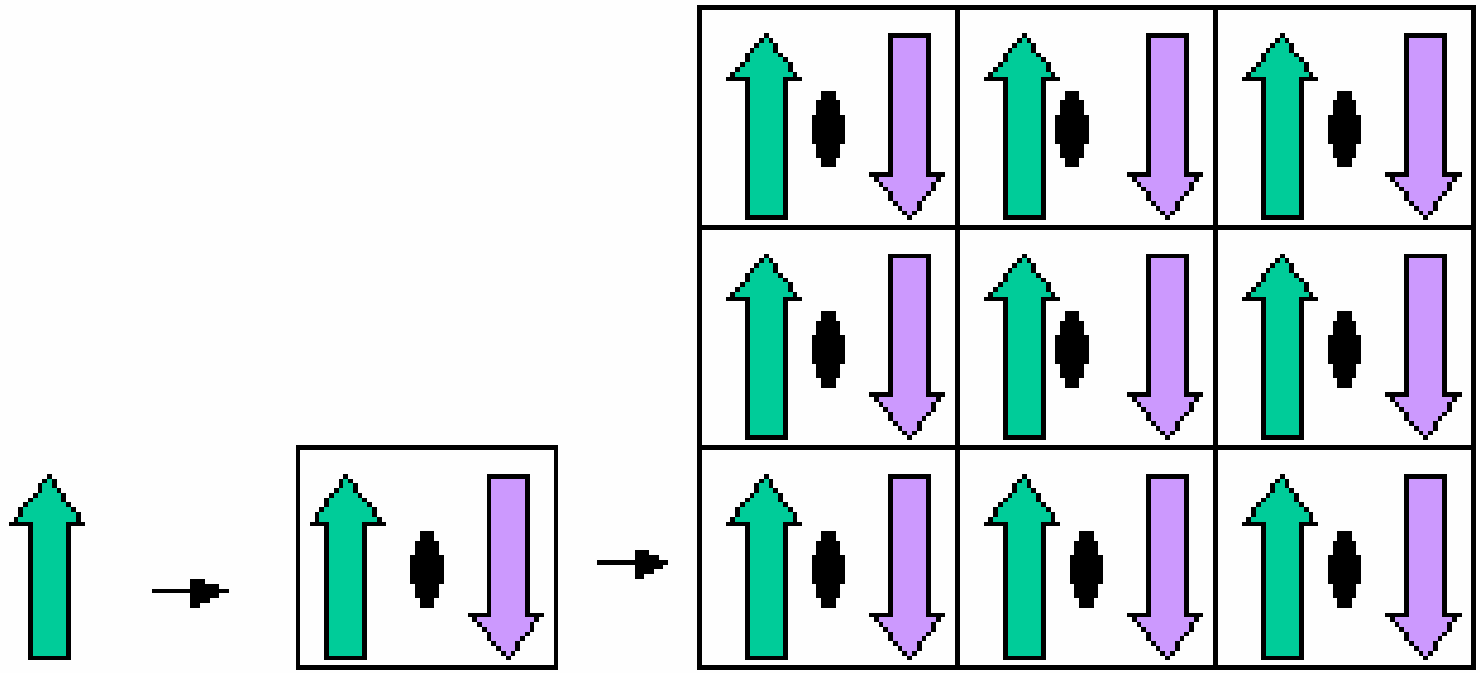
<< Biological Molecule >>



## Images and Visualization

<< Asymmetric Unit >>




Asymmetric Unit
Unit Cell
Entire Crystal

Structure summery包括基本和推导数据，蓝色部分为基本数据，数据由实验直接测得；红色部分为导出数据，或叫二级数据，来自基本数据的解释。

# Structure summery page

| | |
|---|---|
| **Title** | STRUCTURE OF THE E.COLI ATP-PHOSPHORIBOSYLTRANSFERASE |
| **Authors** | Lohkamp, B., Mcdermott, G., Coggins, J.R., Lapthorn, A.J. |
| **Primary Citation** | **Lohkamp, B., McDermott, G., Campbell, S.A., Coggins, J.R., Lapthorn, A.J.** (2004) The structure of Escherichia coli ATP-phosphoribosyltransferase: identification of substrate binding sites and mode of AMP inhibition. *J.Mol.Biol.* *336: 131-144* [ Abstract ] |
| **History** | Deposition 2002-08-27 Release 2003-10-03 |
| **Experimental Method** | Type X-RAY DIFFRACTION Data N/A |

**Parameters**

| Resolution[Å] | R-Value | R-Free | Space Group |
|---|---|---|---|
| 2.70 | 0.226 (obs.) | 0.277 | H 3 2 |

**Unit Cell**

| | | | | | | |
|---|---|---|---|---|---|---|
| Length [Å] | a | 133.65 | b | 133.65 | c | 114.12 |
| Angles [°] | alpha | 90.00 | beta | 90.00 | gamma | 120.00 |

**Molecular Description Asymmetric Unit**

Polymer: 1 Molecule: ATP-PHOSPHORIBOSYLTRANSFERASE Chains: A EC no.: 2.4.2.17

**Classification** Transferase

**Source**

Polymer: 1 Scientific Name: **Escherichia coli** Expression system: **Escherichia coli**

**Ligand Chemical Component**

| Identifier | Name | Formula | Drug Similarity |
|---|---|---|---|
| AMP | ADENOSINE MONOPHOSPHATE | $C_{10}H_{14}N_5O_7P$ | |

| Primary Citation | Lohkamp, B., McDermott, G., Campbell, S.A., Coggins, J.R., Lapthorn, A.J. (2004) The structure of Escherichia coli ATP-phosphoribosyltransferase: identification of substrate binding sites and mode of AMP inhibition. *J.Mol.Biol.* *336: 131-144* [ Abstract ] |
|---|---|

**Article Title**
The structure of Escherichia coli ATP-phosphoribosyltransferase: identification of substrate binding sites and mode of AMP inhibition.

**Abstract**
ATP-phosphoribosyltransferase (ATP-PRT), the first enzyme of the histidine pathway, is a complex allosterically regulated enzyme, which controls the flow of intermediates through this biosynthetic pathway. The crystal structures of Escherichia coli ATP-PRT have been solved in complex with the inhibitor AMP at 2.7A and with product PR-ATP at 2.9A (the ribosyl-triphosphate could not be resolved). On the basis of binding of AMP and PR-ATP and comparison with type I PRTs, the PRPP and parts of the ATP-binding site are identified. These structures clearly identify the AMP as binding in the 5-phosphoribosyl-alpha-1-pyrophosphate (PRPP)-binding site, with the adenosine ring occupying the ATP-binding site. Comparison with the recently solved Mycobacterium tuberculosis ATP-PRT structures indicates that histidine is solely responsible for the large conformational changes observed between the hexameric forms of the enzyme. The role of oligomerisation in inhibition and the structural basis for the synergistic inhibition by histidine and AMP are discussed.

**Keywords**
ATP Phosphoribosyltransferase, Adenosine Monophosphate, Amino Acid Sequence, Binding Sites, Catalytic Domain, Escherichia coli, Escherichia coli Proteins, Histidine, Models, Molecular, Molecular Sequence Data, Molecular Structure, Protein Structure, Quaternary, Protein Structure, Tertiary, Sequence Alignment

**Related Structures**
Primary Citation of: **1H3D** **1Q1K**

**Authors**
Lohkamp, B., McDermott, G., Campbell, S.A., Coggins, J.R., Lapthorn, A.J.

**Organizational Affiliation**
Division of Biochemistry and Molecular Biology, Institute of Biomedical and Life Sciences, University of Glasgow, Glasgow, G12 8QQ, Scotland, UK.

**Journal**
J.Mol.Biol. v336 pp. 131-44, 2004

**Pubmed ID**
14741209

***Click on abstract words and keywords to add them to the search box.***
Histidine Submit Query

| SCOP Classification (version 1.71) | Domain Info | Class | Fold | Superfamily | Family | Domain | Species |
|---|---|---|---|---|---|---|---|
| | d1h3da1 | Alpha and beta proteins (a/b) | Periplasmic binding protein-like II | Periplasmic binding protein-like II | Phosphate binding protein-like | ATP phosphoribosyltransferase (ATP-PRTase, HisG), catalytic domain | Escherichia coli |
| | d1h3da2 | Alpha and beta proteins (a+b) | Ferredoxin-like | GlnB-like | ATP phosphoribosyltransferase (ATP-PRTase, HisG), regulatory C- terminal domain | ATP phosphoribosyltransferase (ATP-PRTase, HisG), regulatory C- terminal domain | Escherichia coli |

- 在数据部分中，蓝色字部分可以作为新的关键词查询，如Ferredoxin-like 铁氧化还原样蛋白

☑ 1a0o

## CHEY-BINDING DOMAIN OF CHEA IN COMPLEX WITH CHEY

*Characteristics* Release Date: 30-Dec-1998 Exp. Method: X Ray Diffraction
Resolution: 2.95 Å

*Classification* Chemotaxis

*Compound* Polymer: 1 Molecule: CHEY Chains: A,C,E,G
Polymer: 2 Molecule: CHEA Fragment: CHEA 124-257 Chains: B,D,F,H EC no.: 2.7.3.-

*Authors* Welch, M., Chinardet, N., Mourey, L., Birck, C., Samama, J.P.

☑ 1a6l

## T14C MUTANT OF AZOTOBACTER VINELANDII FDI

*Characteristics* Release Date: 27-May-1998 Exp. Method: X Ray Diffraction
Resolution: 2.10 Å

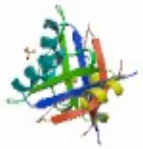
*Classification* Electron Transport

*Compound* Polymer: 1 Molecule: FERREDOXIN Mutation: T14C Chains: A

*Authors* Gao-Sheridan, H.S., Kemper, M.A., Khayat, R., Tilley, G.J., Armstrong, F.A., Sridhar, V., Prasad, G.S., Stout, C.D., Burgess, B.K.

☑ 1a7g

## THE CRYSTAL STRUCTURE OF THE E2 DNA-BINDING DOMAIN FROM HUMAN PAPILLOMAVIRUS AT 2.4 ANGSTROMS



*Characteristics* Release Date: 27-Apr-1999 Exp. Method: X Ray Diffraction
Resolution: 2.40 Å

*Classification* Transcription Regulation

*Compound* Polymer: 1 Molecule: REGULATORY PROTEIN E2 Fragment: DNA-BINDING DOMAIN Chains: E

*Authors* Bussiere, D.E., Kong, X., Egan, D.A., Walter, K., Holzman, T.F., Lindh, F., Robins, T., Giranda, V.L.

☑ 1a9n

## CRYSTAL STRUCTURE OF THE SPLICEOSOMAL U2B''-U2A' PROTEIN COMPLEX BOUND TO A FRAGMENT OF U2 SMALL NUCLEAR RNA

*Characteristics* Release Date: 23-Sep-1998 Exp. Method: X Ray Diffraction
Resolution: 2.38 Å

*Classification* RNA Binding Protein/rna

- **Biology & Chemistry** 中包括结构详细信息、蛋白详细信息、基因详细信息及相关文章详细信息
- 1.结构详细信息： 结构关键词、多聚体分子、配体及辅基。
- 2.蛋白详细信息: UniProt 信息、功能域.
- 3.基因详细信息:基因来源.基因组信息
- 4.相关文章详细信息: Pubmed ID、主题词、文章网络.
- 以上详细信息都可以通过点击斜向上的箭头直接连接到其它相关数据库.
- **Materials & Methods** 包括:X射线材料及方法报道、晶体数据、衍射、软件及计算等

- **Sequence Details** 中包括蛋白名称、链类型、Uniprot索引号、长度、SCOP结构域分配、DSSP二级结构及其它一些信息。

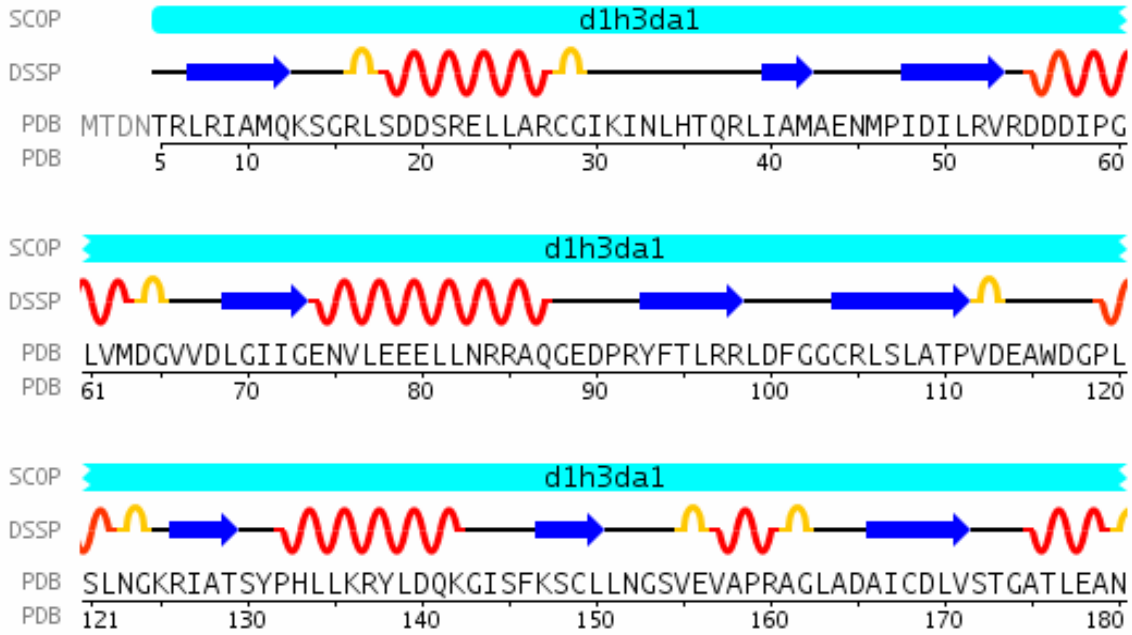
- **Geometry** 包括结构方差分析、键长、键角、二面角等信息。

# Sequence Details

**Chain A** (polymer 1)

| | |
|---|---|
| **Description** | ATP-PHOSPHORIBOSYLTRANSFERASE |
| **Chain Type** | polypeptide(L) |
| **UniProt reference** | P60757<br>[show this sequence below] |
| **Length** | 299 residues |
| **SCOP domain assignment**<br>[hide] [reference] | d1h3da1 ATP phosphoribosyltransferase (ATP-PRTase, HisG), catalytic domain: 220 residues<br>d1h3da2 ATP phosphoribosyltransferase (ATP-PRTase, HisG), regulatory C-terminal domain: 68 residues |
| **DSSP secondary structure**<br>[hide] [reference] | 31% helical (11 helices; 95 residues)<br>25% beta sheet (16 strands; 77 residues) |
| **More annotations** | |

