

Protein Data Bank Tutorial

Matthew Lang 20.310

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www.rcsb.org

PDB structures...

- <http://www.rcsb.org/pdb/>
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Can search for structures

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The Protein Data Bank (PDB) is operated by Rutgers, The State University of New Jersey; the San Diego Supercomputer Center at the University of California, San Diego; and the Center for Advanced Research in Biotechnology of the National Institute of Standards and Technology -- three members of the [Research Collaboratory for Structural Bioinformatics \(RCSB\)](#).

The RCSB PDB is supported by funds from the National Science Foundation (NSF), the National Institute of General Medical Sciences (NIGMS), the Department of Energy (DOE), the National Library of Medicine (NLM), the National Cancer Institute (NCI), the National Center for Research Resources (NCRR), the National Institute of Biomedical Imaging and Bioengineering (NIBIB), and the National Institute of Neurological Disorders and Stroke (NINDS).

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PROTEIN DATA BANK

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30-Mar-2004
[RCSB PDB at RECOMB and National Science Teachers Association's National Convention](#) A demonstration on using the re-engineered RCSB PDB web site will be given and an RCSB PDB Poster Prize will be awarded at the Eighth Annual International Conference on Research in Computational Molecular Biology (RECOMB 2004, March 27-31, San Diego, CA). [\[MORE\]](#)

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In citing the PDB please refer to:

H.M. Berman, J. Westbrook, Z. Feng, G. Gilliland, T.N. Ehat, H. Weissig, I.N. Shindyalov, P.E. Bourne: [The Protein Data Bank](#), *Nucleic Acids Research*, 28 pp. 235-242 (2000)

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 RCSB

Crystal file

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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 CDS1;
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
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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.JOACHIMIYAK,S.L.GOODMAN,M.A.ARNAOUT
REVDTAT    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.JOACHIMIYAK,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
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REMARK     3 DATA CUTOFF HIGH (ABS(F)) : NULL
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.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

