Protein Data Bank Tutorial

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Google search “protein Data Bank”

www.rcsb.org

PDB structures…

- http://www.rcsb.org/pdb/
- Viewers: Rasmol, Swiss-Pdb Viewer,

- Find your favorite protein, save as a text file or save with a .pdb extension

Can search for structures

Crystal file

```
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<BODY><PRE>HEADER    CELL ADHESION                           28-AUG-01   1JV2
TITLE     CRYSTAL STRUCTURE OF THE EXTRACELLULAR SEGMENT OF INTEGRIN
TITLE    2 ALPHAVBETA3
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: INTEGRIN, ALPHA V;
COMPND   3 CHAIN: A;
COMPND   4 FRAGMENT: RESIDUES 31-987;
COMPND   5 SYNONYM: VITRONECTIN RECEPTOR, ALPHA POLYPEPTIDE, ANTIGEN
COMPND   6 CD51;
COMPND   7 ENGINEERED: YES;
COMPND   8 MOL_ID: 2;
COMPND   9 MOLECULE: PLATELET MEMBRANE GLYCOPROTEIN IIIA BETA SUBUNIT;
COMPND  10 CHAIN: B;
COMPND  11 FRAGMENT: RESIDUES 27-718;
COMPND  12 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   3 ORGANISM_COMMON: HUMAN;
SOURCE   4 EXPRESSION_SYSTEM: SPODOPTERA FRUGIPERDA;
SOURCE   5 EXPRESSION_SYSTEM_COMMON: FALL ARMYWORM;
SOURCE   6 MOL_ID: 2;
SOURCE   7 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   8 ORGANISM_COMMON: HUMAN;
SOURCE   9 EXPRESSION_SYSTEM: SPODOPTERA FRUGIPERDA;
SOURCE  10 EXPRESSION_SYSTEM_COMMON: FALL ARMYWORM
KEYWDS    GENU, HYBRID DOMAIN, BETA-TAIL DOMAIN, PSI DOMAIN, EGF
KEYWDS   2 DOMAIN, MIDAS, ADMIDAS, CAGE MOTIF, PROPELLER, A-DOMAIN,
KEYWDS   3 THIGH DOMAIN, CALF DOMAIN
EXPDTA    X-RAY DIFFRACTION
AUTHOR    J.P.XIONG,T.STEHLE,B.DIEFENBACH,R.ZHANG,R.DUNKER,D.SCOTT,
AUTHOR   2 A.JOACHIMIAK,S.L.GOODMAN,M.A.ARNAOUT
REVDAT   1   17-OCT-01 1JV2    0
JRNL        AUTH   J.-P.XIONG,T.STEHLE,B.DIEFENBACH,R.ZHANG,R.DUNKER,
JRNL        AUTH 2 D.L.SCOTT,A.JOACHIMIAK,S.L.GOODMAN,M.A.ARNAOUT
JRNL        TITL   CRYSTAL STRUCTURE OF THE EXTRACELLULAR SEGMENT OF
JRNL        TITL 2 INTEGRIN {ALPHA}V{BETA}3
JRNL        REF    SCIENCE                       V. 294   339 2001
JRNL        REFN   ASTM SCIEAS  US ISSN 0036-8075
REMARK   1
REMARK   2
REMARK   2 RESOLUTION. 3.10 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : X-PLOR 3.851
REMARK   3   AUTHORS     : BRUNGER
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 3.10
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 20.00
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 2.000
REMARK   3   DATA CUTOFF HIGH         (ABS(F)) : NULL
```