Select



# PDB图形分析软件

KiNG

Jmol

Webmol

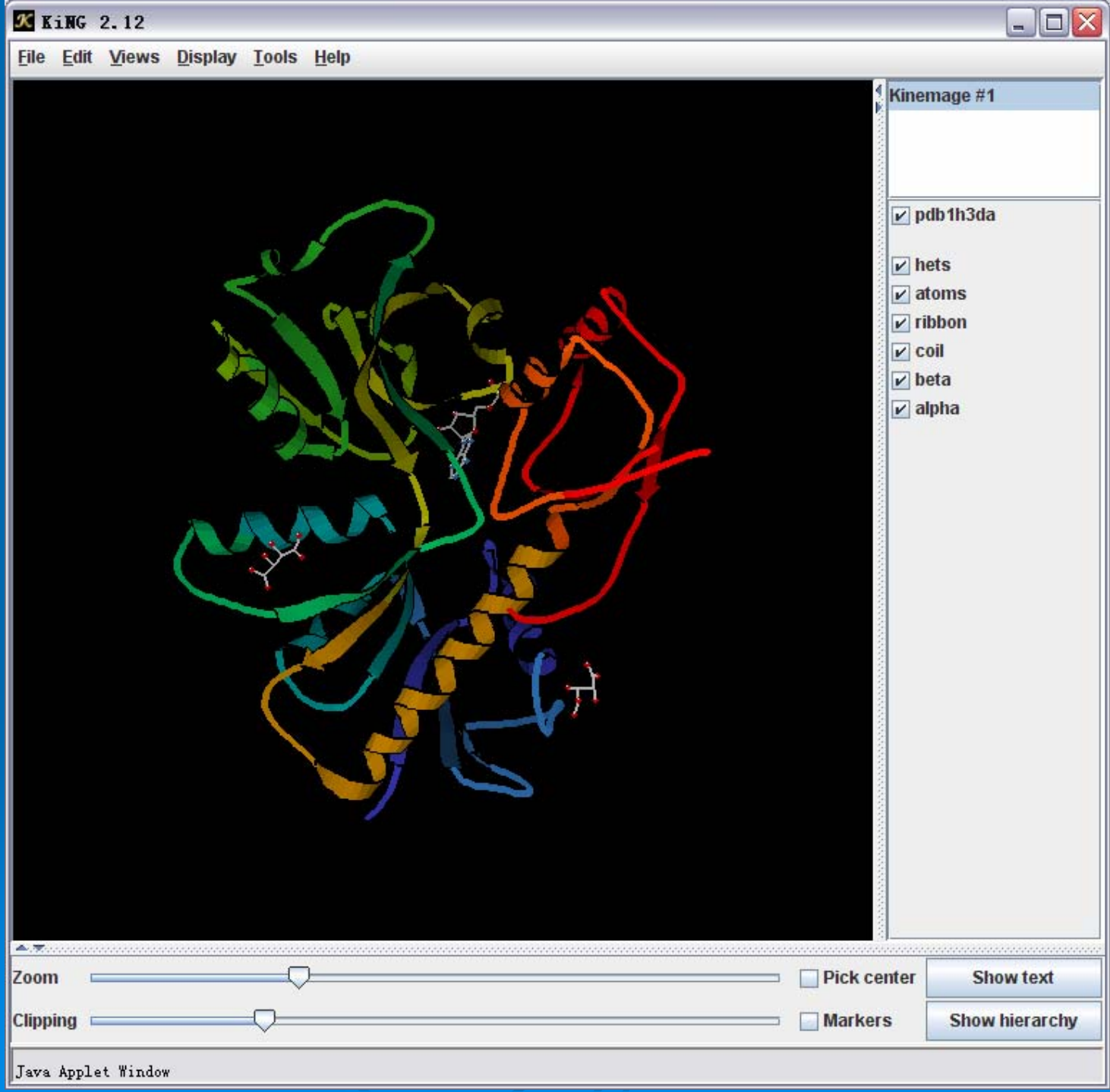
MBT SimpleViewer & Protein Workshop

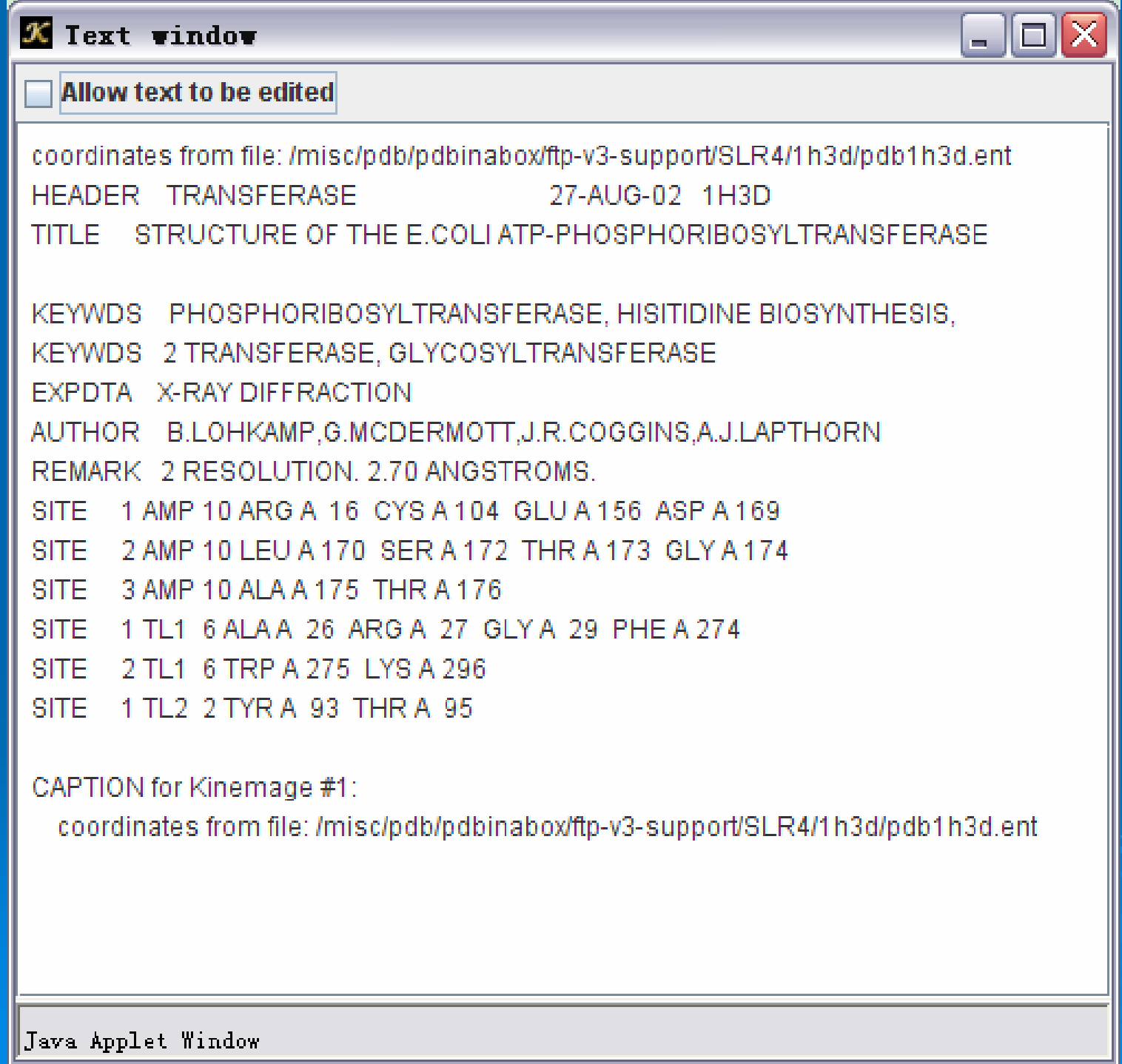
QuickPDB

# KiNG

软件优点：可操作性强；功能丰富；图形显示比较好

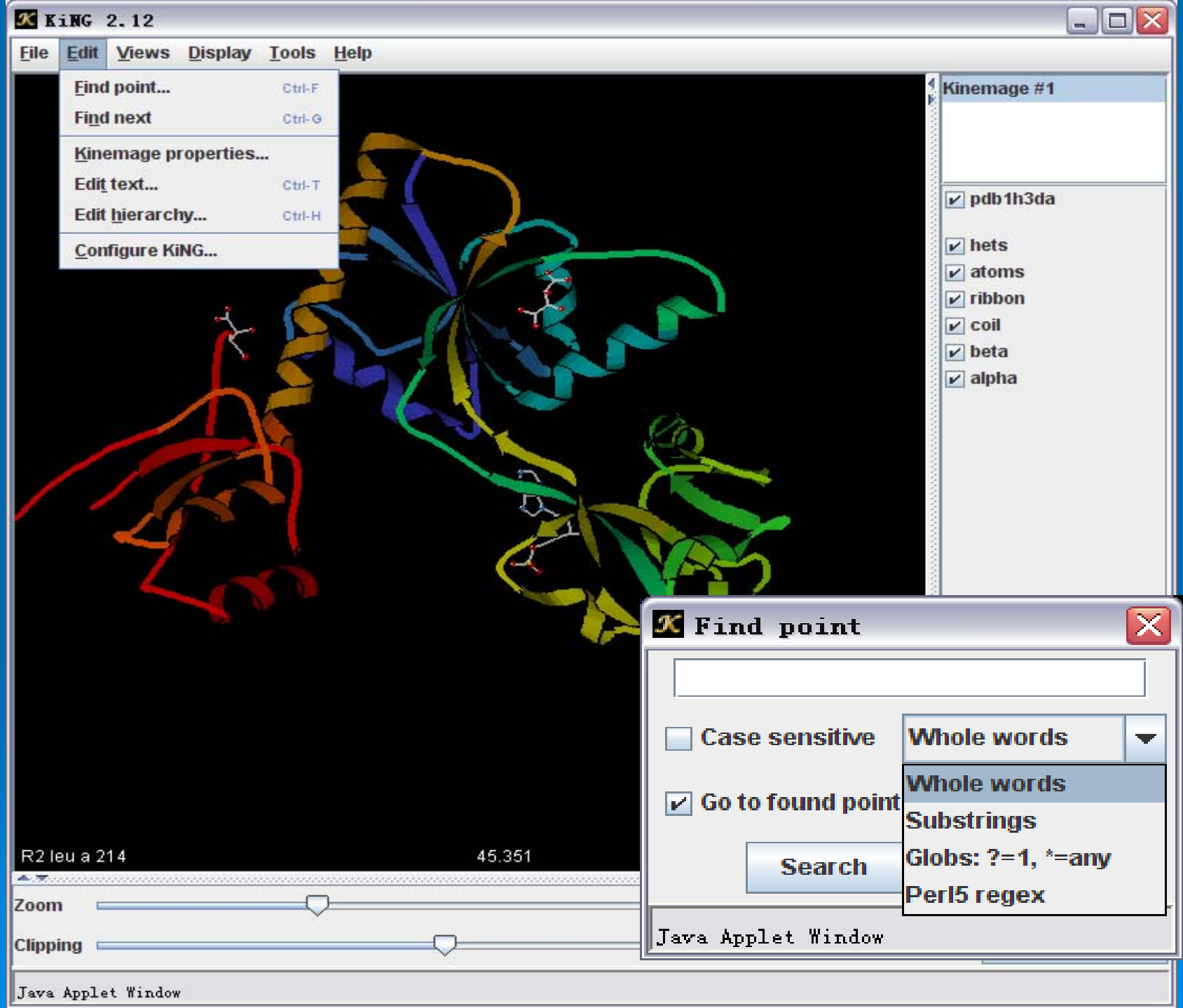
软件缺点：没有列出蛋白质的所有氨基酸残基；距离和角度测量后没有显示所测的氨基酸残基


KiNG 2.12
File Edit Views Display Tools Help
Kinemage #1
pdb1h3da
hets
atoms
ribbon
coil
beta
alpha
Zoom
Clipping
Pick center
Markers
Show text
Show hierarchy
Java Applet Window


Text window
Allow text to be edited
coordinates from file: /misc/pdb/pdbinabox/ftp-v3-support/SLR4/1h3d/pdb1h3d.ent
HEADER TRANSFERASE 27-AUG-02 1H3D
TITLE STRUCTURE OF THE E.COLI ATP-PHOSPHORIBOSYLTRANSFERASE
KEYWDS PHOSPHORIBOSYLTRANSFERASE, HISITIDINE BIOSYNTHESIS,
KEYWDS 2 TRANSFERASE, GLYCOSYLTRANSFERASE
EXPDTA X-RAY DIFFRACTION
AUTHOR B.LOHKAMP,G.MCDERMOTT,J.R.COGGINS,A.J.LAPTHORN
REMARK 2 RESOLUTION. 2.70 ANGSTROMS.
SITE 1 AMP 10 ARG A 16 CYS A 104 GLU A 156 ASP A 169
SITE 2 AMP 10 LEU A 170 SER A 172 THR A 173 GLY A 174
SITE 3 AMP 10 ALA A 175 THR A 176
SITE 1 TL1 6 ALA A 26 ARG A 27 GLY A 29 PHE A 274
SITE 2 TL1 6 TRP A 275 LYS A 296
SITE 1 TL2 2 TYR A 93 THR A 95
CAPTION for Kinemage #1:
coordinates from file: /misc/pdb/pdbinabox/ftp-v3-support/SLR4/1h3d/pdb1h3d.ent
Java Applet Window

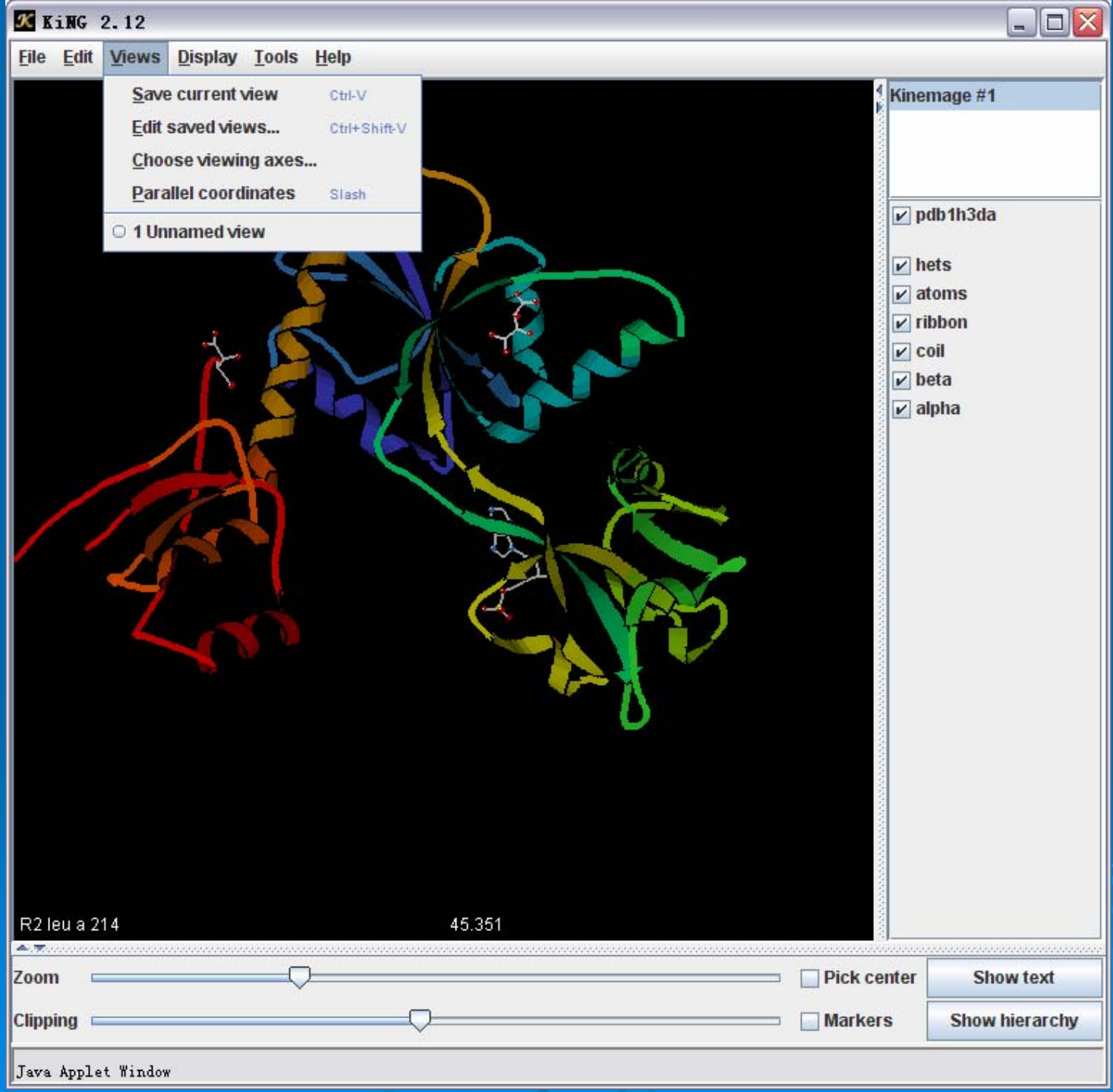
# 常用基本操作：

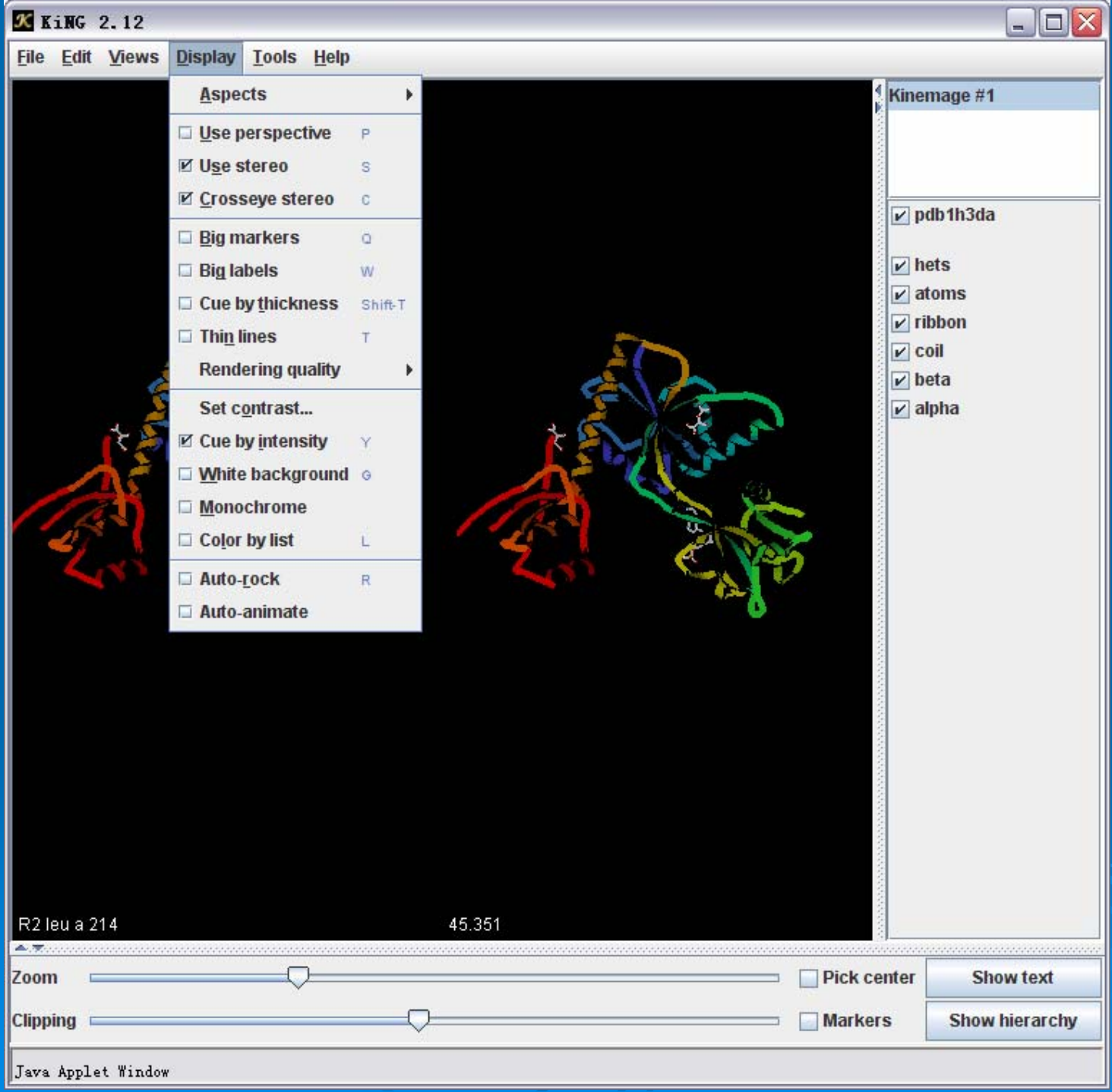
旋转： 鼠标拖动。
移动：ctrl+鼠标左键拖拉 or alt+鼠标左键拖动。
放大缩小： 鼠标滚轮 or shift+鼠标左键拖动 or 鼠标右键垂直拖动。
沿Z轴旋转：在图形顶端拖动
图形位于中心： 鼠标右键 or shift+鼠标左键


KiNG 2.12
File
Edit
Views
Display
Tools
Help
Find point... Ctrl-F
Find next Ctrl-G
Kinemage properties...
Edit text... Ctrl-T
Edit hierarchy... Ctrl-H
Configure KiNG...
Kinemage #1
pdb1h3da
hets
atoms
ribbon
coil
beta
alpha
R2 leu a 214
45.351
Zoom
Clipping
Find point
Case sensitive
Whole words
Whole words
Substrings
Globs: ?=1, *=any
Perl5 regex
Go to found point
Search
Java Applet Window
Java Applet Window

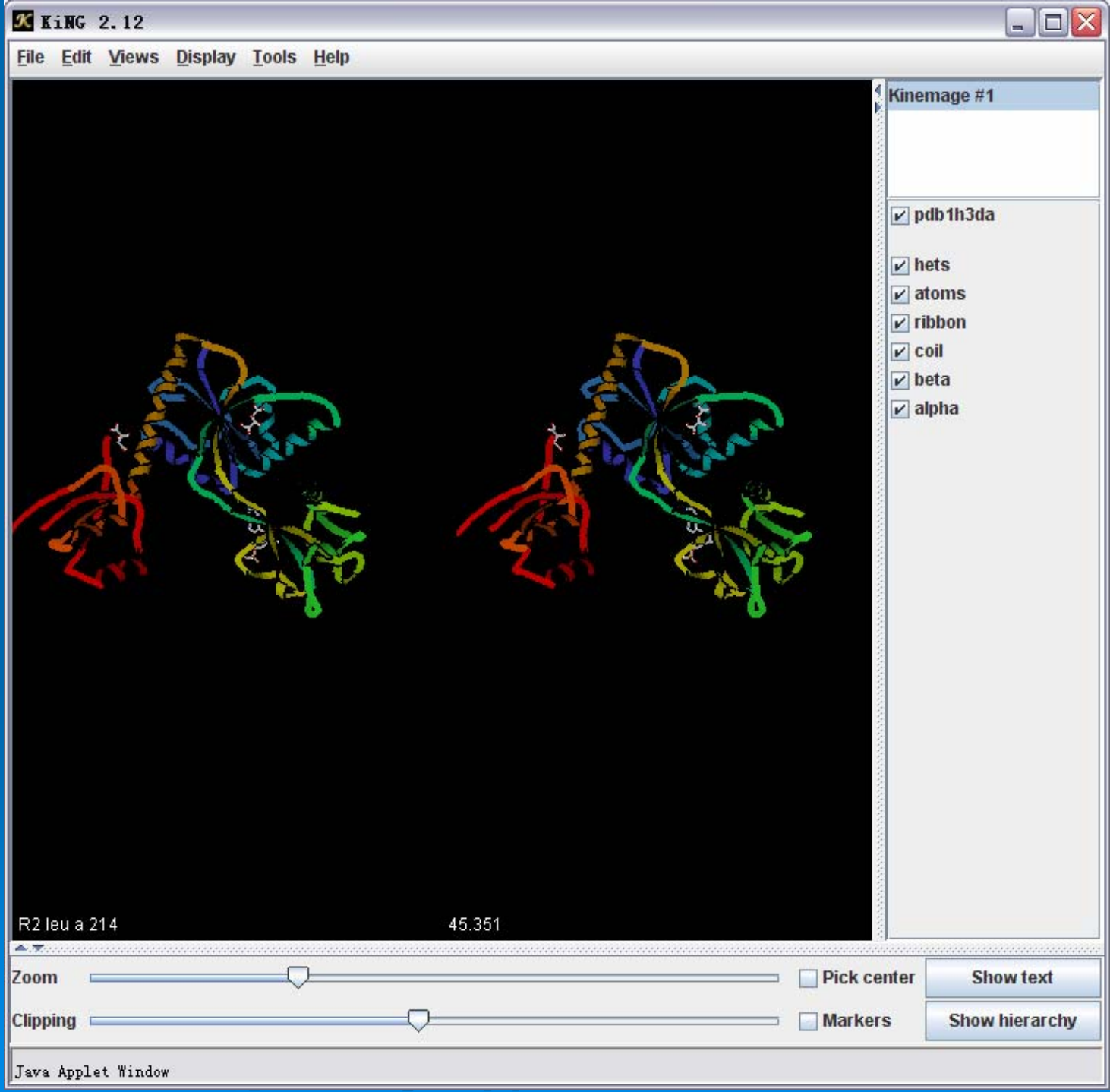
Whole words 是最简单的搜寻模式，会搜出包含输入词的所有氨基酸残基。输入词的顺序不影响输入结果。

Substrings类似于Whole words，会搜出包含输入词的所有氨基酸残基，顺序影响输入结果。


KiNG 2.12
File Edit Views Display Tools Help
Save current view Ctrl-V
Edit saved views... Ctrl+Shift-V
Choose viewing axes...
Parallel coordinates Slash
1 Unnamed view
Kinemage #1
pdb1h3da
hets
atoms
ribbon
coil
beta
alpha
R2 leu a 214
45.351
Zoom
Clipping
Pick center
Markers
Show text
Show hierarchy
Java Applet Window


KiNG 2.12
File Edit Views Display Tools Help
Aspects
Use perspective P
Use stereo S
Crosseye stereo C
Big markers Q
Big labels W
Cue by thickness Shift-T
Thin lines T
Rendering quality
Set contrast...
Cue by intensity Y
White background G
Monochrome
Color by list L
Auto-rock R
Auto-animate
Kinemage #1
pdb1h3da
hets
atoms
ribbon
coil
beta
alpha
R2 leu a 214
45.351
Zoom
Clipping
Pick center
Markers
Show text
Show hierarchy
Java Applet Window

