

PDB's, protein structure, and dynamics

A few additional details about the RCSB and structural biology

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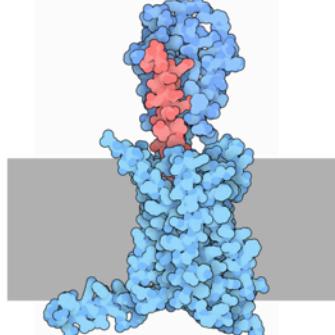
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A Structural View of Biology
This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.
As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.
The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

Structure and Health Focus: HIV


April Molecule of the Month

Glucagon

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STRUCTURE OF THE FIRST C2-DOMAIN OF SYNAPTOTAGMIN I: A NOVEL CA₂₊(SLASH)PHOSPHOLIPID BINDING FOLD

DOI:10.2210/pdb1rsy/pdb

Primary Citation

Structure of the first C2 domain of synaptotagmin I: a novel Ca₂₊/phospholipid-binding fold.

Sutton, R.B. , Davletov, B.A. , Berghuis, A.M. , Sudhof, T.C. , Sprang, S.R. 

Journal: (1995) Cell(Cambridge,Mass.) **80**: 929-938

PubMed: [7697723](#)  Search Related Articles in PubMed 

PubMed Abstract:

C2 domains are regulatory sequence motifs that occur widely in nature. Synaptotagmin I, a synaptic vesicle protein involved in the Ca₂₊ regulation of exocytosis, contains two C2 domains, the first of which acts as a Ca₂₊ sensor. We now describe the three-dimensional structure of this C2 domain at 1.9 Å resolution in both the Ca(2+)-bound and Ca(2+)-free forms. The C2 polypeptide forms an eight-stranded beta sandwich constructed around a conserved four-stranded motif designated as a C2 key. Ca₂₊ binds in a cup-shaped depression between two polypeptide loops located at the N- and C-termini of the C2-key motif.

Keywords:
Amino Acid Sequence, Base Sequence, Binding Sites, Calcium, Calcium-Binding Proteins, Conserved Sequence, Exocytosis, Liposomes, Membrane Glycoproteins, Models, Molecular, Molecular Sequence Data, Mutagenesis, Site-Directed, Nerve Tissue Proteins, Oligodeoxyribonucleotides, Phosphatidylcholines, Phosphatidylserines, Phospholipids, Protein Folding, Protein Structure, Secondary, Recombinant Proteins, Sequence Homology, Amino Acid, Synaptic Vesicles, Synaptotagmin I, Synaptotagmins

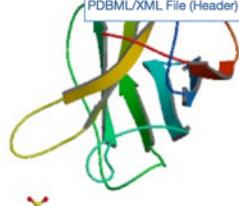
Related Structures:
Also Cited By: [4WEE](#)

Organizational Affiliation:
Department of Biochemistry, University of Texas Southwestern Medical Center, Dallas 75235.

1RSY  

Bio

- FASTA Sequence
- PDB File
- PDB File (Header)
- mmCIF File
- mmCIF File (Header)
- PDBML/XML File
- PDBML/XML File (Header)



 [3D View](#) [More Images...](#)

Stoichiometry: Monomer
Biological assembly 1 assigned by authors

Downloadable viewers:
[Simple Viewer](#) [Protein Workshop](#) [Kiosk Viewer](#)

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The most important values are on the right

Click on abstract words and keywords to add them to the search box.

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Molecular Description

Classification: Calcium/phospholipid Binding Protein [P](#)

Structure Weight: 17194.56 [?](#)

Molecule: SYNAPTOTAGMIN I

Polymer: 1 **Type:** protein **Length:** 152

Chains: A

Organism: Rattus norvegicus [P](#)

Gene Name: Syt1

UniProtKB: [Protein Feature View](#) | Search PDB [P](#) | P21707 [?](#)

UniProtKB

- P21707
- Molec. Processing
- Motif
- UP Sites
- SCOP domains
- PDB Sites
- Secstruc
- 1RSY.A

Deposition Summary

Authors: Sutton, R.B. [P](#), Sprang, S.R. [P](#)

Deposition: 1995-02-01

Release: 1995-05-08

Last Modified (REVDAT): 2009-02-24

Revision History

Mouse over text for details

2011-07-13
Version format compliance

Experimental Details

Method: X-RAY DIFFRACTION

Exp. Data: N/A

Resolution[Å]:	1.90
R-Value:	0.186 (obs.)
R-Free:	0.249
Space Group:	P 1 2 1 1 P

Unit Cell:

Length [Å]	Angles [°]
a = 42.30	α = 90.00
b = 38.90	β = 96.90
c = 44.60	γ = 90.00

Structure Validation

View the full validation report [?](#)

Metric	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		2.6%

■ Percentile relative to all X-ray structures
□ Percentile relative to X-ray structures of similar resolution