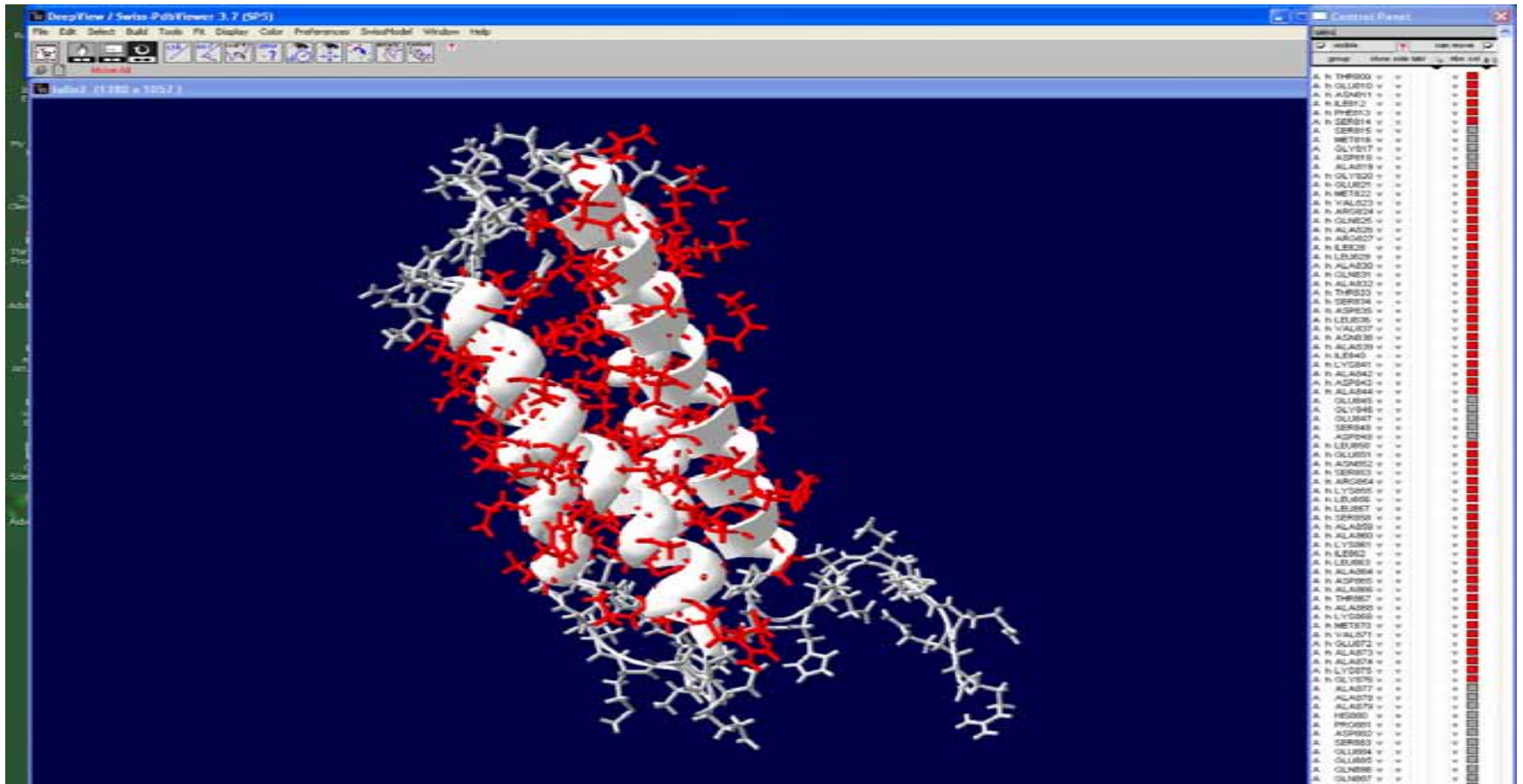
CYS #168

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

Ribbon display, and many others

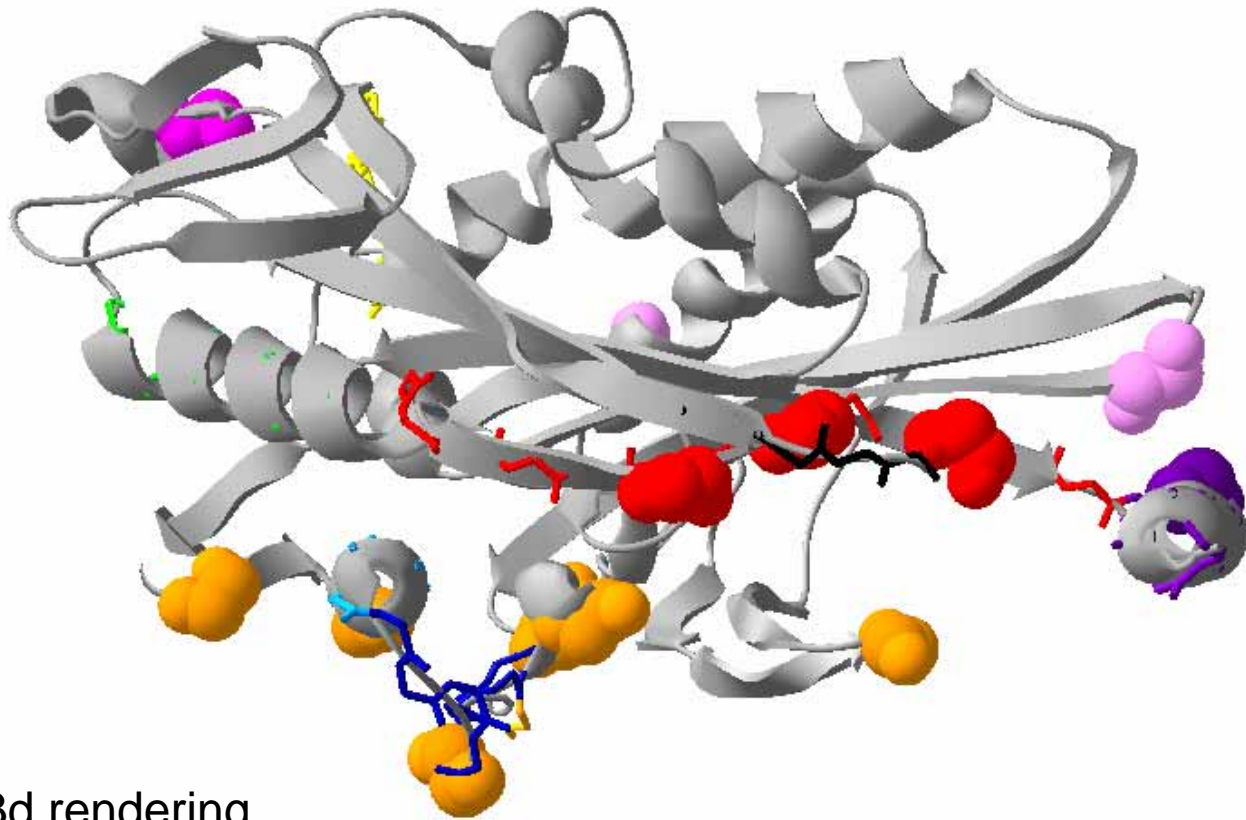


Swiss PDB viewer



Many other viewers, Rasmol, VIPER (virus structures)

MT binding to kinesin



Turn on 3d rendering

Highlight residues of interest

Align structures

Align

? ?

2KIN LAGSEKVAKNI NKSL SALGNVI SALAEETTHVPT RDKMTRI LQDSLDGNCRTT
1BG2 GSEKVS TGAEGAVL DEAKNI NKSL SALGNVI SALAEETTYVPT RDKMTRI LQD

1BG2: GLU236 rms: 37.21

Compare species