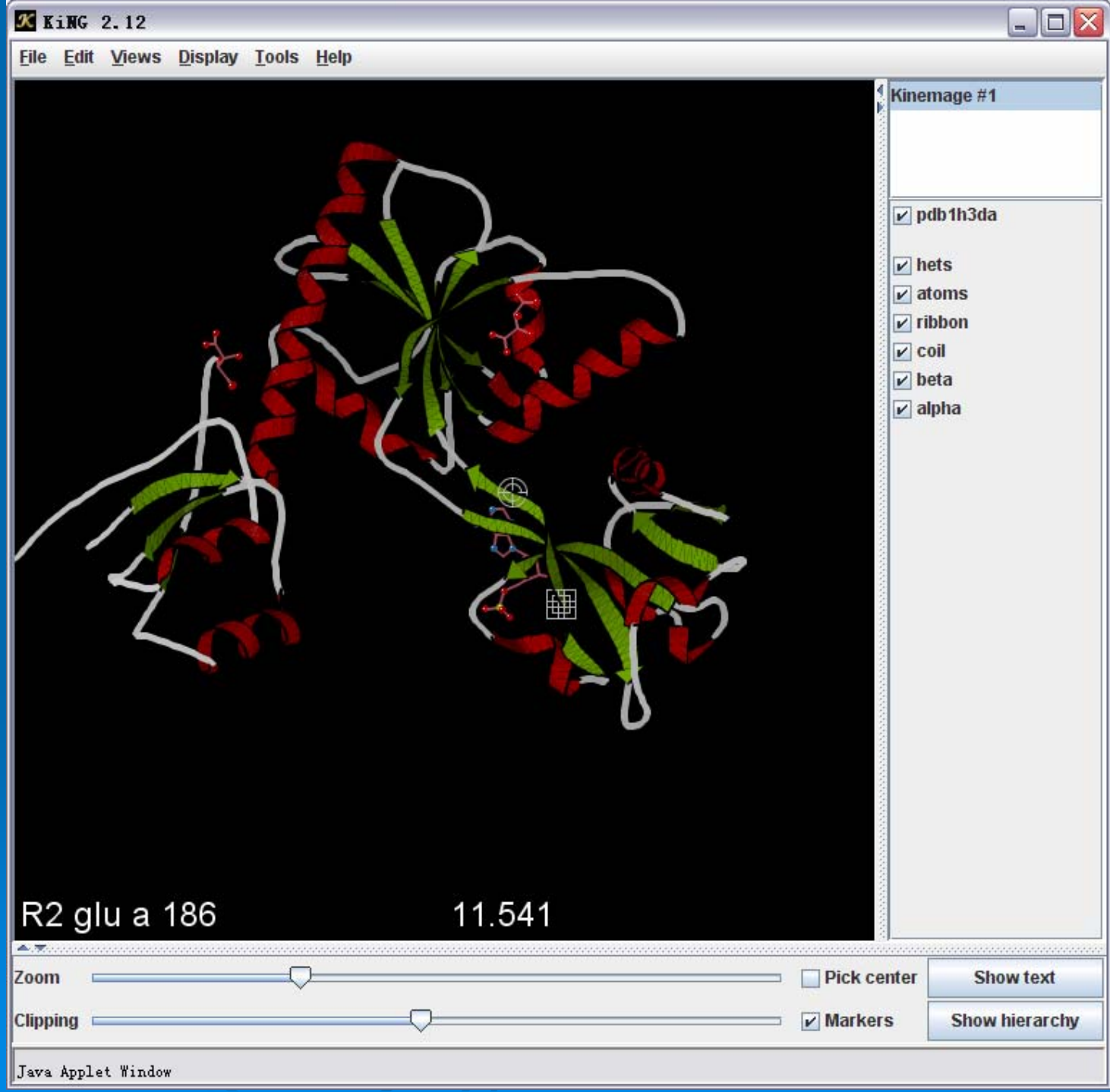
Crosseye stereo

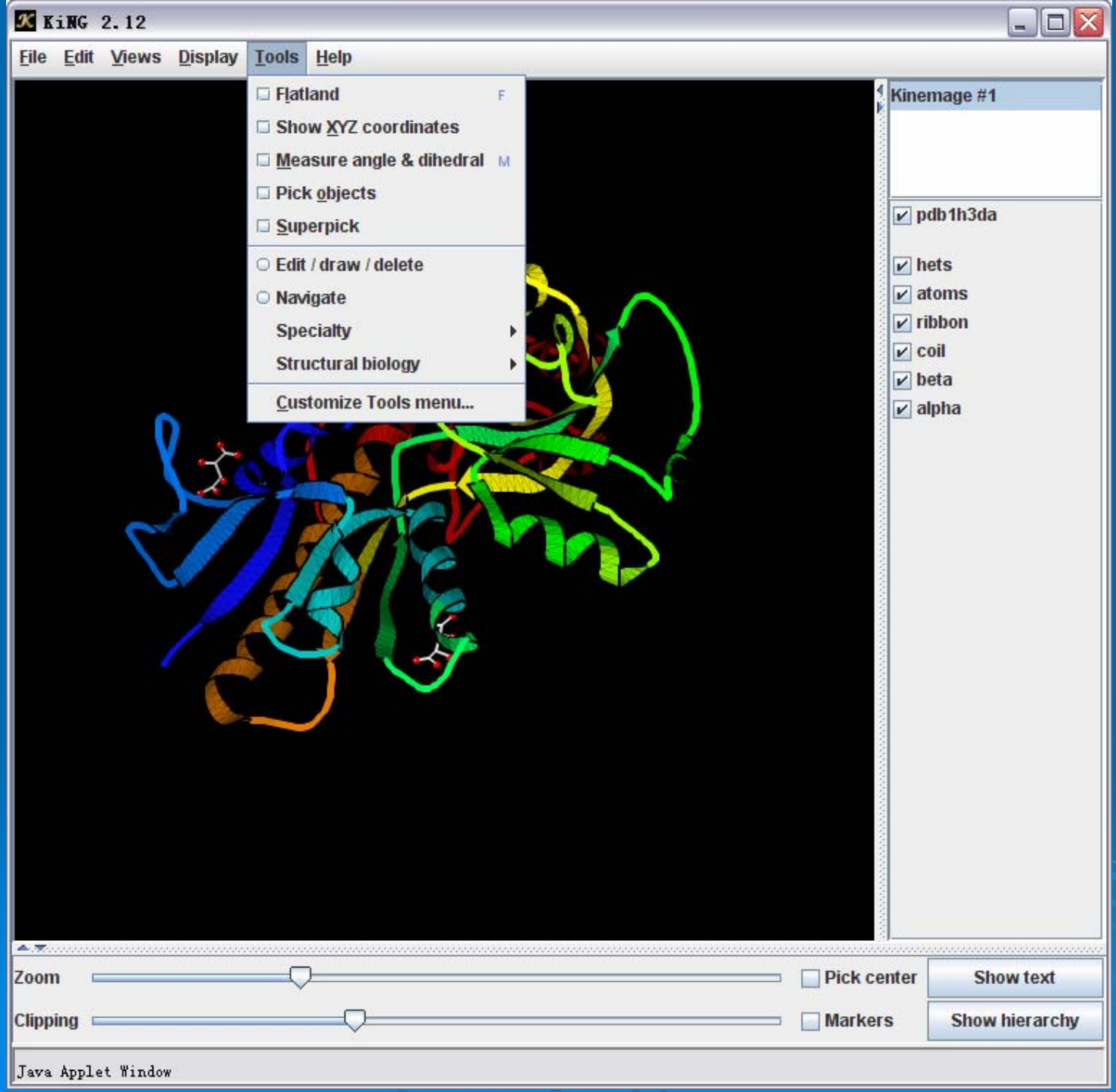


Color by list

Big Markers

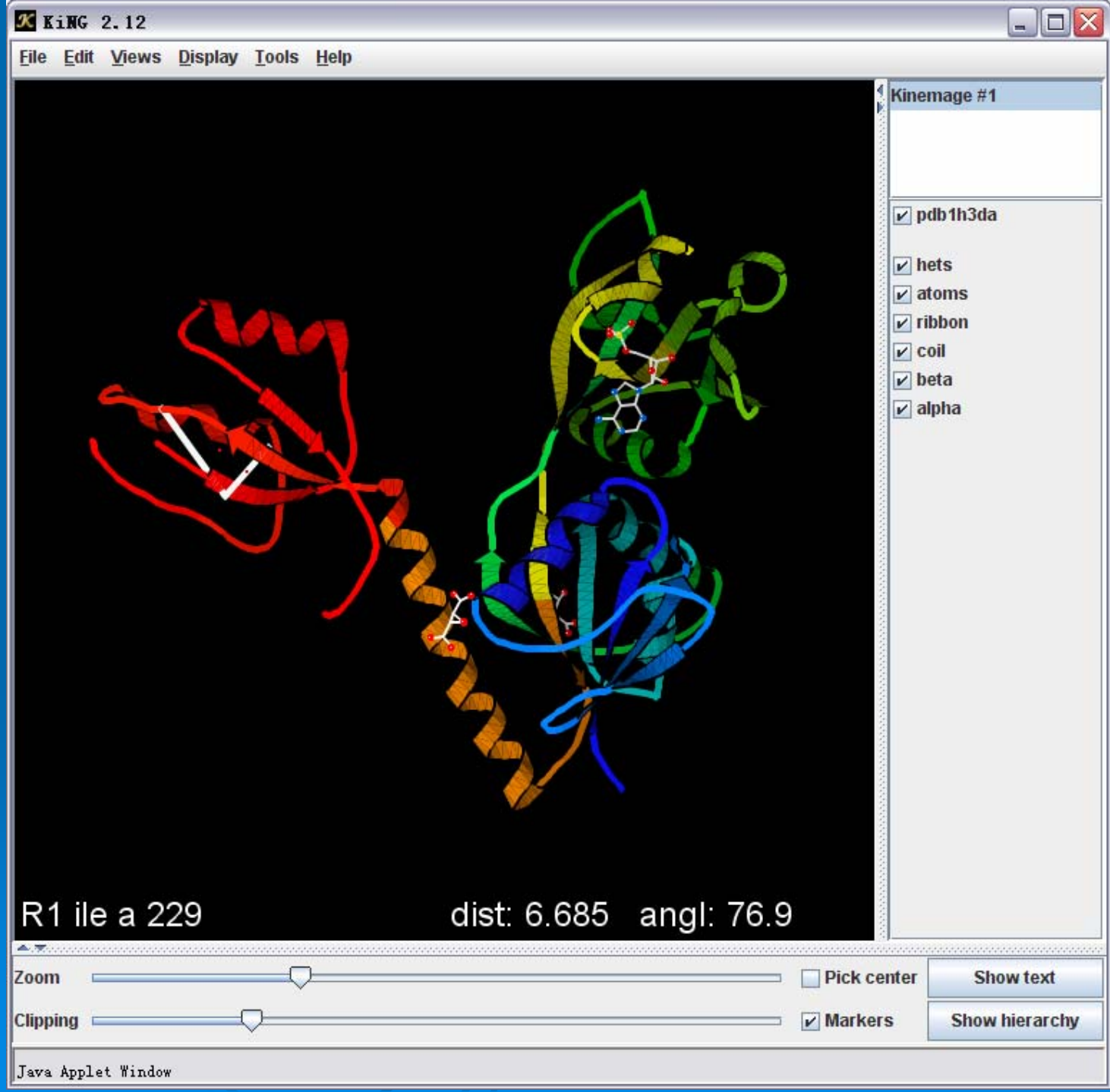
Big labels




KiNG 2.12
File
Edit
Views
Display
Tools
Help
Flatland
F
Show XYZ coordinates
Measure angle & dihedral
M
Pick objects
Superpick
Edit / draw / delete
Navigate
Specialty
Structural biology
Customize Tools menu...
Kinemage #1
pdb1h3da
hets
atoms
ribbon
coil
beta
alpha
Zoom
Clipping
Pick center
Markers
Show text
Show hierarchy
Java Applet Window