.pdb reference code

species

Authors, look up the papers

resolution

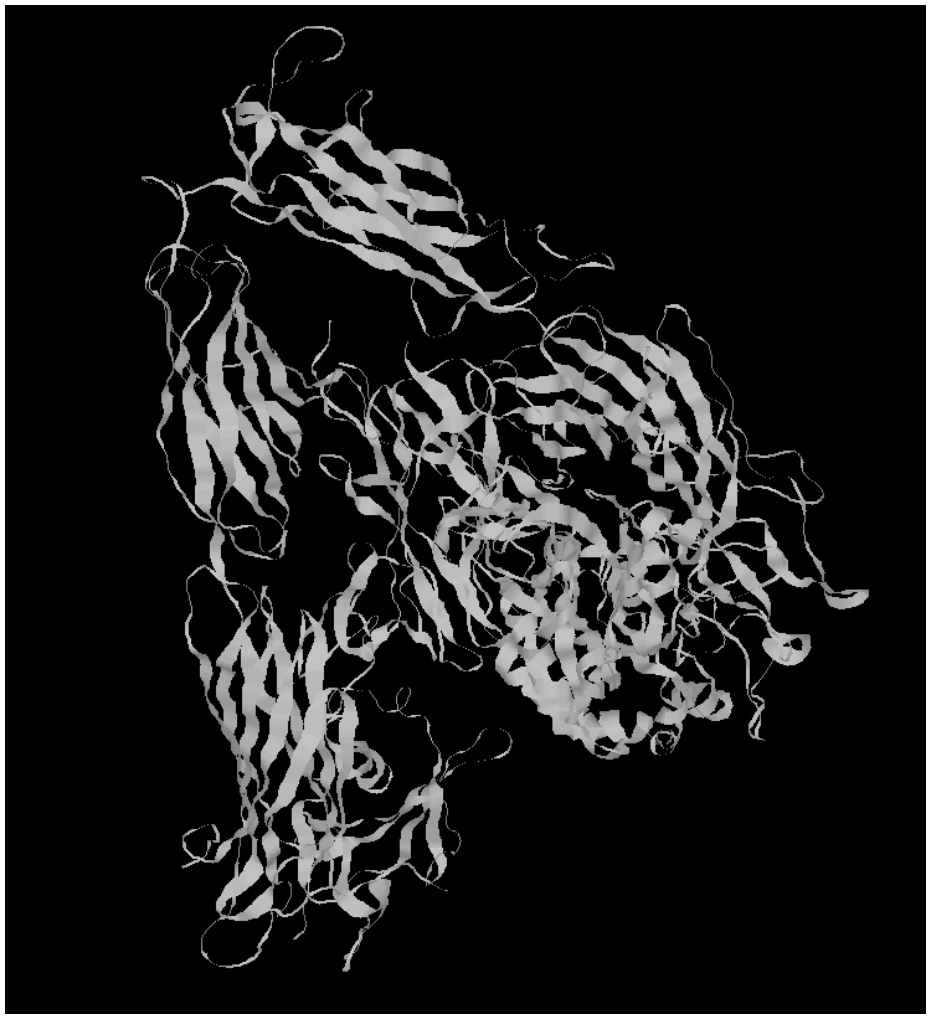
Coordinate information available

		x	y	z		
ATOM 1334 N	**CYS 168**	**31.690**	**17.042**	**22.831**	**1.00**	**24.35 N**
ATOM 1335 CA	**CYS 168**	**30.949**	**17.421**	**24.027**	**1.00**	**23.50 C**
ATOM 1336 C	**CYS 168**	**31.590**	**18.646**	**24.666**	**1.00**	**21.29 C**
ATOM 1337 O	**CYS 168**	**32.812**	**18.714**	**24.849**	**1.00**	**20.60 O**
ATOM 1338 CB	**CYS 168**	**30.878**	**16.279**	**25.047**	**1.00**	**18.87 C**
ATOM 1339 SG	**CYS 168**	**29.632**	**16.551**	**26.342**	**1.00**	**21.22 S**