Measure distance

Measure angle



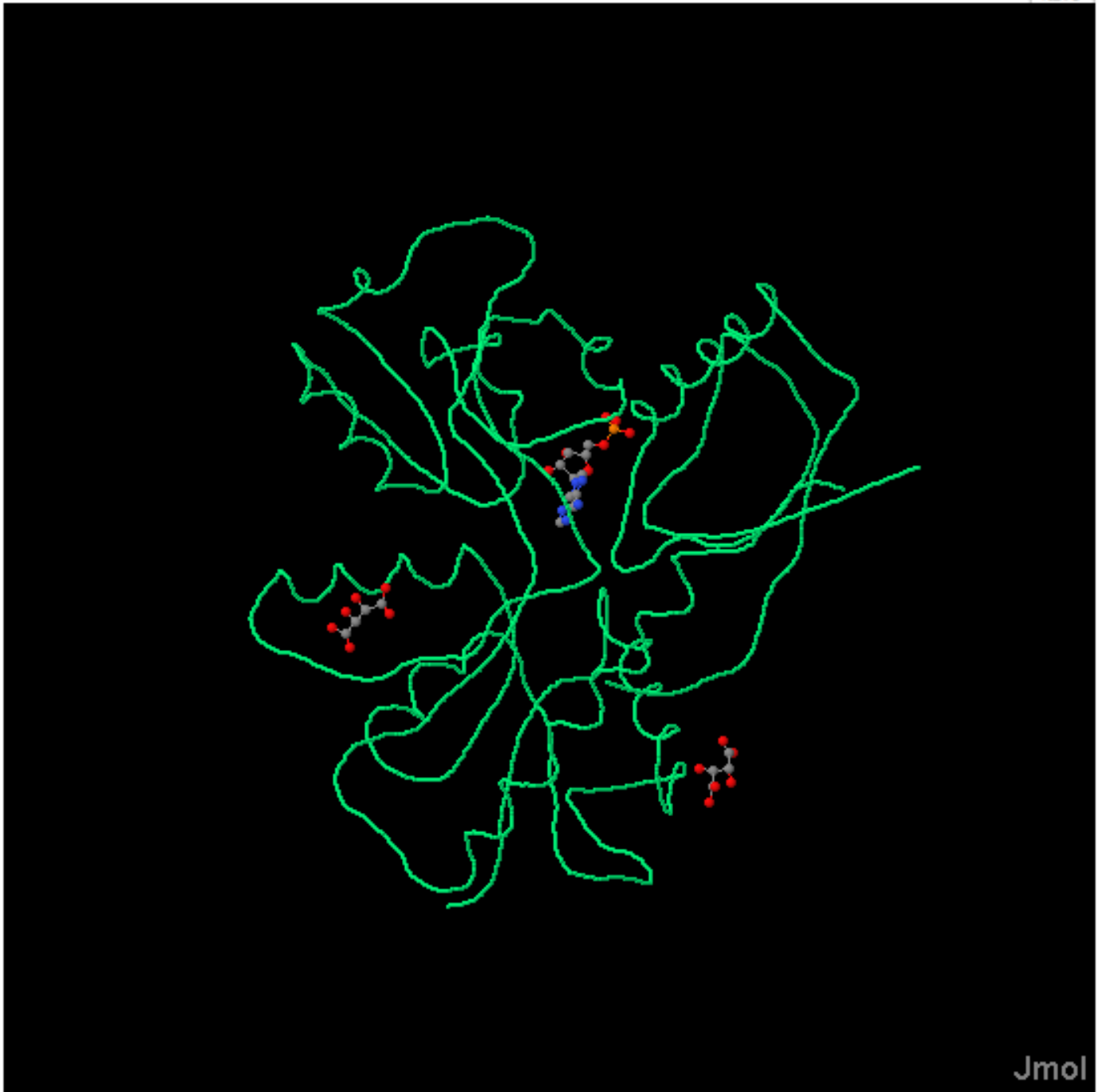
# Jmol

软件优点：图形显示占用资源少；可以显示有关晶体方面的图形；测量单位可以选择；具有图形自动旋转功能

软件缺点：选项不丰富；部分操作过于繁琐；测量时，选取位置有时不能准确定位。

Jmol

1h3d



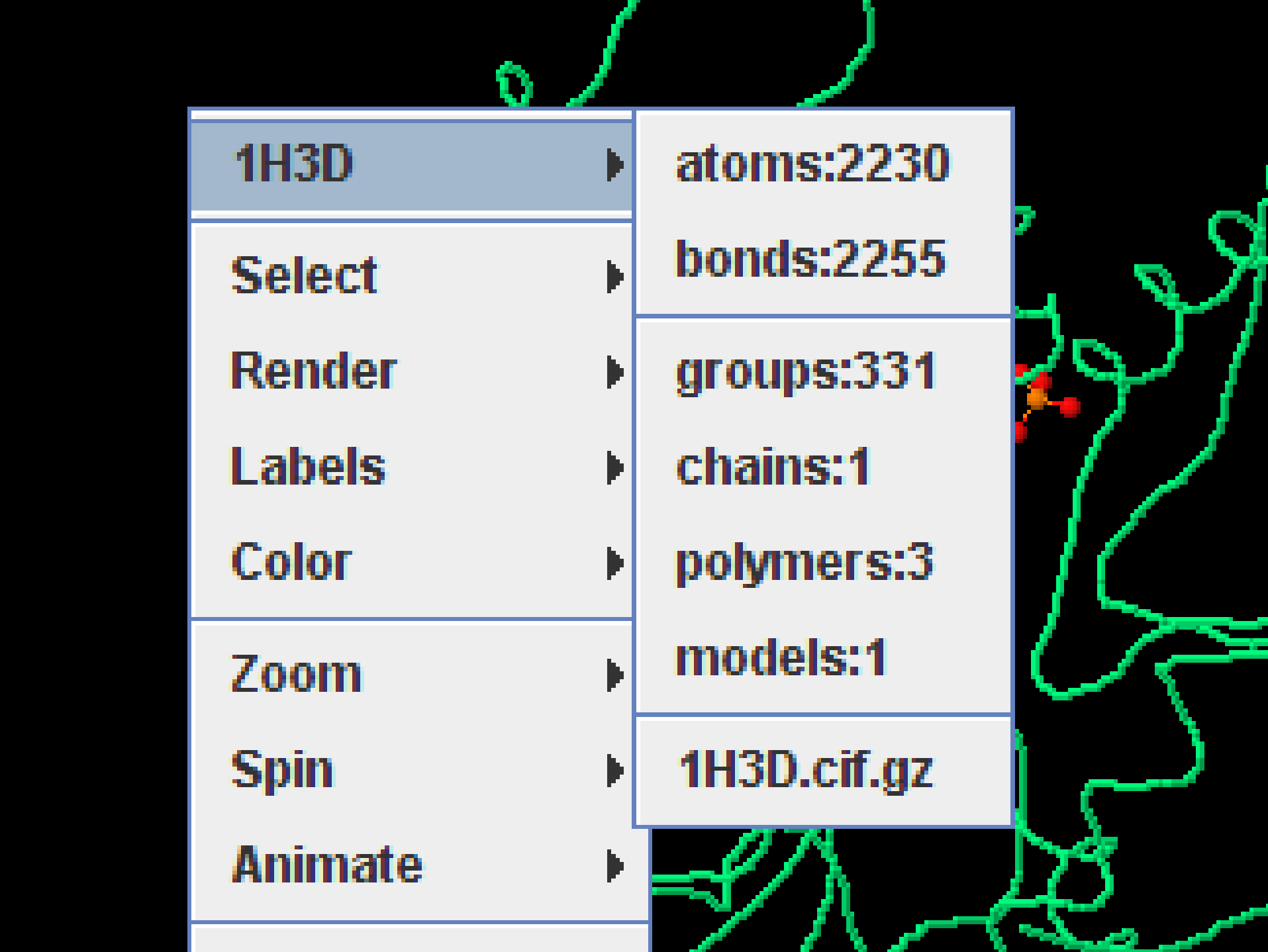
# 常用基本操作：

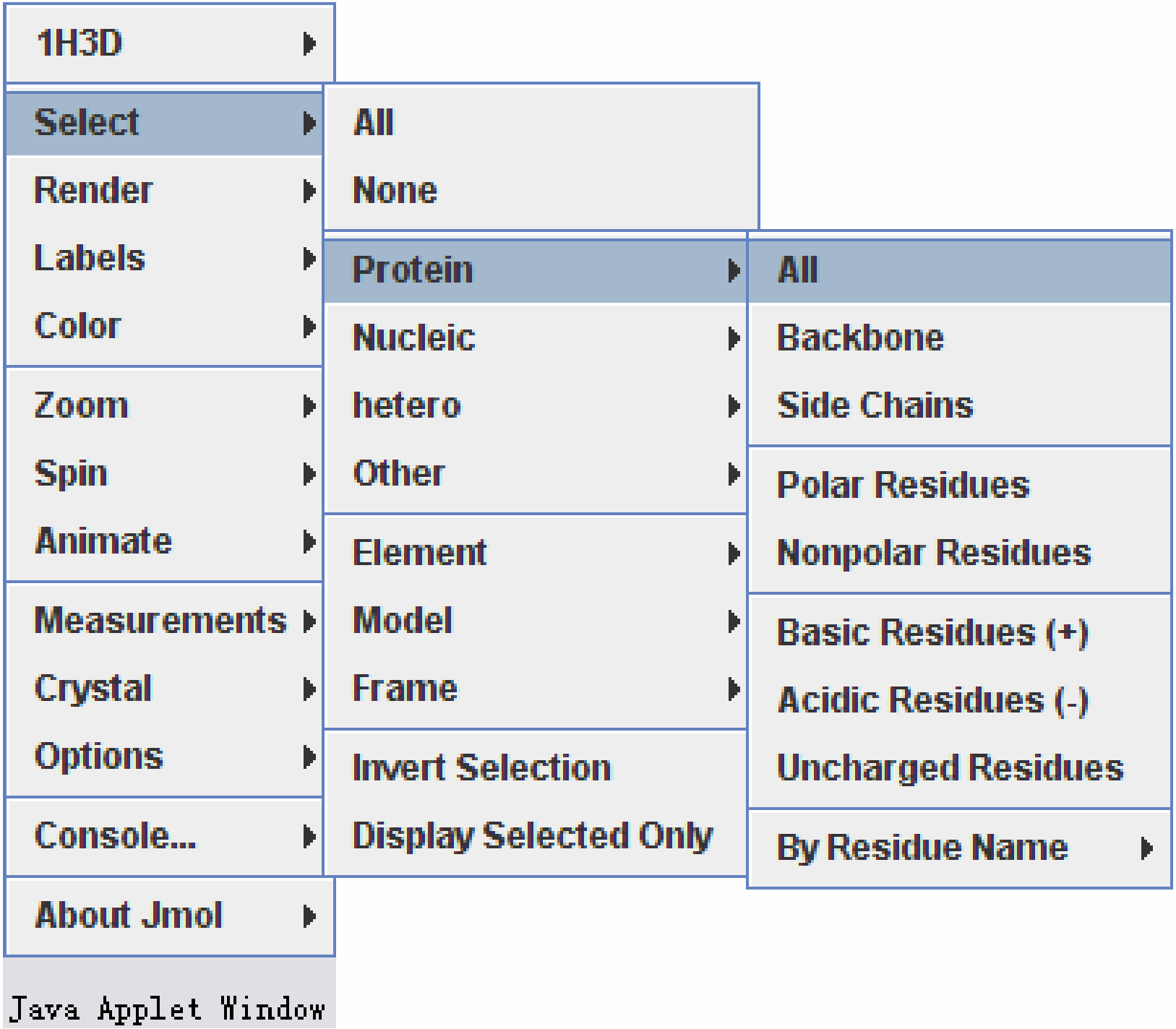
旋转： 鼠标拖动

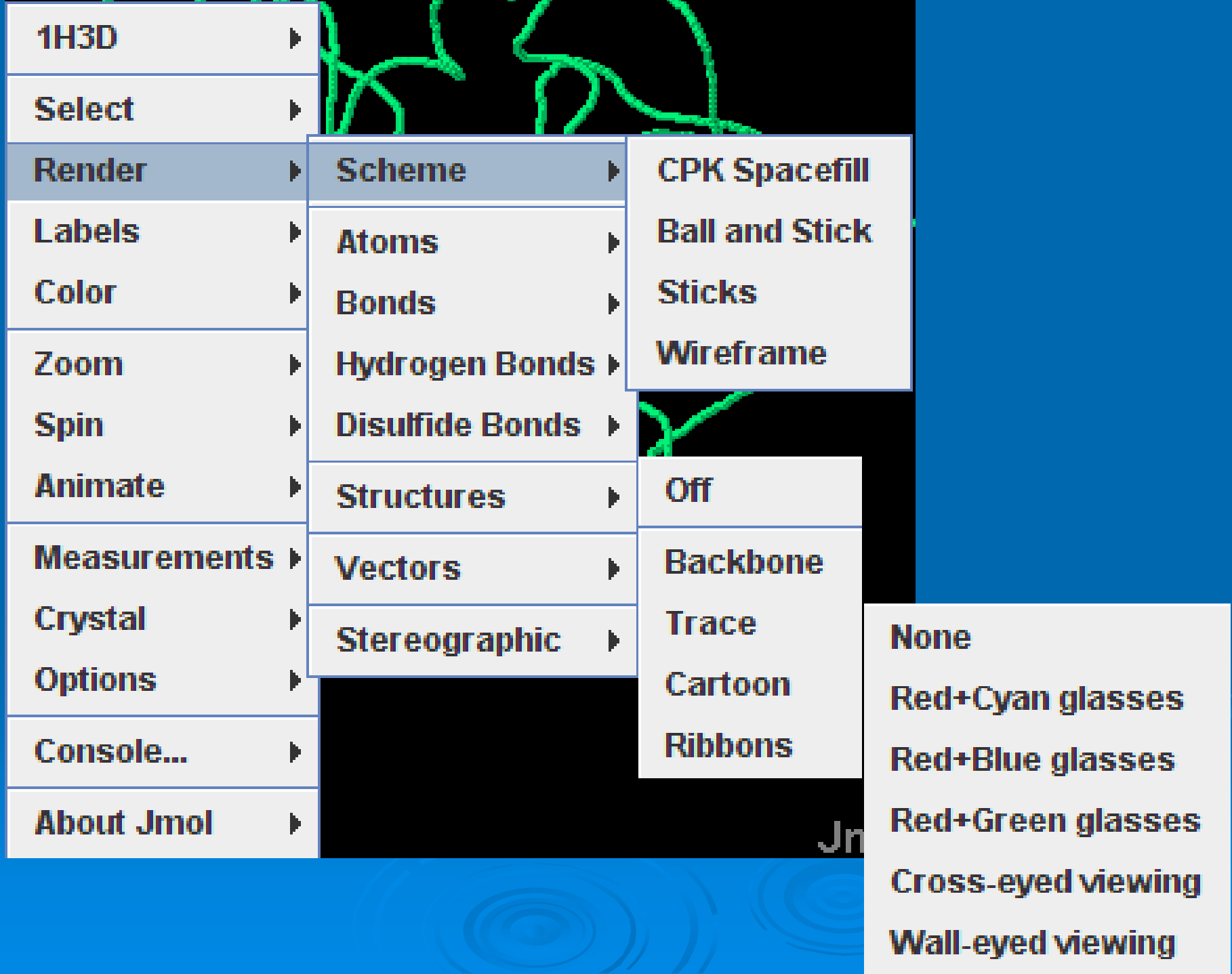
移动：ctrl+鼠标右键拖拉

放大缩小： 鼠标滚轮 or shift+鼠标左键垂直拖动 or alt+鼠标左键垂直拖动

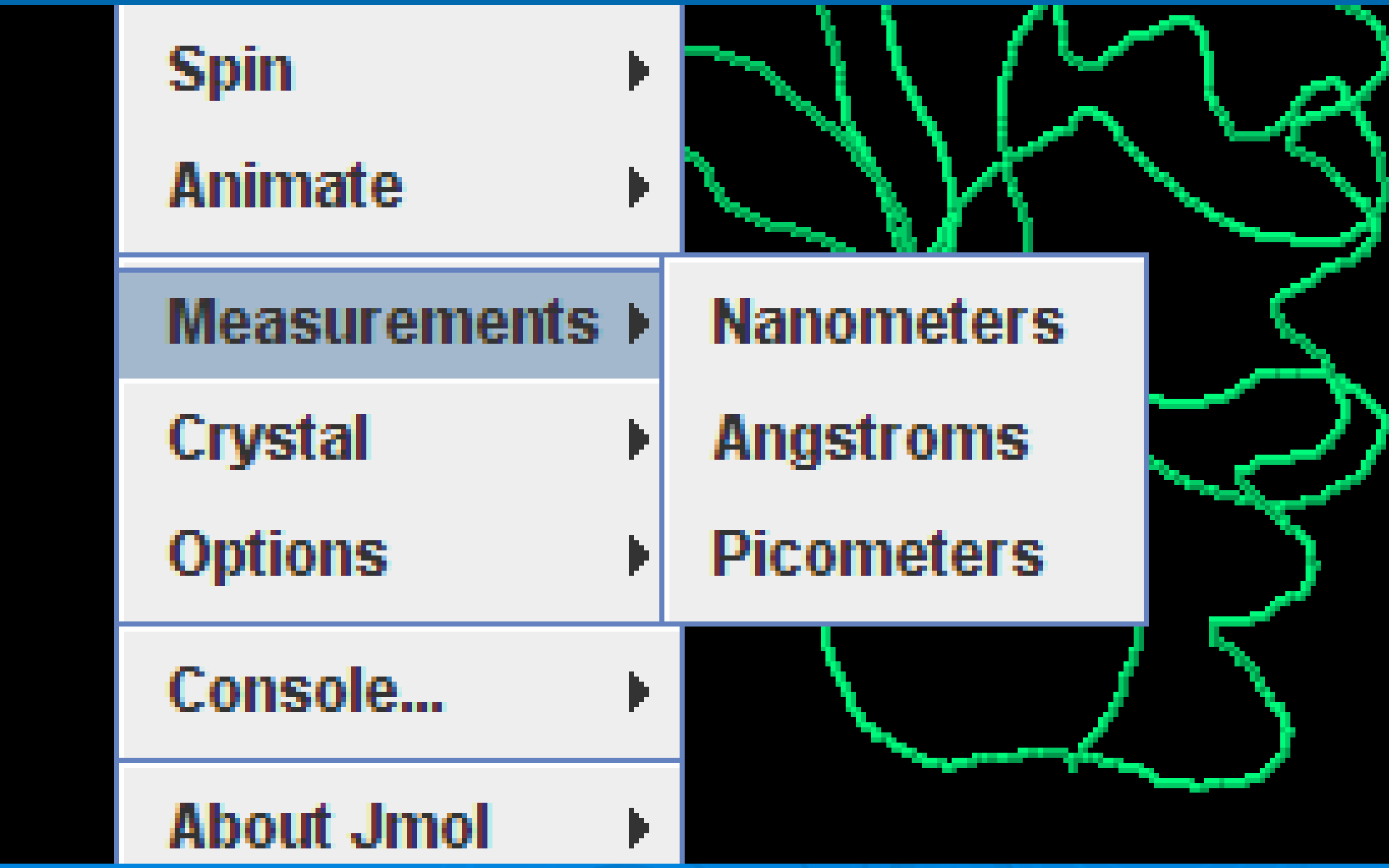
沿Z轴旋转： 鼠标滚轮 or shift+鼠标左键水平拖动 or alt+鼠标左键水平拖动

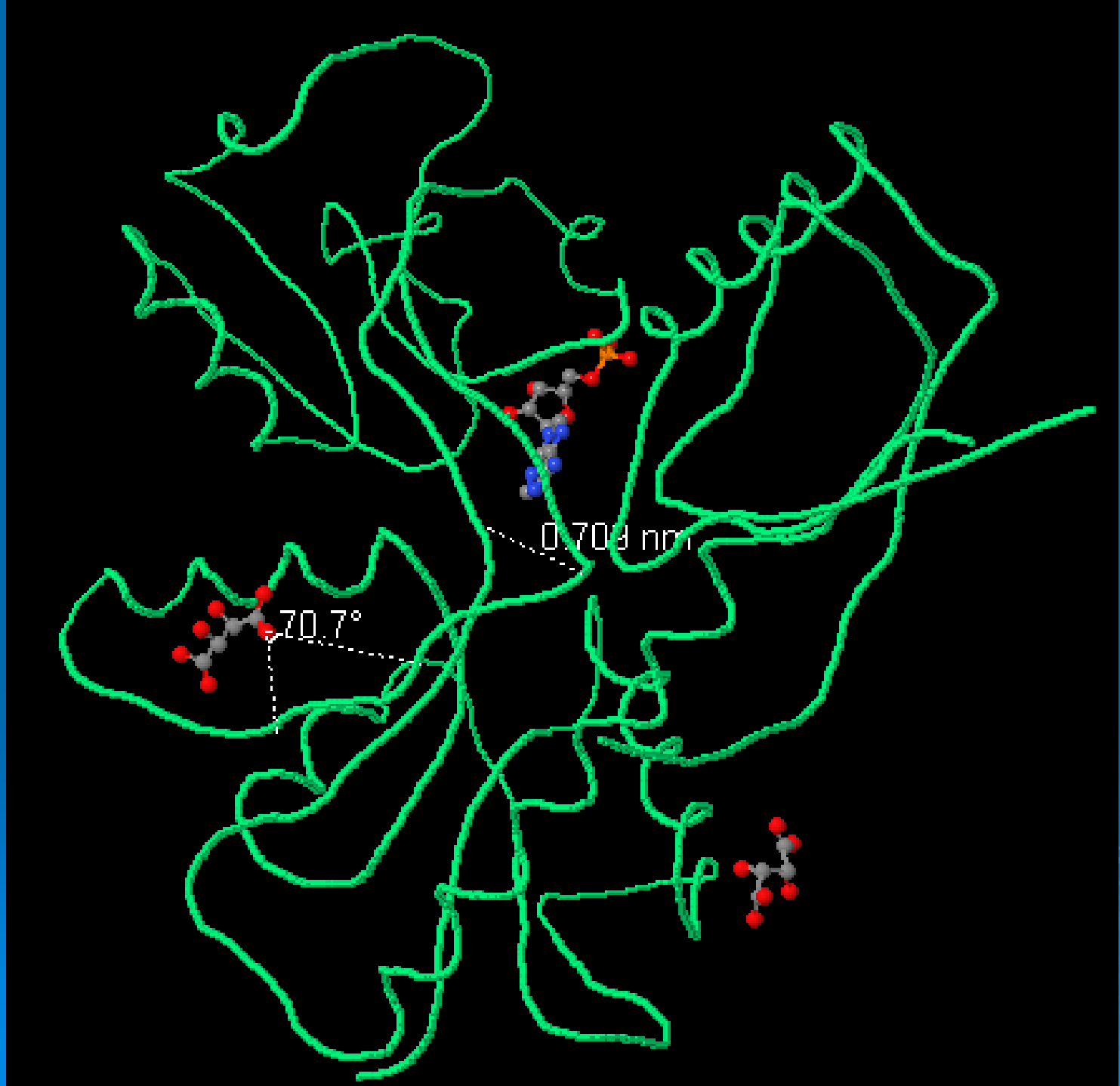

1H3D
Select
Render
Labels
Color
Zoom
Spin
Animate
atoms:2230
bonds:2255
groups:331
chains:1
polymers:3
models:1
1H3D.cif.gz

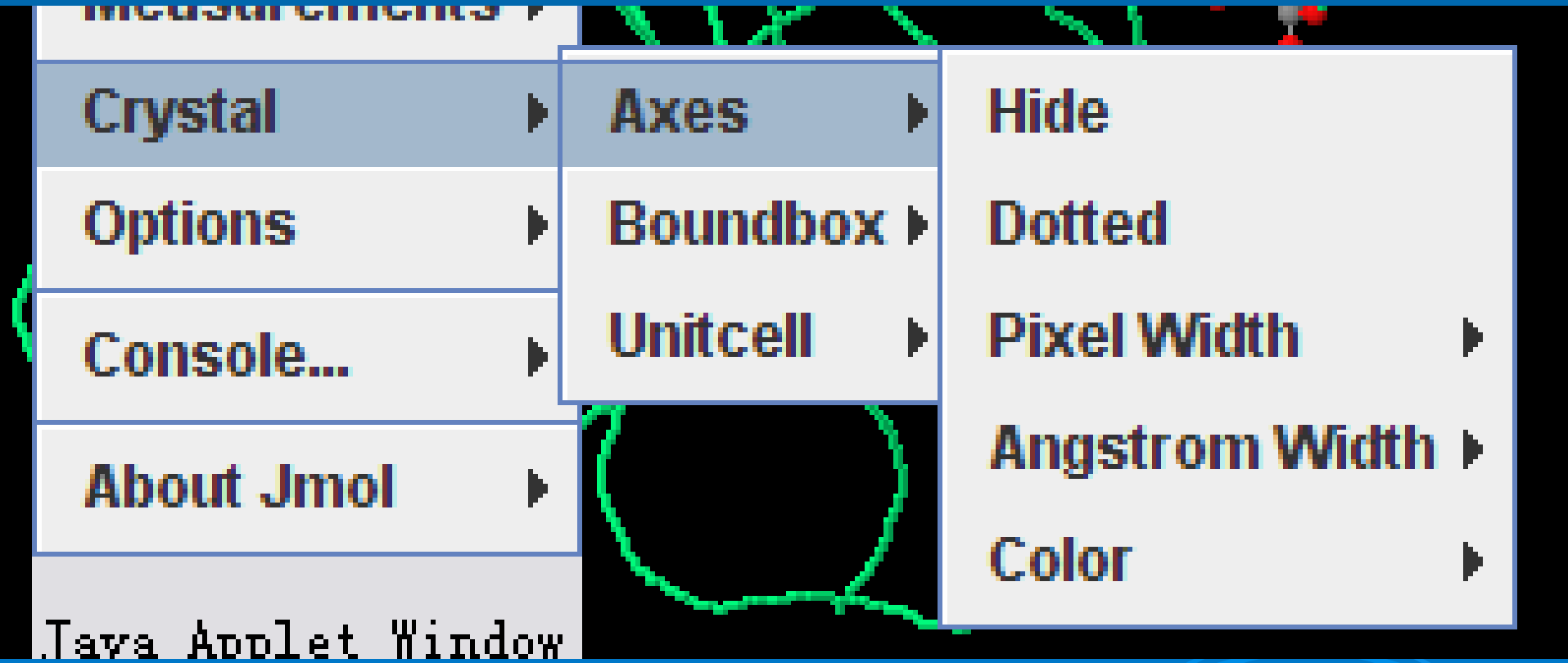

1H3D
Select
Render
Labels
Color
Zoom
Spin
Animate
Measurements
Crystal
Options
Console...
About Jmol
All
None
Protein
Nucleic
hetero
Other
Element
Model
Frame
Invert Selection
Display Selected Only
All
Backbone
Side Chains
Polar Residues
Nonpolar Residues
Basic Residues (+)
Acidic Residues (-)
Uncharged Residues
By Residue Name
Java Applet Window

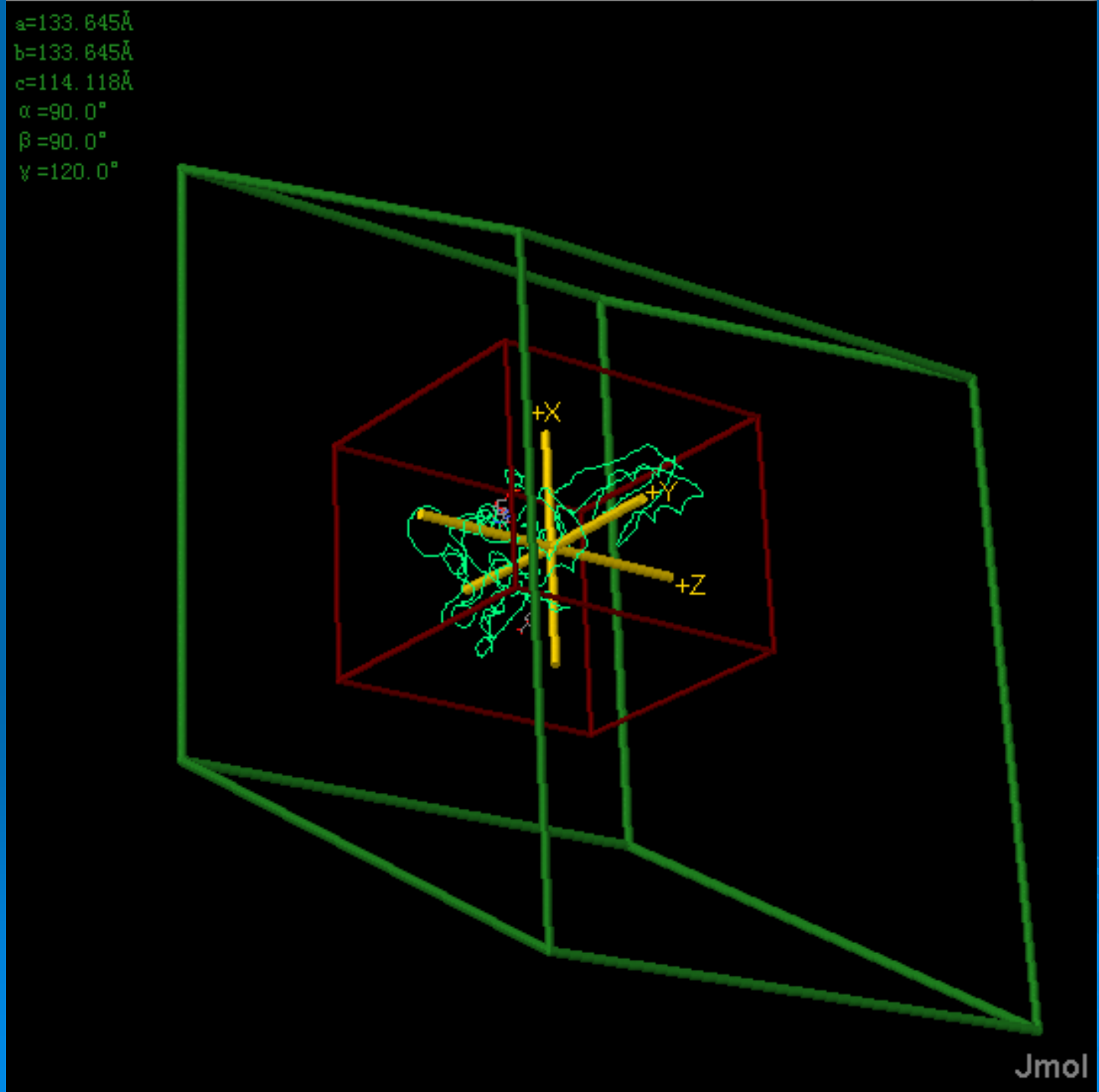

1H3D
Select
Render
Labels
Color
Zoom
Spin
Animate
Measurements
Crystal
Options
Console...
About Jmol
Scheme
Atoms
Bonds
Hydrogen Bonds
Disulfide Bonds
Structures
Vectors
Stereographic
CPK Spacefill
Ball and Stick
Sticks
Wireframe
Off
Backbone
Trace
Cartoon
Ribbons
None
Red+Cyan glasses
Red+Blue glasses
Red+Green glasses
Cross-eyed viewing
Wall-eyed viewing

Red + blue glasses


Spin
Animate
Measurements
Crystal
Options
Console...
About Jmol
Nanometers
Angstroms
Picometers


0.704 nm
70.7°


Crystal
Options
Console...
About Jmol
Axes
Boundbox
Unitcell
Hide
Dotted
Pixel Width
Angstrom Width
Color
Java Applet Window


a=133.645Å
b=133.645Å
c=114.118Å
α=90.0°
β=90.0°
γ=120.0°
+X
+Y
+Z
Jmol

# Webmol

软件优点：用户界面良好；操作方便；功能丰富，具有一些独特分析功能

软件缺点：图形显示性不好；使用说明解释不够详细

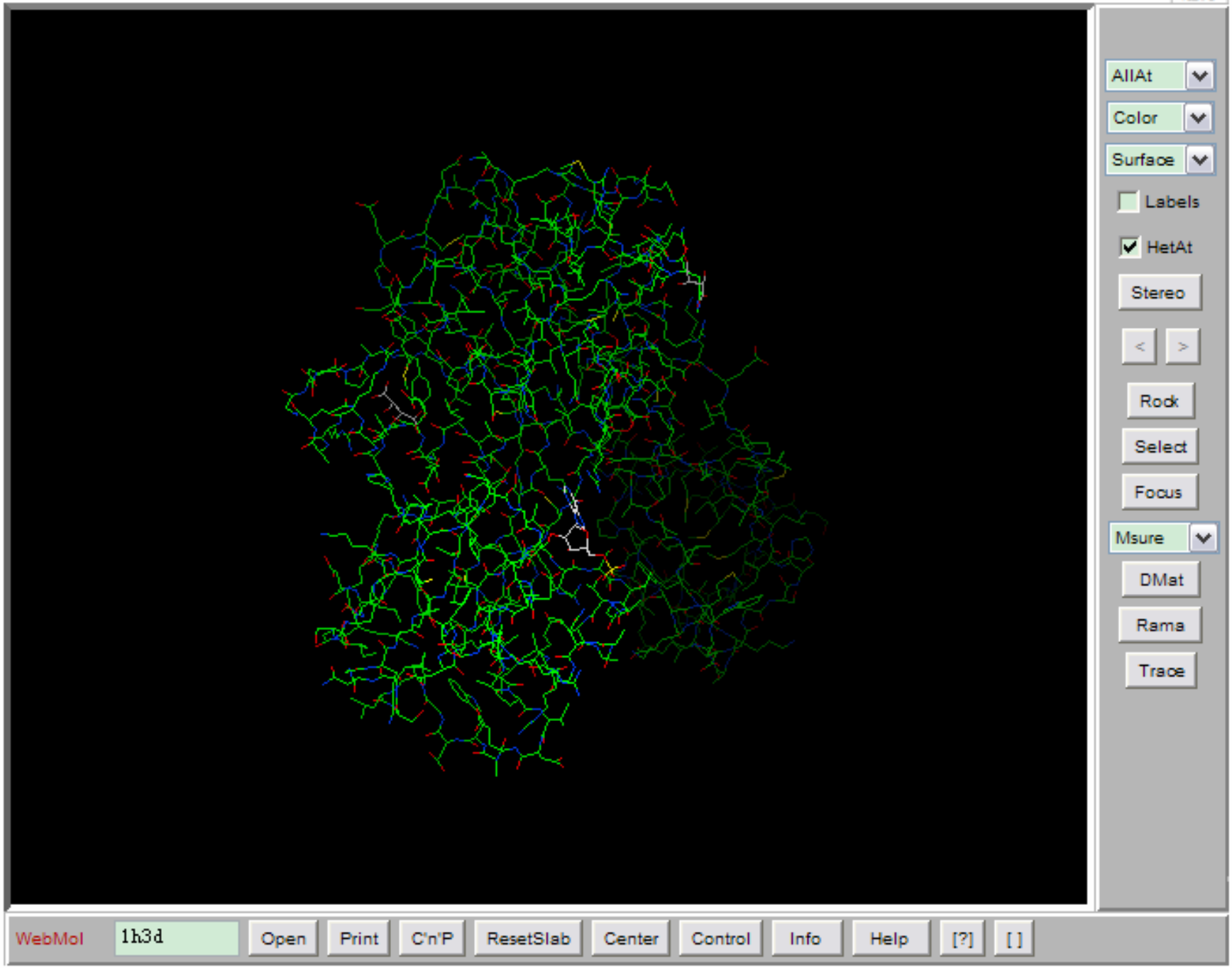
# 常用基本操作：

旋转：左键鼠标拖动

移动：alt+鼠标左键拖拉

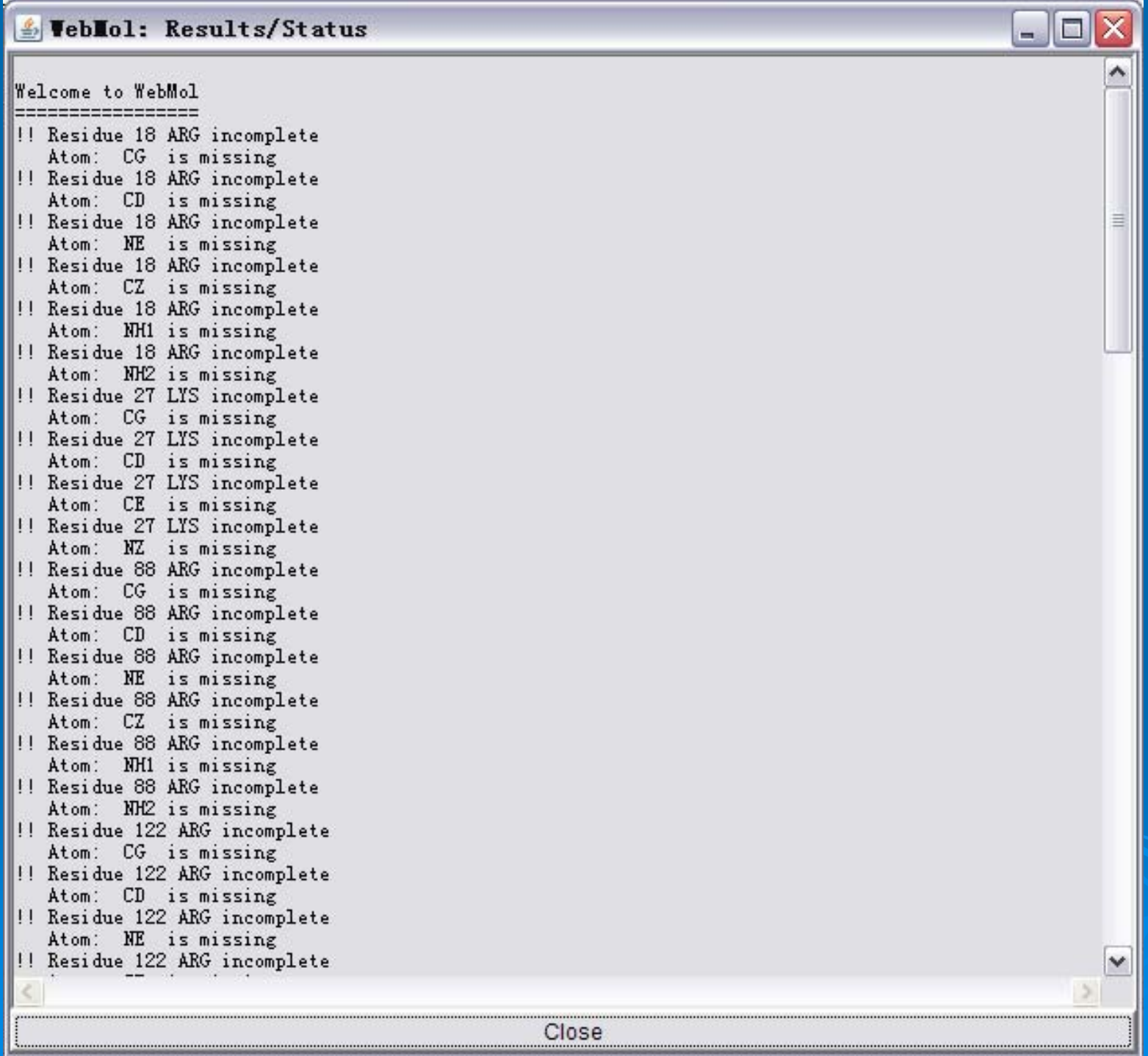
放大缩小：鼠标右键垂直拖动

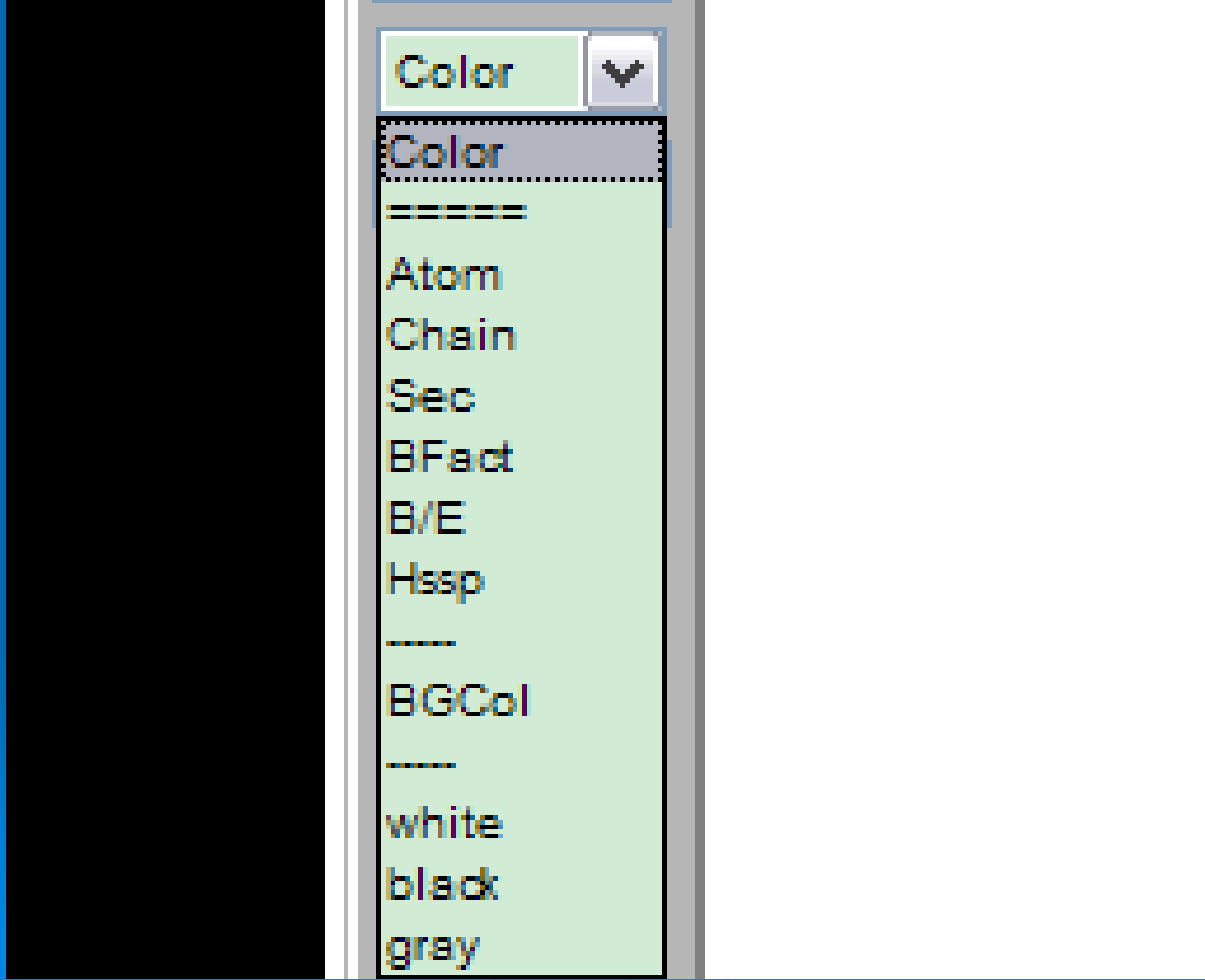
沿Z轴旋转：shift+鼠标左键水平拖动 or ctrl+鼠标左键水平拖动

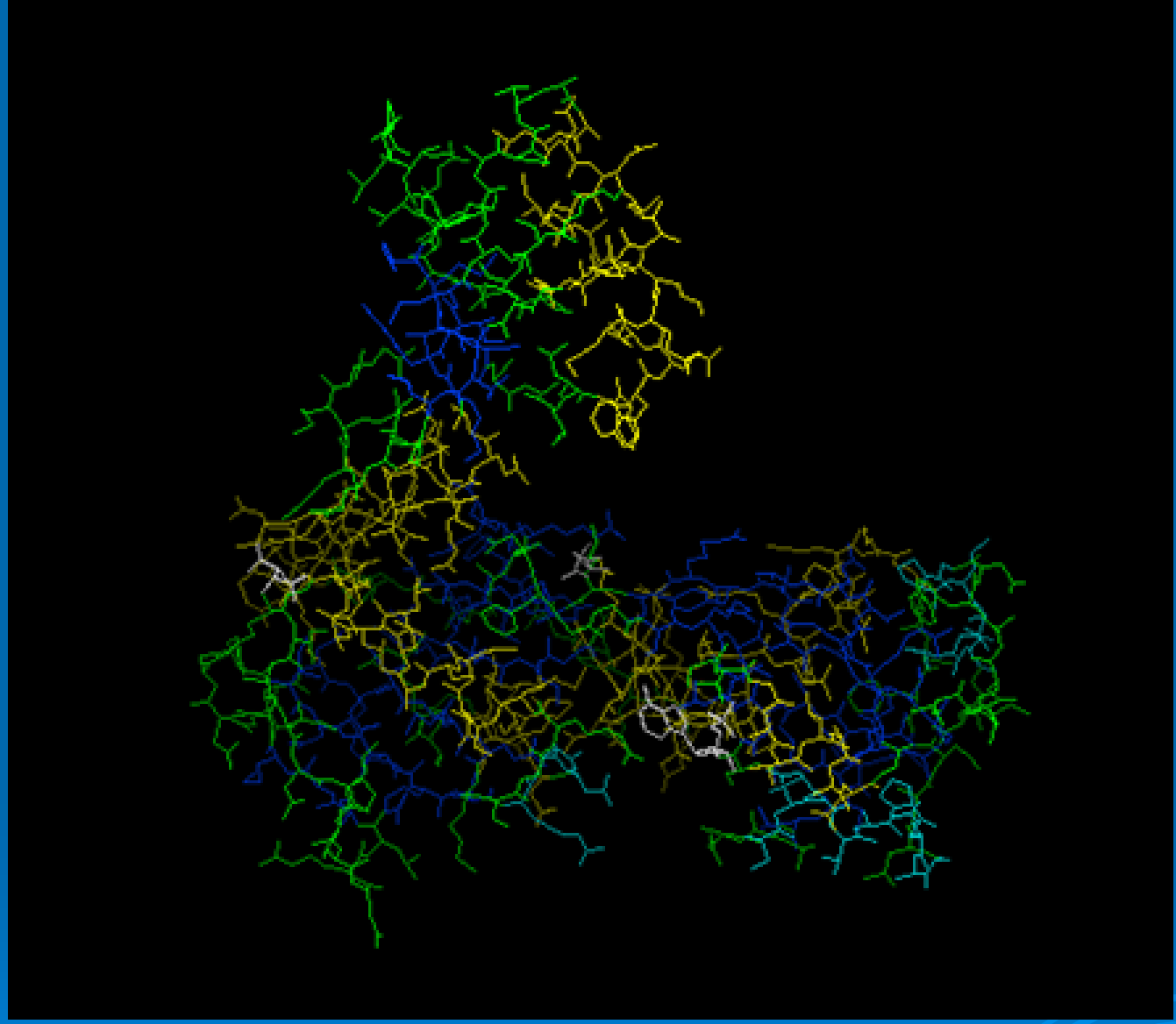

WebMol
1h3d
AllAt
Color
Surface
Labels
HetAt
Stereo
Rock
Select
Focus
Msure
DMat
Rama
Trace
WebMol
1h3d
Open
Print
C'n'P
ResetSlab
Center
Control
Info
Help
[?]
[ ]

# 功能按钮

C‘n’P：复制并黏贴PDB文件到viewer中。
Center：使图形位于中间
Control：控制面板
[?]：显示或隐藏 WebMol 文件的状态信息

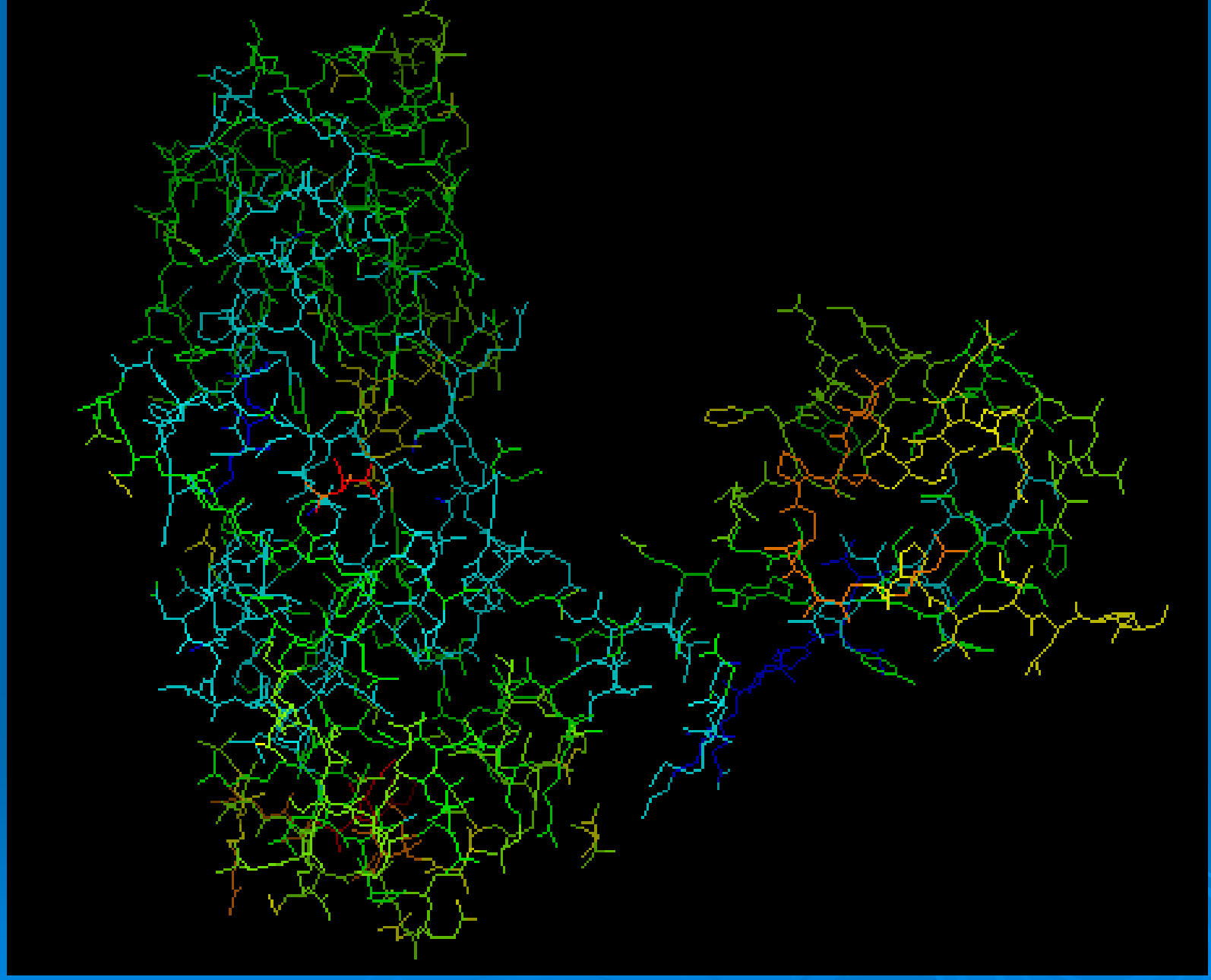

WebMol: Results/Status
Welcome to WebMol
==========
!! Residue 18 ARG incomplete
Atom: CG is missing
!! Residue 18 ARG incomplete
Atom: CD is missing
!! Residue 18 ARG incomplete
Atom: NE is missing
!! Residue 18 ARG incomplete
Atom: CZ is missing
!! Residue 18 ARG incomplete
Atom: NH1 is missing
!! Residue 18 ARG incomplete
Atom: NH2 is missing
!! Residue 27 LYS incomplete
Atom: CG is missing
!! Residue 27 LYS incomplete
Atom: CD is missing
!! Residue 27 LYS incomplete
Atom: CE is missing
!! Residue 27 LYS incomplete
Atom: NZ is missing
!! Residue 88 ARG incomplete
Atom: CG is missing
!! Residue 88 ARG incomplete
Atom: CD is missing
!! Residue 88 ARG incomplete
Atom: NE is missing
!! Residue 88 ARG incomplete
Atom: CZ is missing
!! Residue 88 ARG incomplete
Atom: NH1 is missing
!! Residue 88 ARG incomplete
Atom: NH2 is missing
!! Residue 122 ARG incomplete
Atom: CG is missing
!! Residue 122 ARG incomplete
Atom: CD is missing
!! Residue 122 ARG incomplete
Atom: NE is missing
!! Residue 122 ARG incomplete
Close


Color
Color
=====
Atom
Chain
Sec
BFact
B/E
Hssp
-----
BGCol
-----
white
black
gray