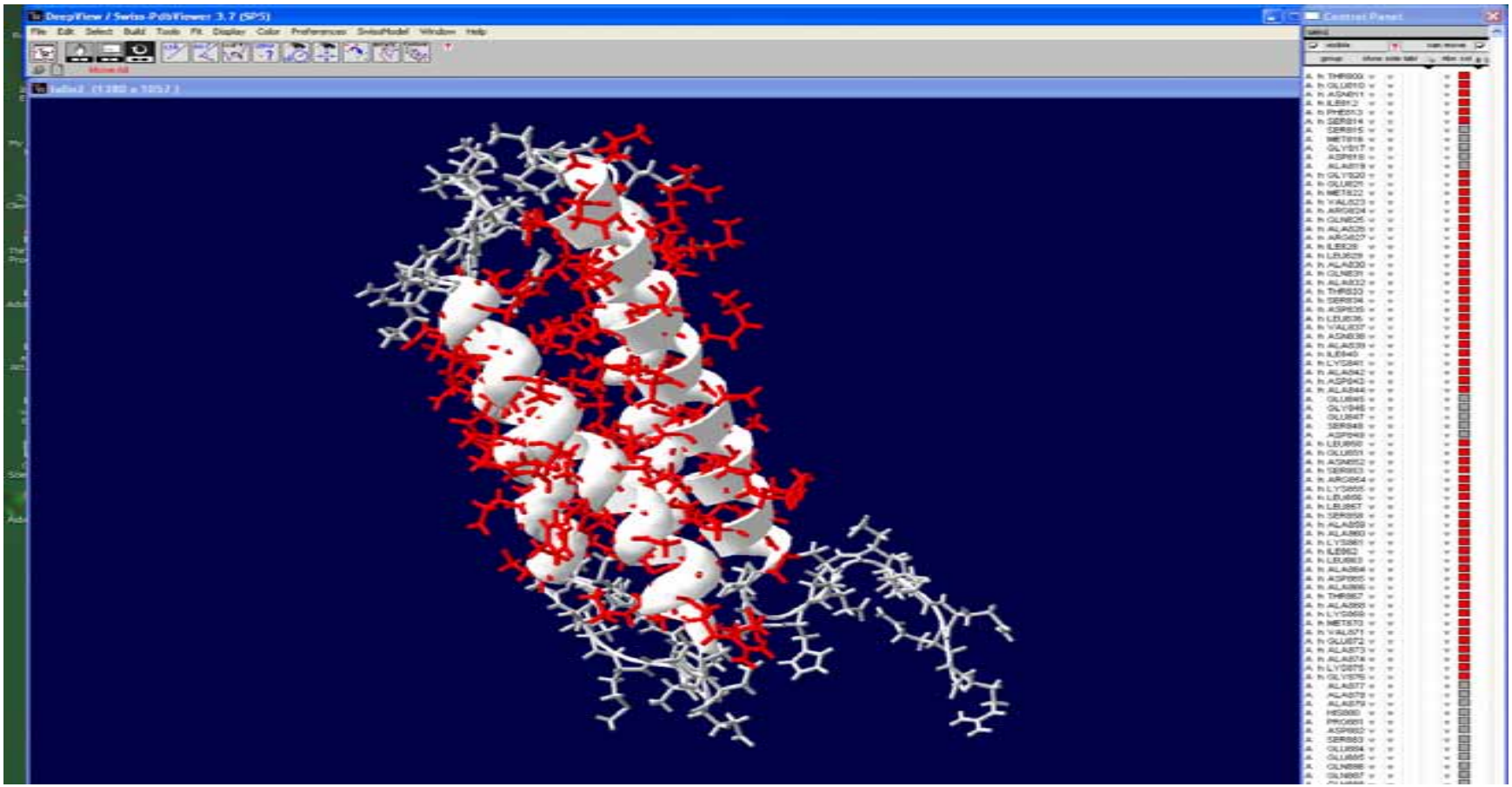
CYS #168

You can do math (distances, angles etc.) directly with this Coordinate info

Ribbon display, and many others

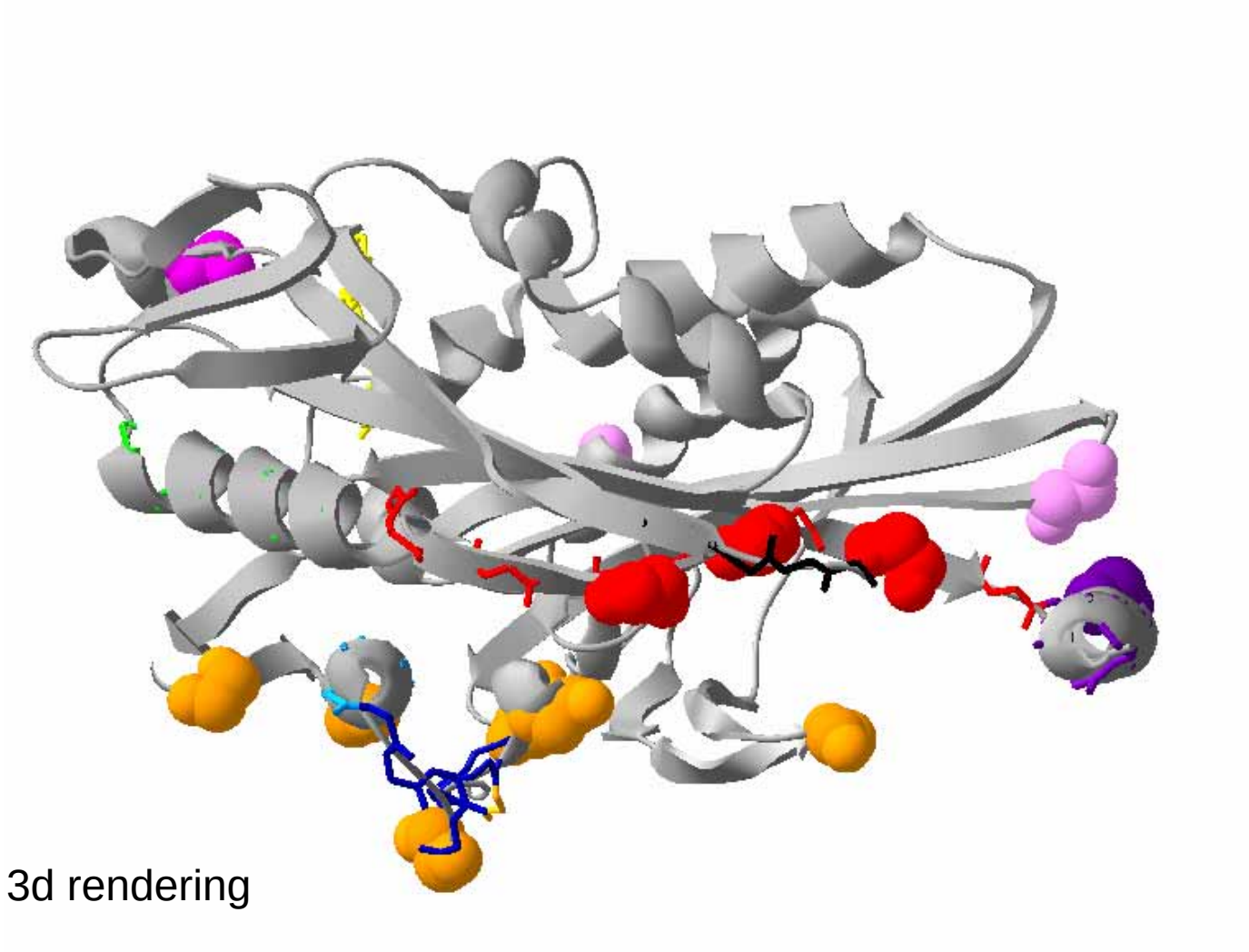


Swiss PDB viewer



Many other viewers, Rasmol, VIPER (virus structures)

MT binding to kinesin



Turn on 3d rendering

Highlight residues of interest

Align structures

Compare species