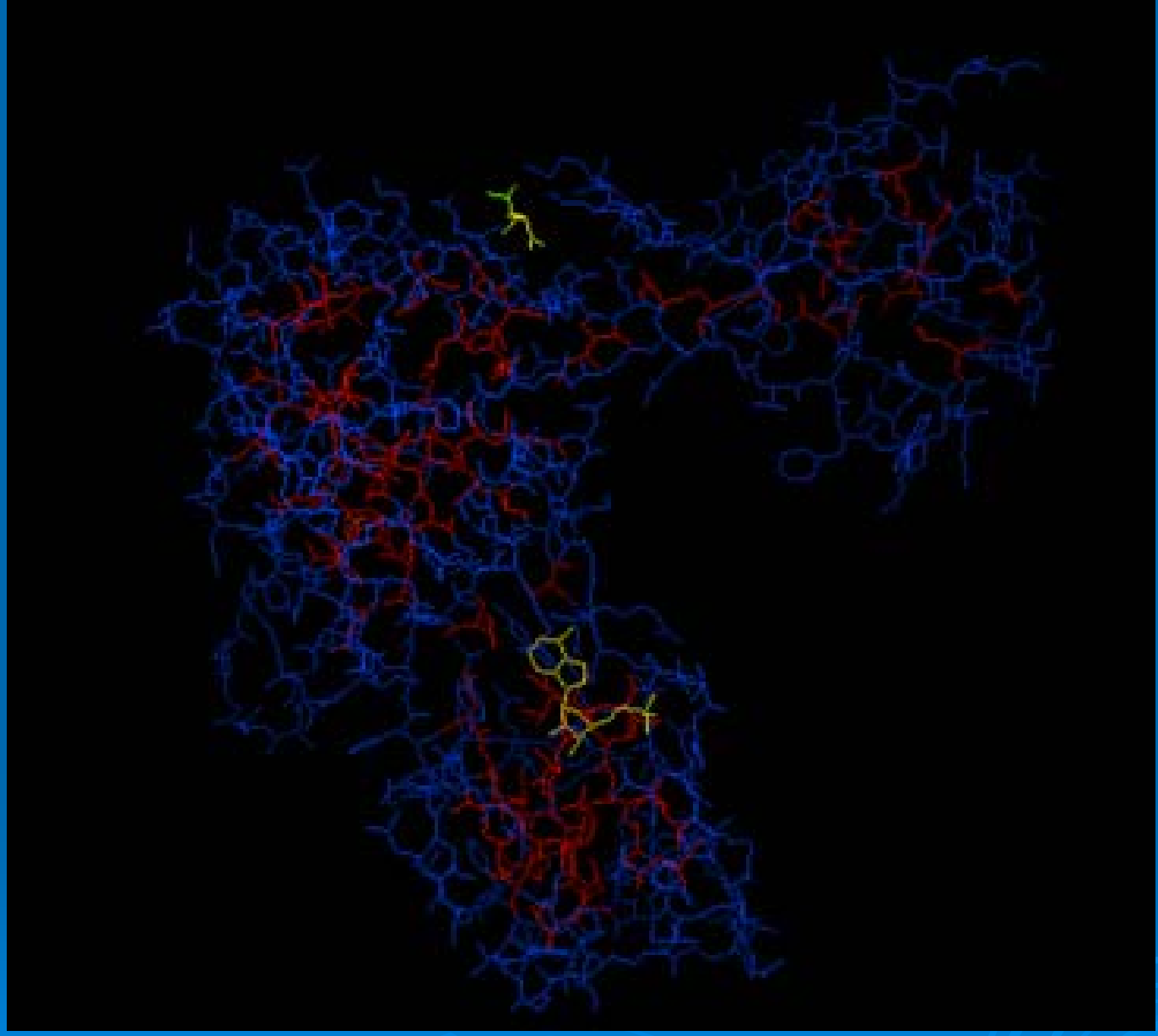


Sec：secondary structure

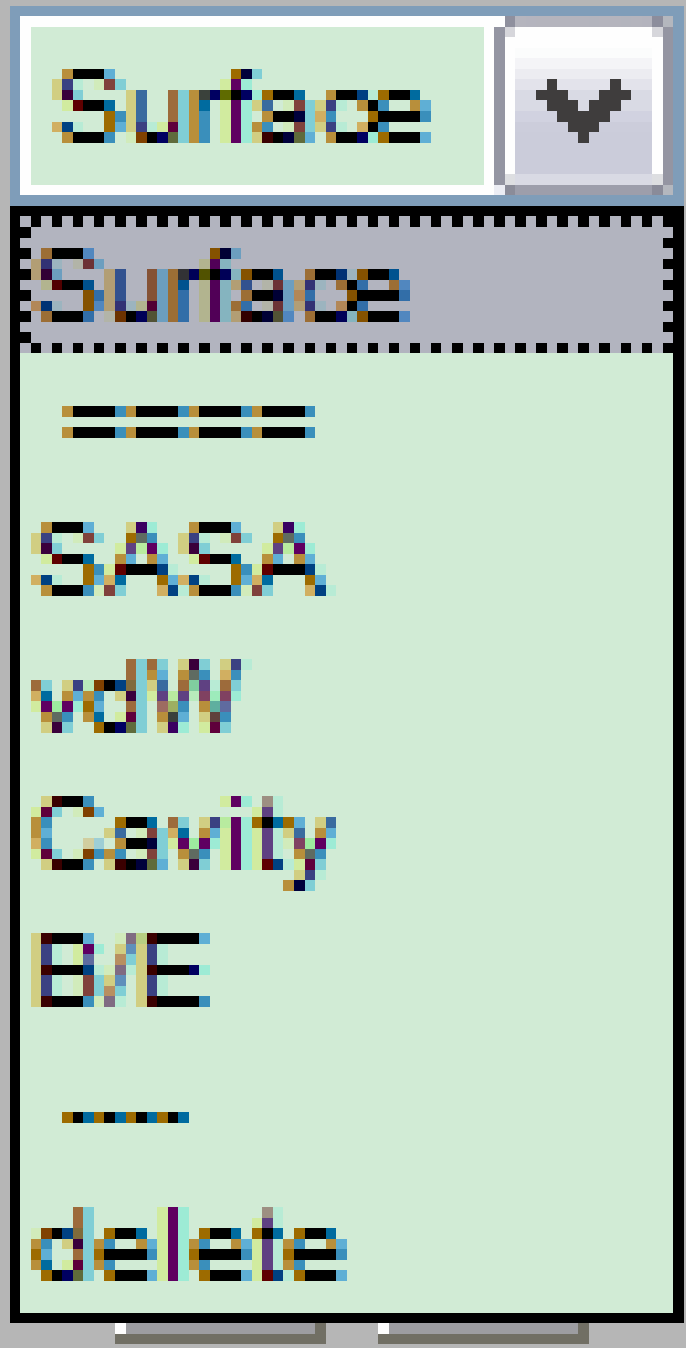
黄色为a螺旋,；蓝色为β折叠；灰色为转角；青色为非a螺旋

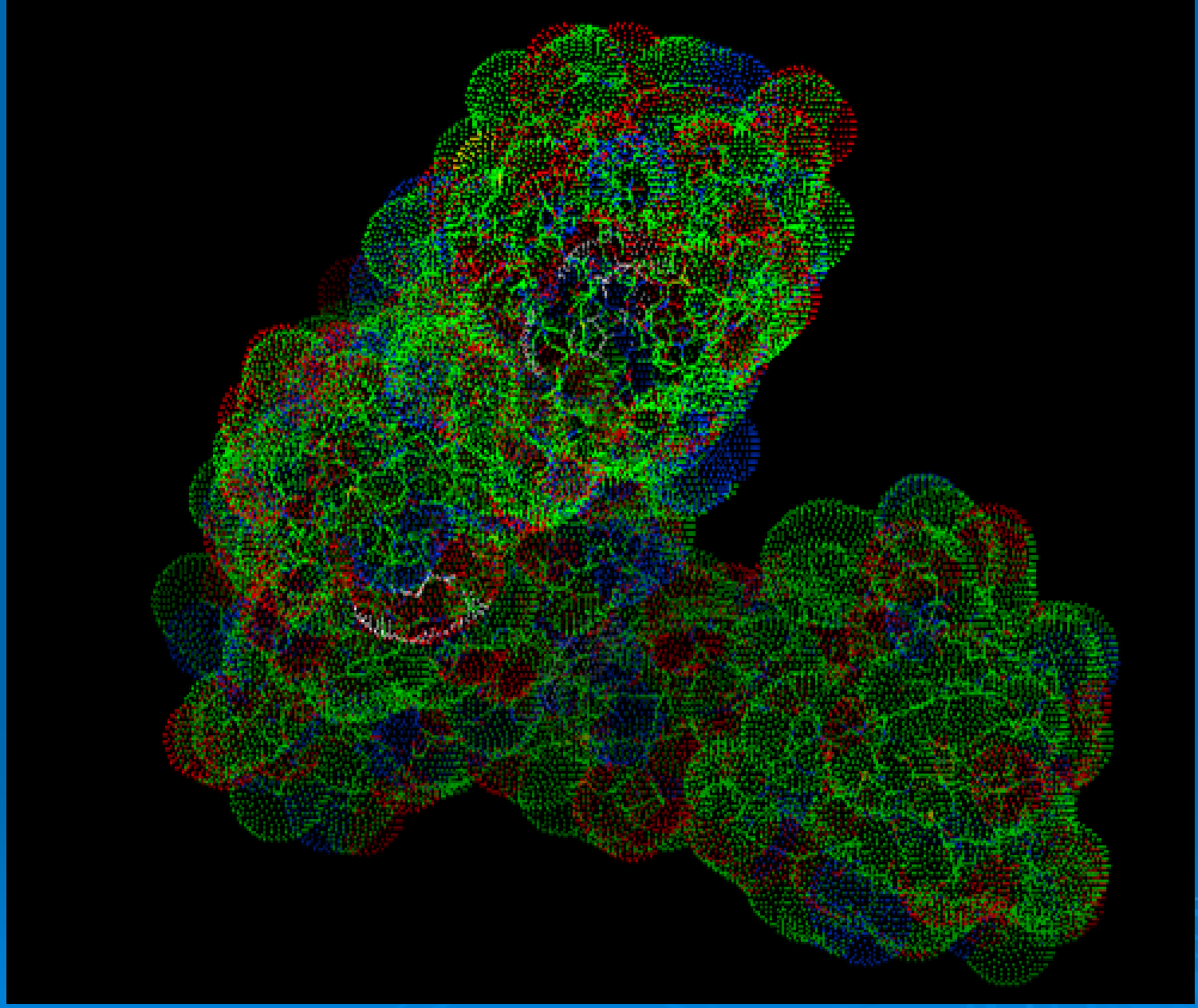


Bfact：B-factors or temperature factors

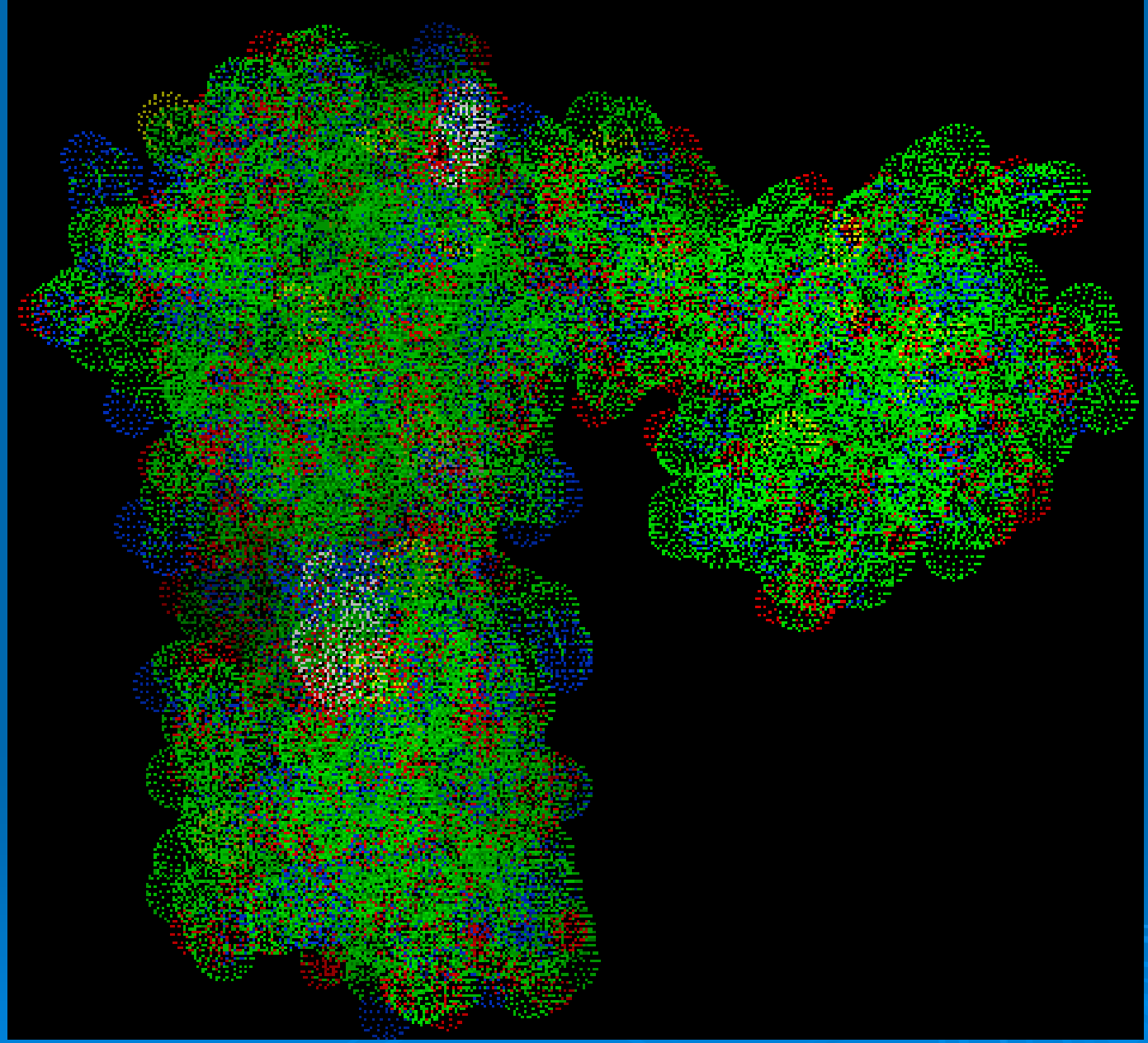


B/E： buried/exposed 当一个残基在溶剂可及表面不到5%时，则被认为包埋于内部，以红色部分显示。

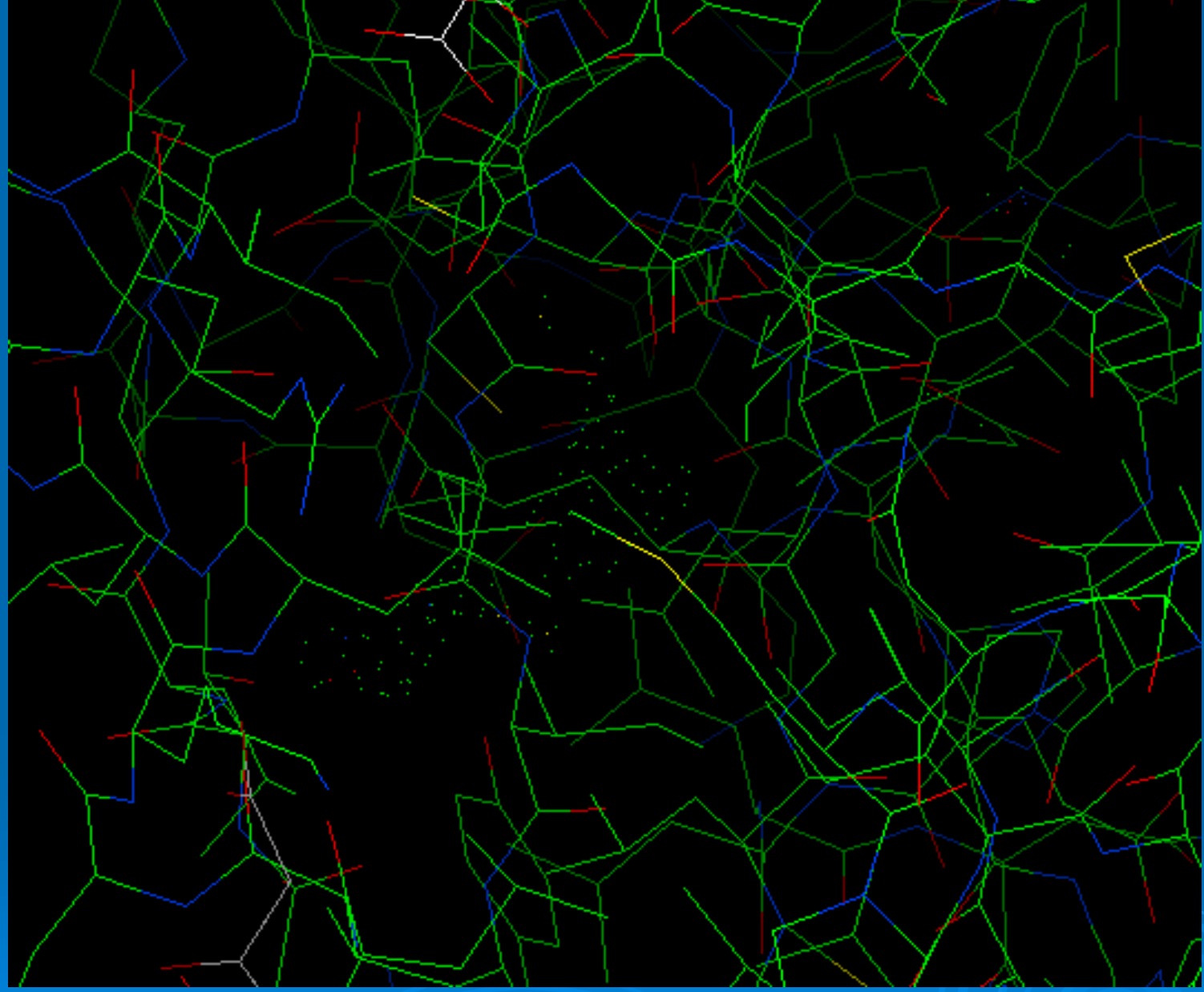

Surface
Surface
SASA
vdW
Cavity
B/E
delete



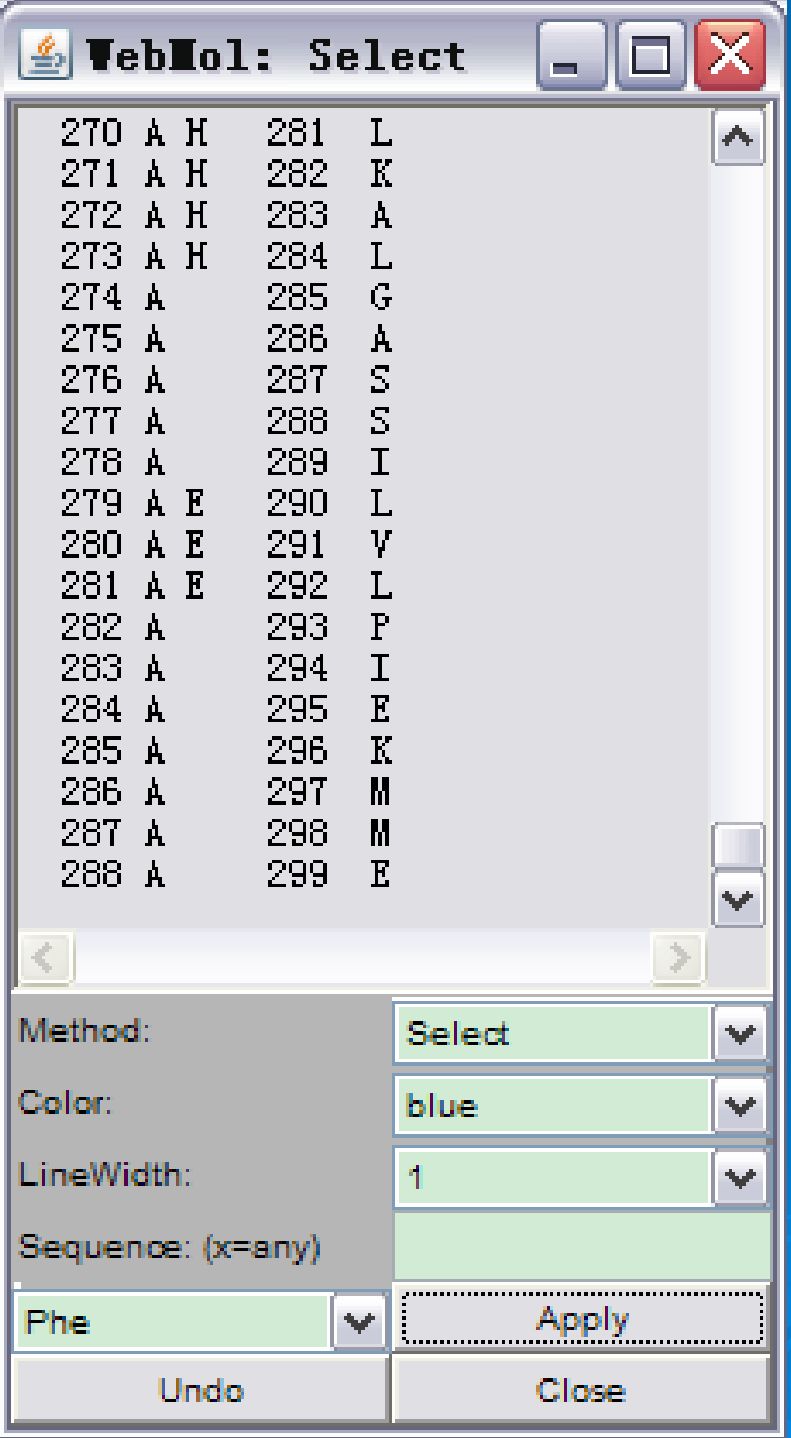
SASA：solvent Accessible Surface Area



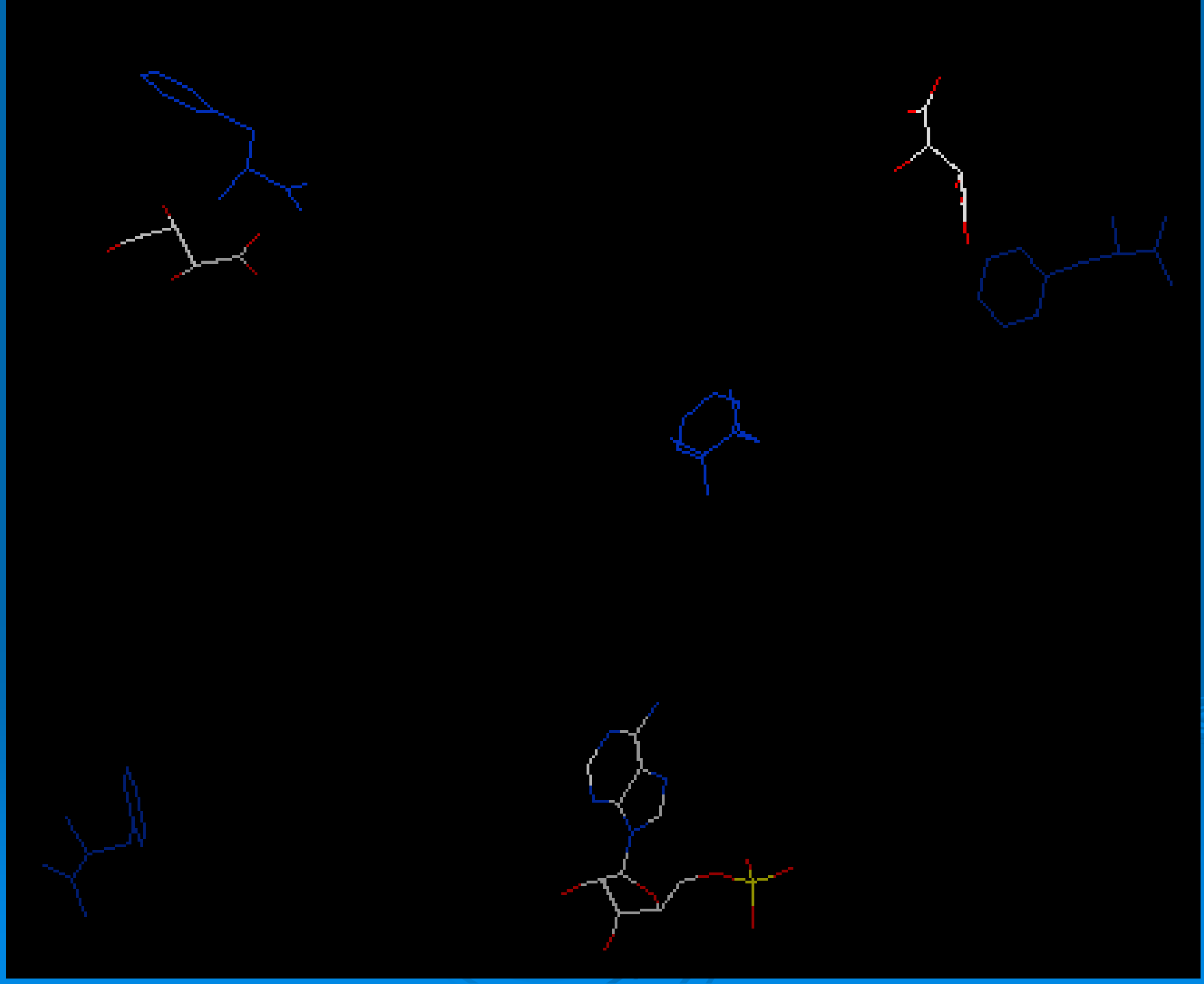
vdW：van der walls 范德华力

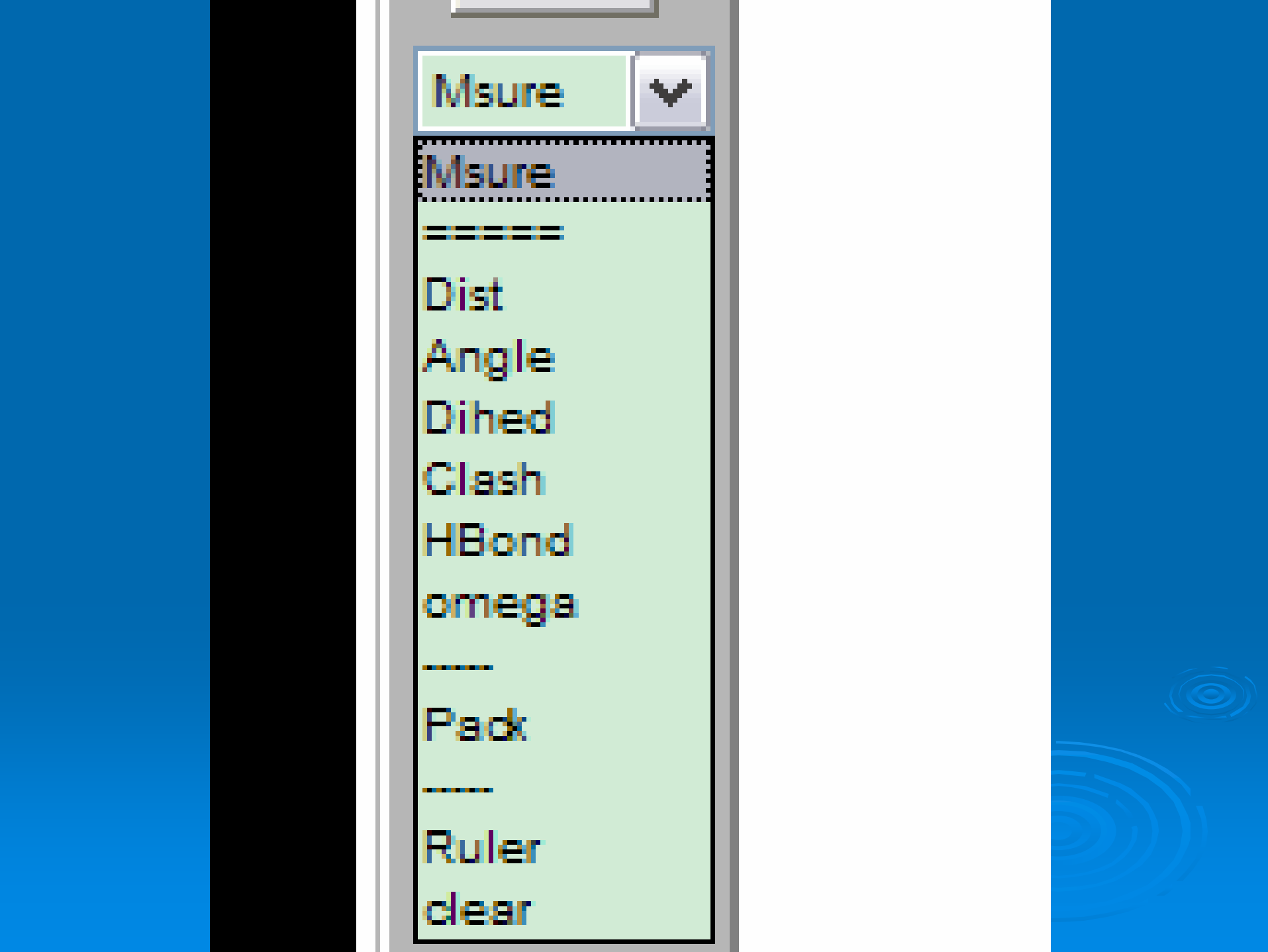


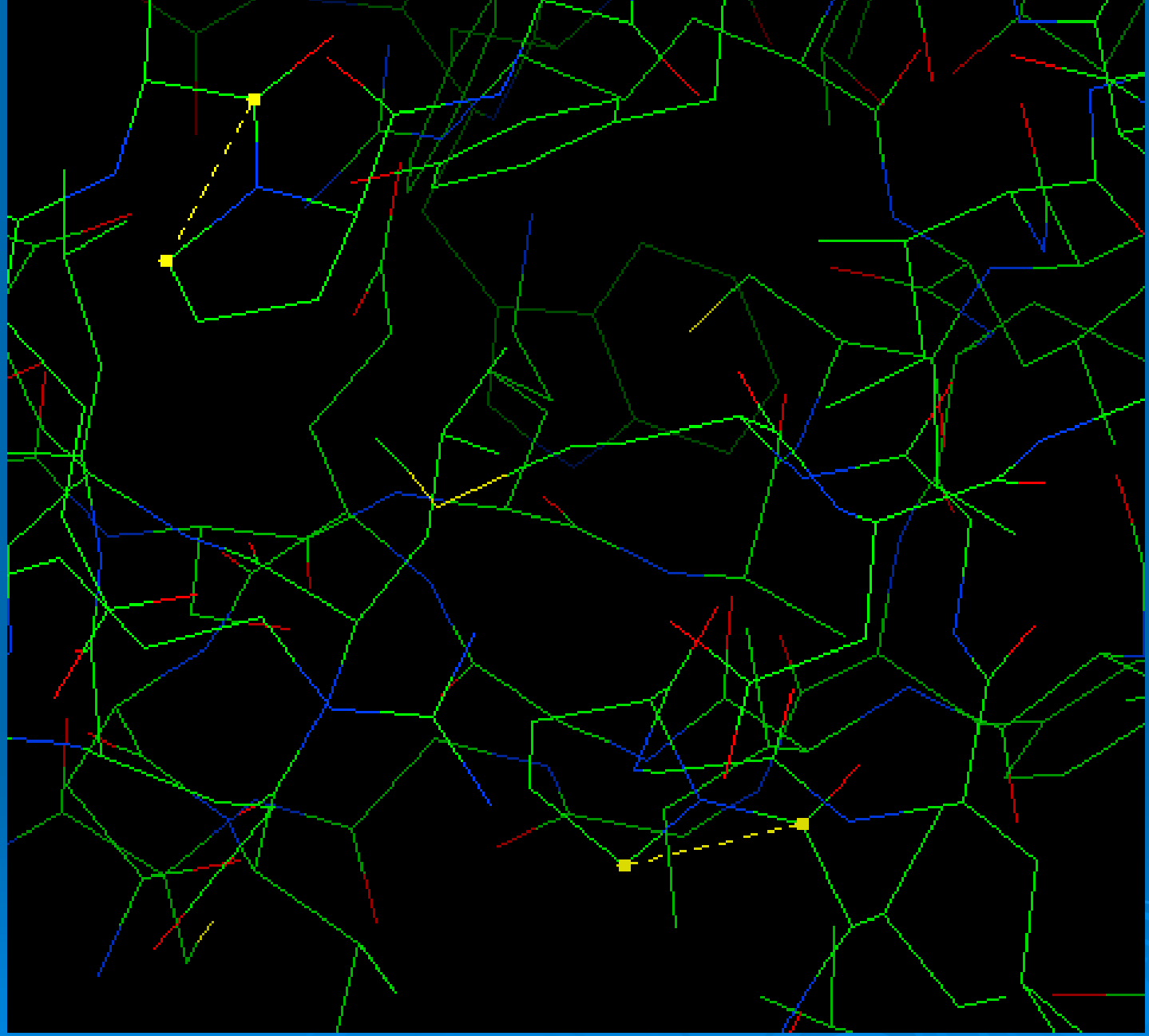
Cavity:相当于包埋于结构内部的solvent accessible surface



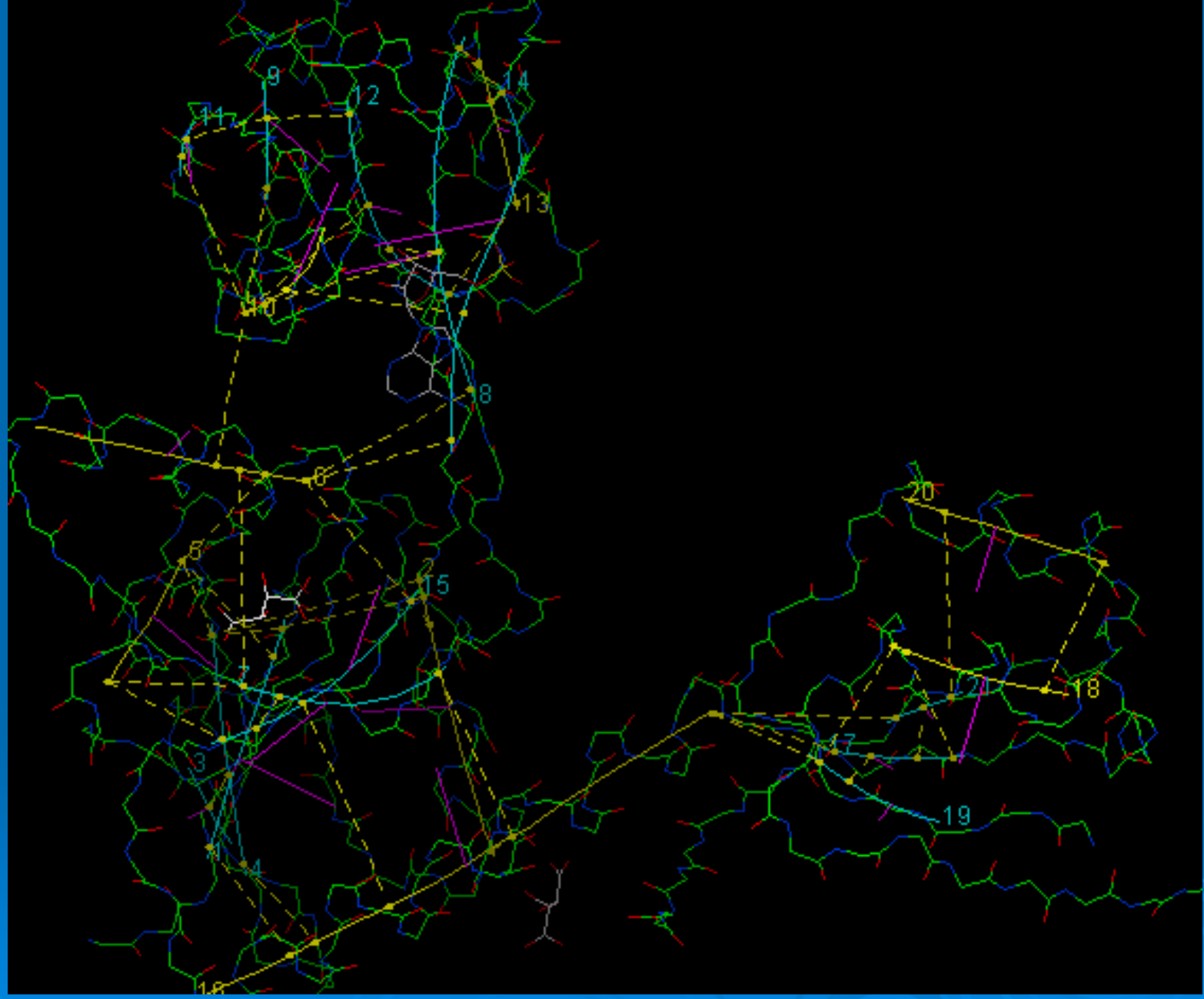

可以选择单一氨基酸种类，
也可以搜索一个序列



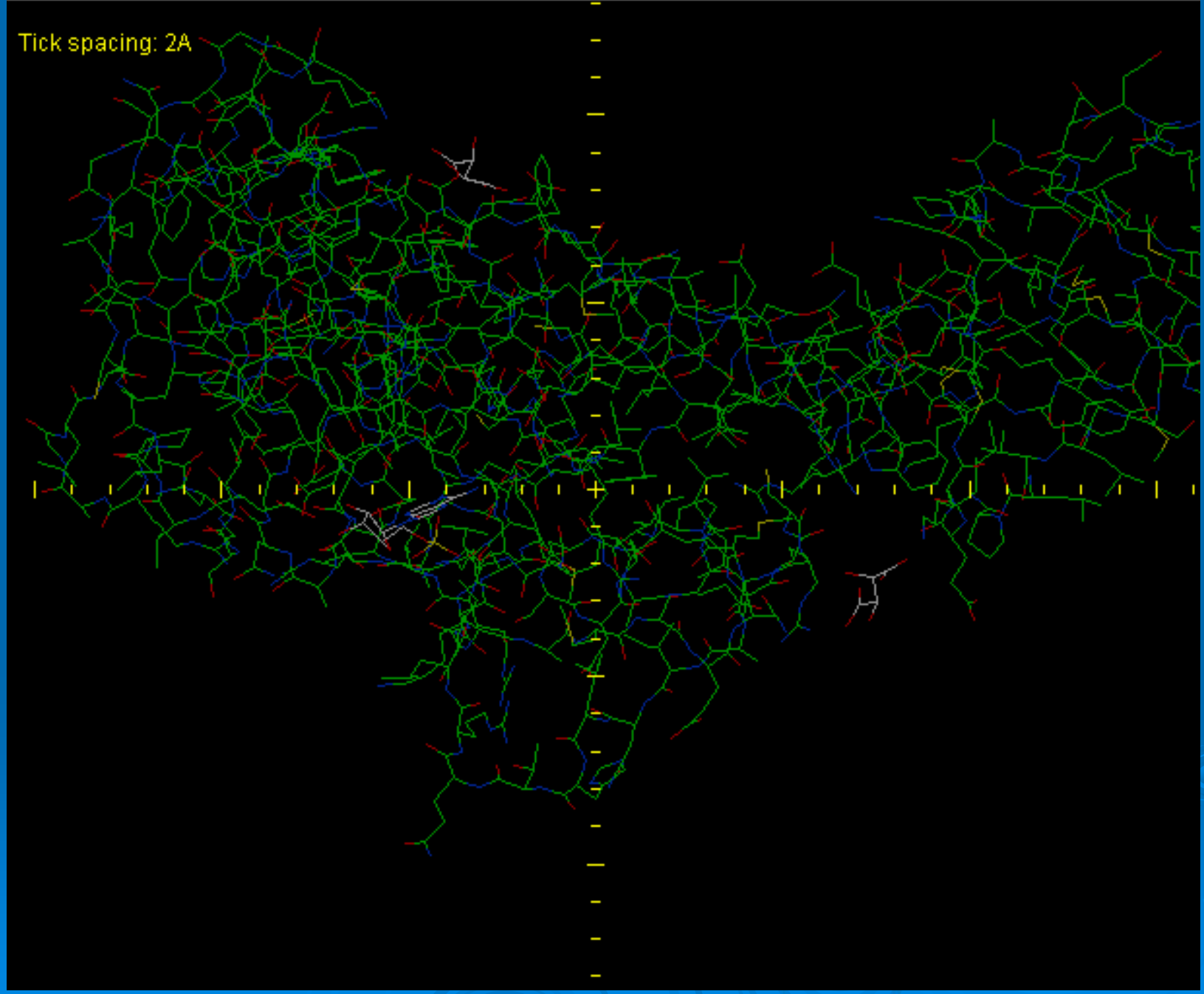

Msure
Msure
=====
Dist
Angle
Dihed
Clash
HBond
omega
----
Pack
----
Ruler
clear



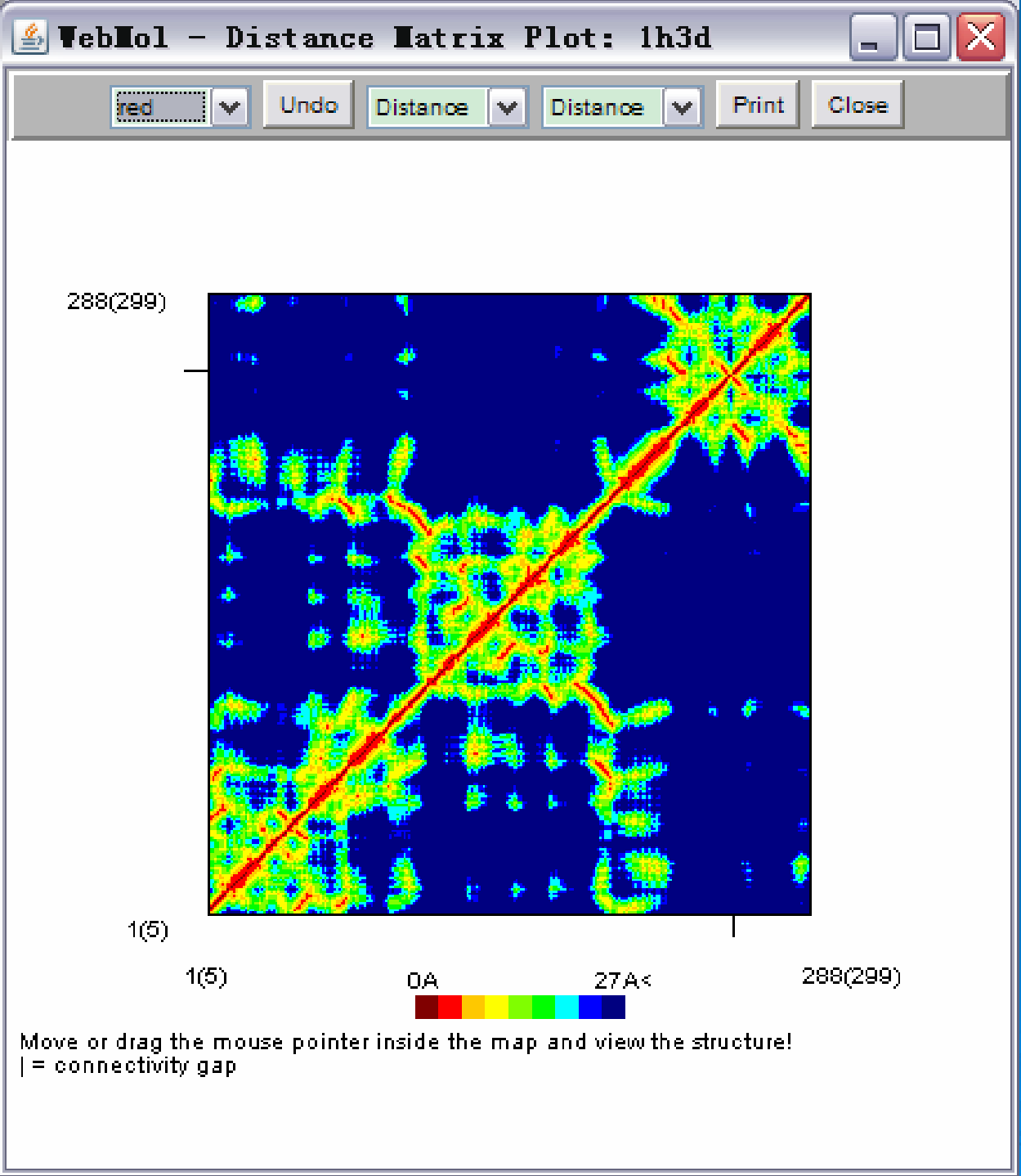
Clash：显示测链和测链的空间重叠




Pack：分析二级结构包装几何学




尺子

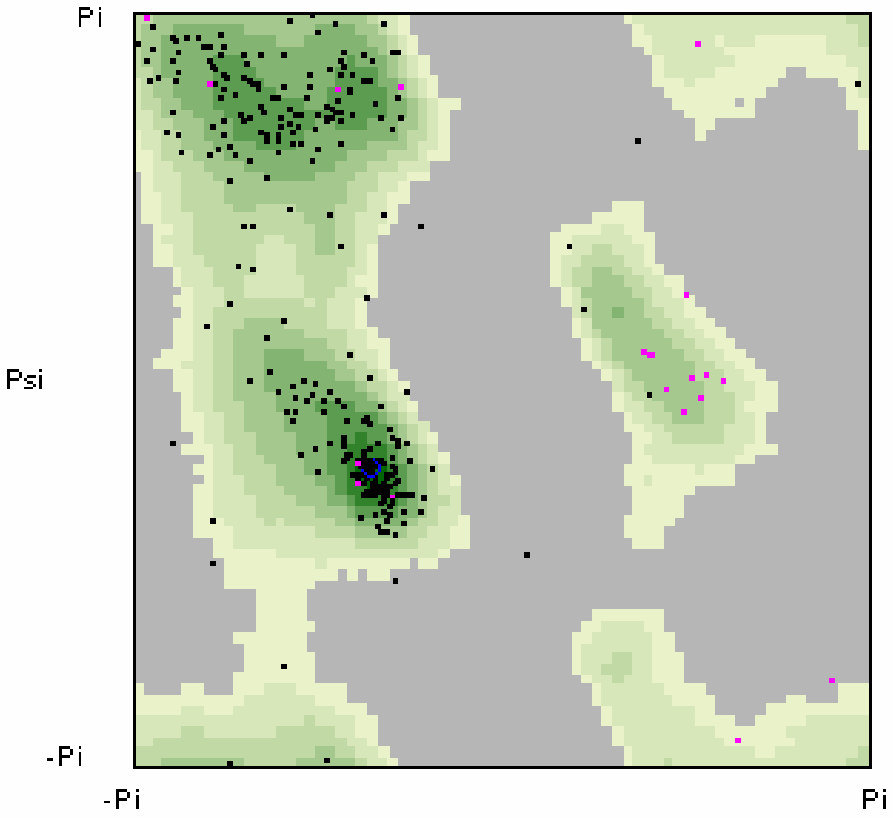



DMat/DMOff Distance Matrix Plot based on Calpha distance range = 0.0A(red) - 27A(blue)

WebMol - Ramachandran Plot: 1h3d

Type: log(N) red Undo Print Close

▪ Gly; Select residue(s) by mouse clicking or dragging either here or in the structure



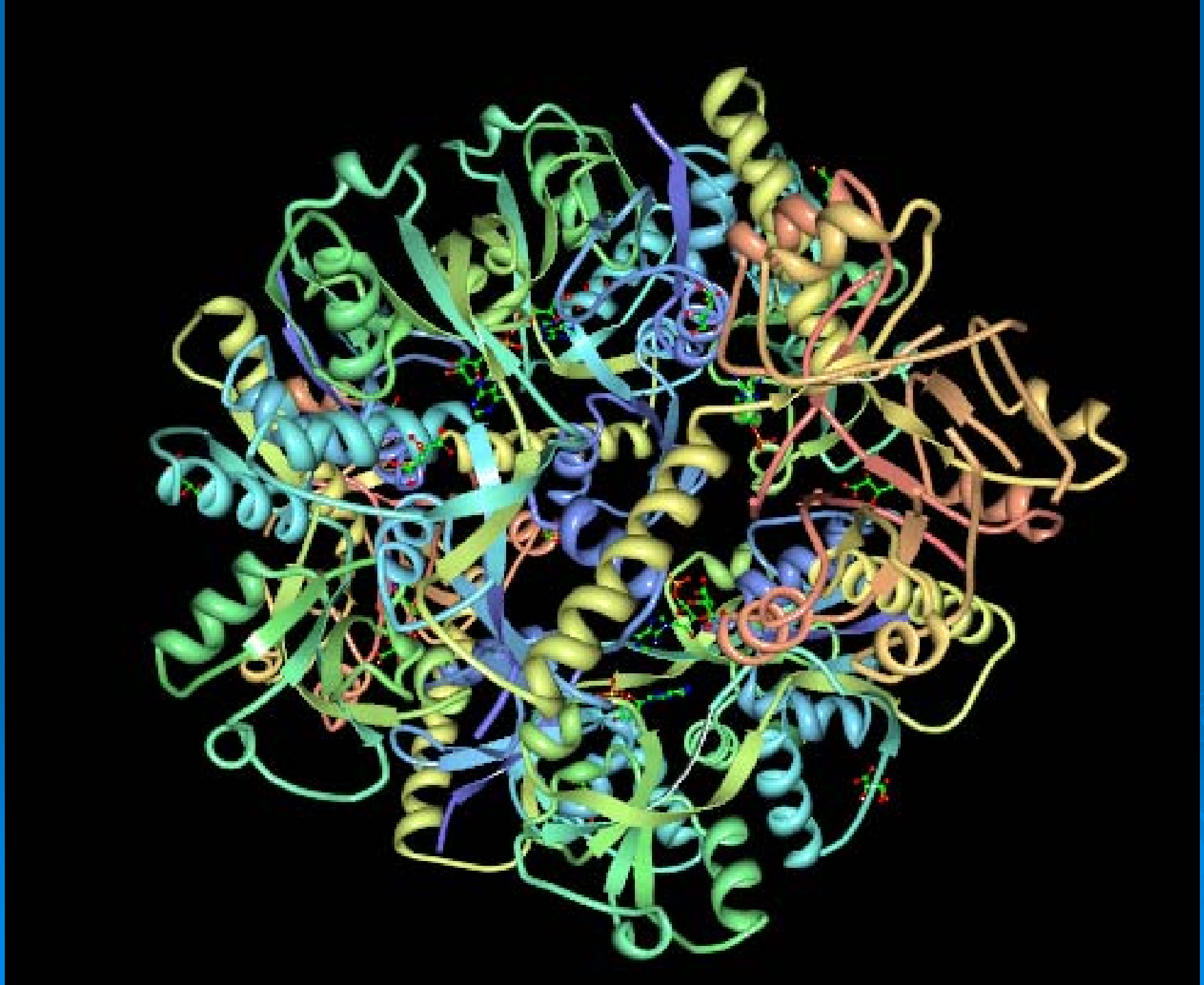

20(16) D -63 -36

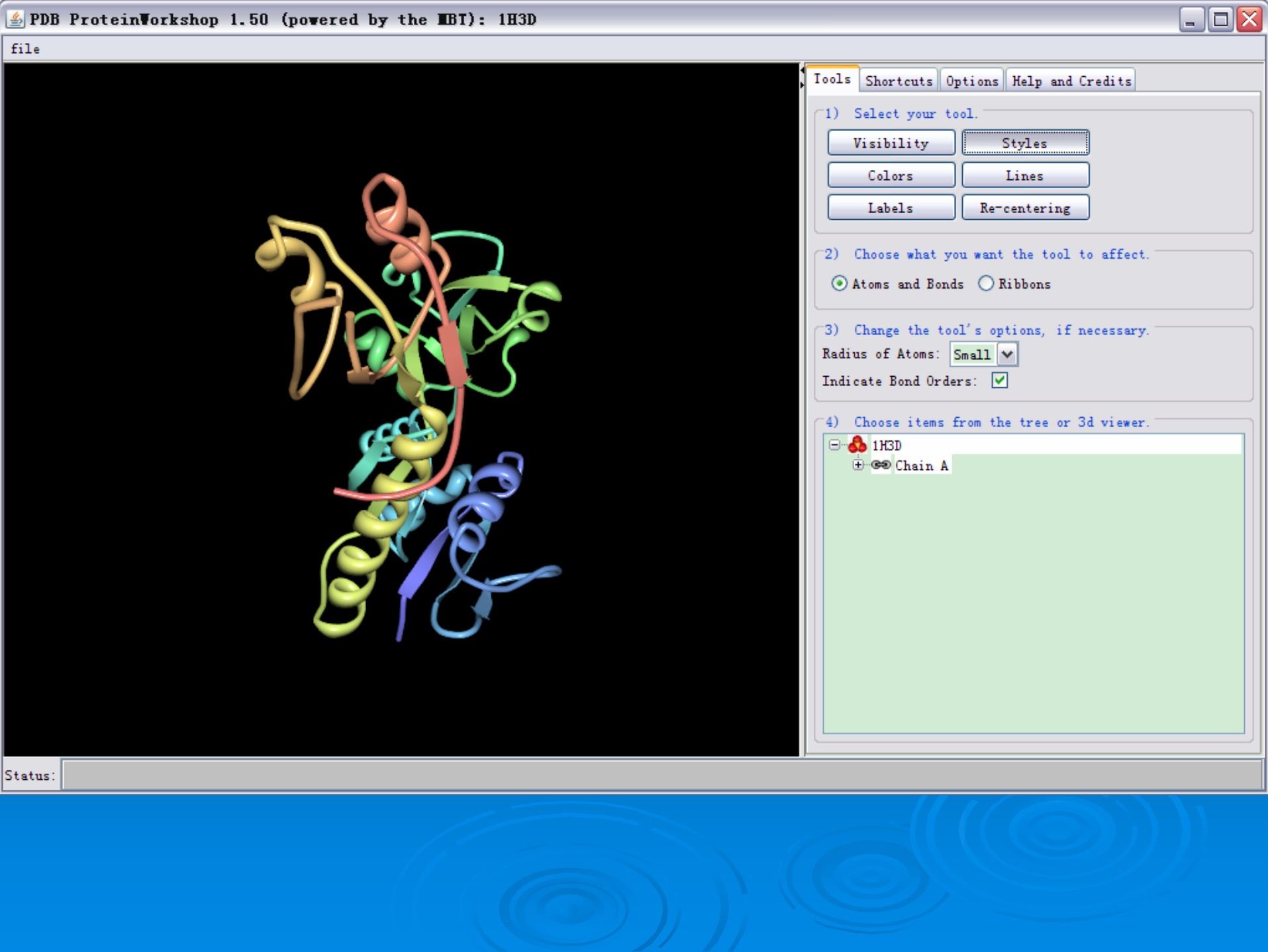
Reference map: heuristic Ramachandran map with color scale according to log(N)

# MBT SimpleViewer & Protein Workshop

软件优点：图形显示好，适合文章图片的使用；可显示分子整体结构；

软件缺点：功能简单，只可进行距离测量和标记等基本功能

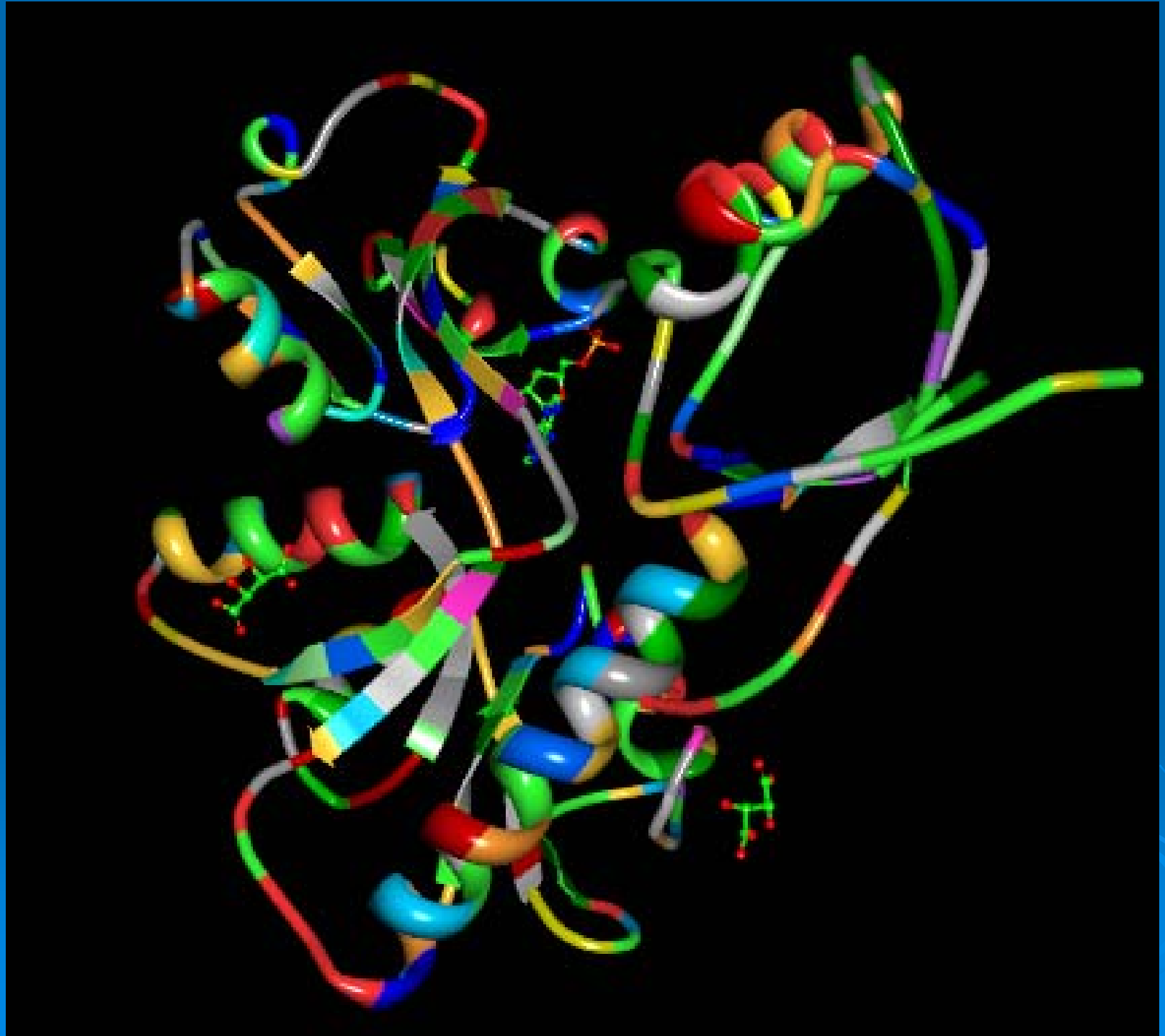



PDB ProteinWorkshop 1.50 (powered by the MBT): 1H3D
file
Tools
Shortcuts
Options
Help and Credits
1) Select your tool.
Visibility
Styles
Colors
Lines
Labels
Re-centering
2) Choose what you want the tool to affect.
Atoms and Bonds
Ribbons
3) Change the tool's options, if necessary.
Radius of Atoms:
Small
Indicate Bond Orders:
4) Choose items from the tree or 3d viewer.
1H3D
Chain A
Status:

Recolor the backbone by...

- Chain Color Ramp
- Conformation Type
- Hydrophobicity
- By Compound

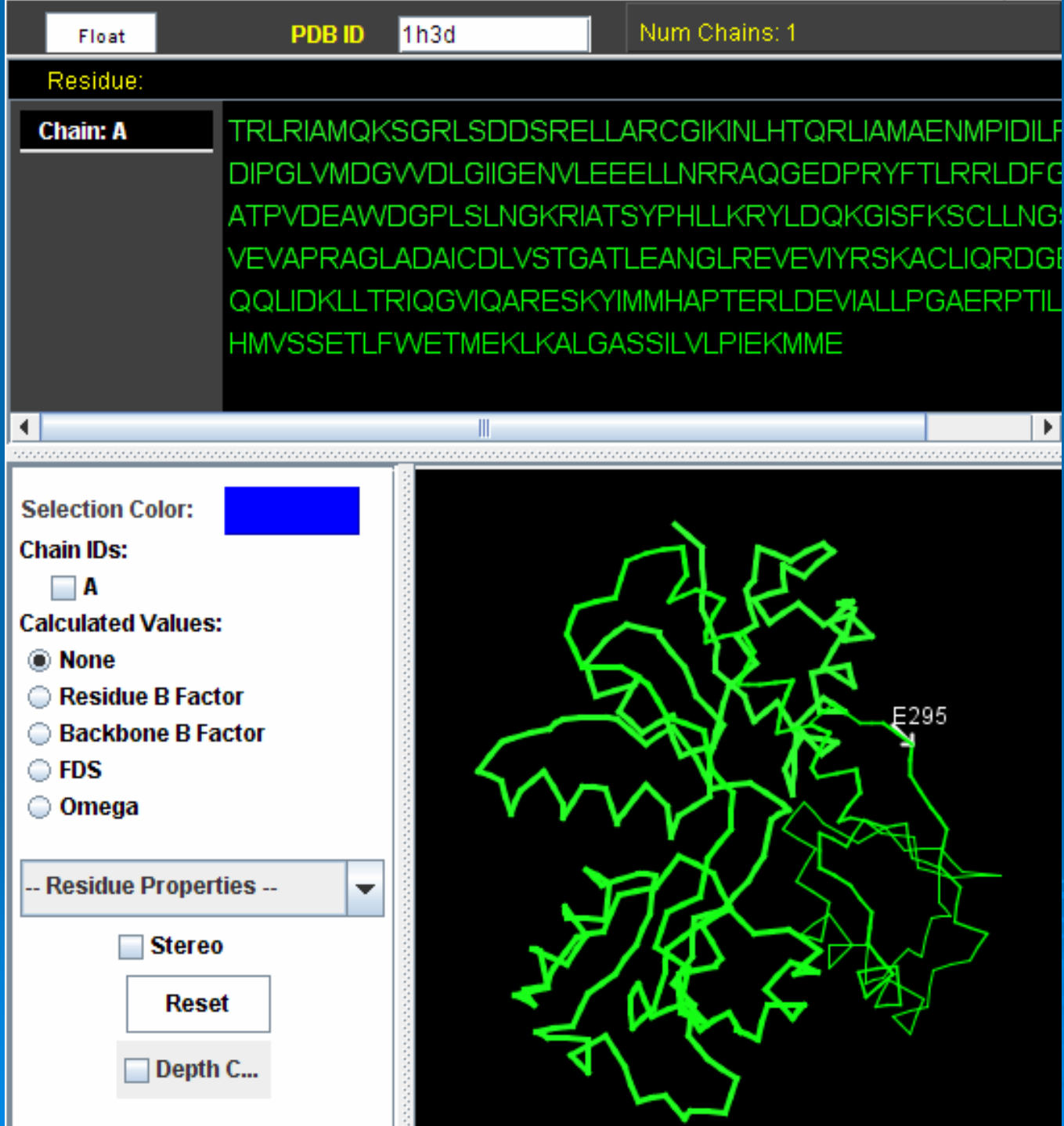
Enact

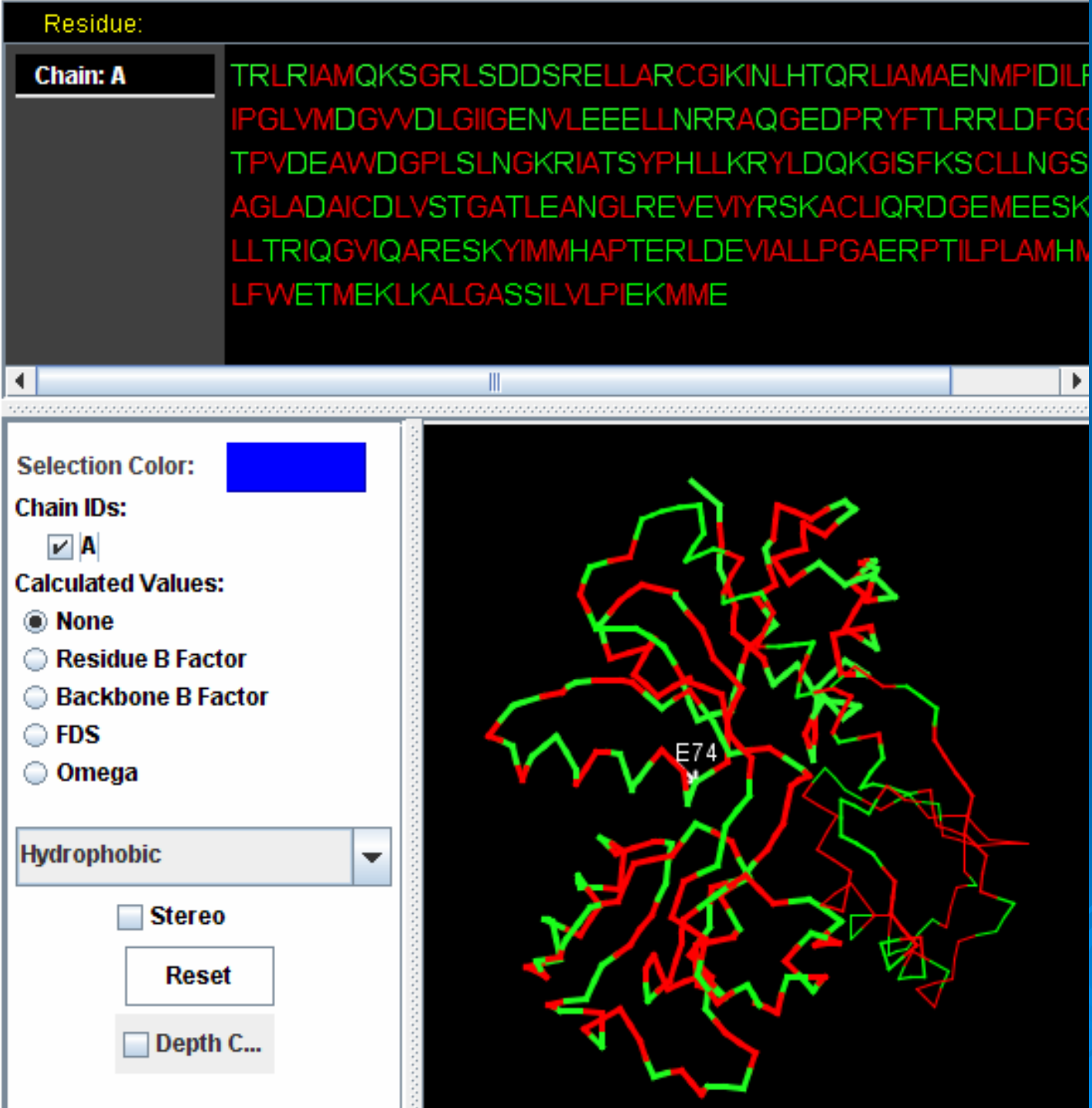


# Quick PDB

软件优点：显示蛋白质的氨基酸序列；操作简单；主要通过颜色显示结构差异

软件缺点：功能单一


Float
PDB ID
1h3d
Num Chains: 1
Residue:
Chain: A
TRLRIAMQKSGRLSDDSRELLARCGIKINLHTQRLIAMAENMPIDILR
DIPGLVMDGVVDLGIIGENVLEEELLNRRAQGEDPRYFTLRRLDFG
ATPVDEAWDGPLSLNGKRIATSYPHLLKRYLDQKGISFKSCLLNG
VEVAPRAGLADAICDLVSTGATLEANGLREVEVIYRSKACLIQRDGE
QQLIDKLLTRIQGVIQARESKYIMMHAPTERLDEVIALLPGAERPTIL
HMVSSETLFWETMEKLKALGASSILVLPIEKMME
Selection Color:
Chain IDs:
A
Calculated Values:
None
Residue B Factor
Backbone B Factor
FDS
Omega
-- Residue Properties --
Stereo
Reset
Depth C...
E295




通过红色显示出该蛋白质的疏水性氨基酸

# 总结

以上五种图形分析软件各有自己的特点，可以在网上直接操作也是其优势之一。我们平时所用的Swiss-Pdbviewer 对以上软件在功能上起到了很好的补充作用。

Thanks!