A reminder: the file contains a 3D position for every atom

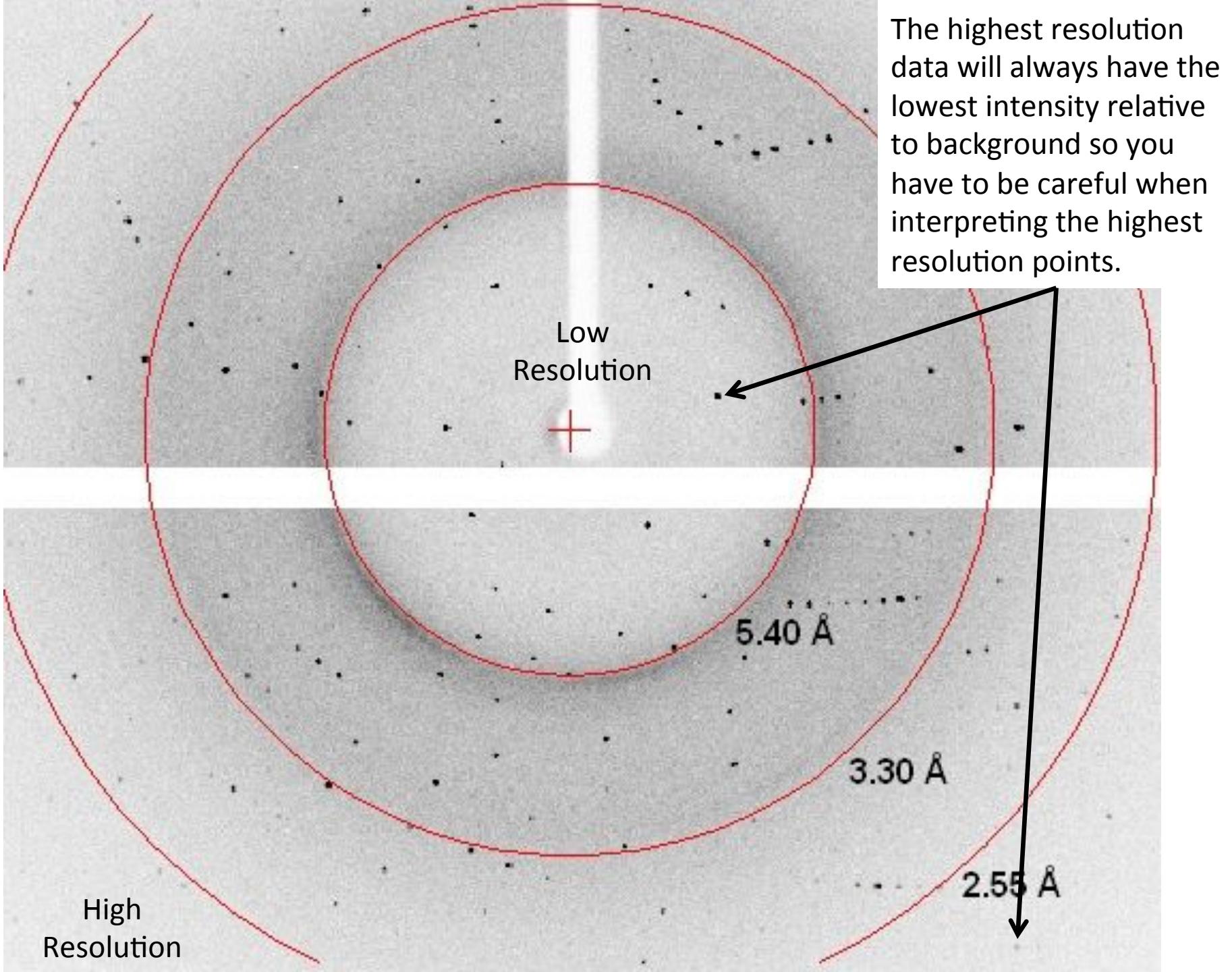
	Atom Number										
	Atom Type	Amino Acid	Residue Number		X	Y	Z		b-factor		
ATOM	58	N	GLU	A	140	17.190	20.090	9.663	1.00	19.75	N
ATOM	59	CA	GLU	A	140	16.873	18.811	10.312	1.00	21.60	C
ATOM	60	C	GLU	A	140	17.310	17.646	9.425	1.00	19.94	C
ATOM	61	O	GLU	A	140	17.241	17.719	8.198	1.00	17.93	O
ATOM	62	CB	GLU	A	140	15.374	18.717	10.600	1.00	20.06	C
ATOM	63	CG	GLU	A	140	14.927	19.739	11.636	1.00	25.25	C
ATOM	64	CD	GLU	A	140	13.449	20.065	11.557	1.00	30.82	C
ATOM	65	OE1	GLU	A	140	12.846	19.863	10.479	1.00	32.21	O
ATOM	66	OE2	GLU	A	140	12.891	20.535	12.577	1.00	31.01	O

The PDB file contains a lot of other info: these are important

REMARK 1
REMARK 1 REFERENCE 1
REMARK 1 AUTH B.A.DAVLETOV,T.C.SUDHOF
REMARK 1 TITL A SINGLE C2 DOMAIN FROM SYNAPTOTAGMIN I IS
REMARK 1 TITL 2 SUFFICIENT FOR HIGH AFFINITY
REMARK 1 TITL 3 CA2+(SLASH)PHOSPHOLIPID BINDING
REMARK 1 REF J.BIOL.CHEM. V. 268 26386 1993
REMARK 1 REFN ISSN 0021-9258
REMARK 2
REMARK 2 RESOLUTION. 1.90 ANGSTROMS.
REMARK 3
REMARK 3 REFINEMENT.
REMARK 3 PROGRAM : X-PLOR 3.1
REMARK 3 AUTHORS : BRUNGER
REMARK 3
REMARK 3 DATA USED IN REFINEMENT.
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 1.90
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 6.00
REMARK 3 DATA CUTOFF (SIGMA(F)) : 2.000
REMARK 3 DATA CUTOFF HIGH (ABS(F)) : NULL
REMARK 3 DATA CUTOFF LOW (ABS(F)) : NULL
REMARK 3 COMPLETENESS (WORKING+TEST) (%) : 90.0
REMARK 3 NUMBER OF REFLECTIONS : 9851
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 CROSS-VALIDATION METHOD : NULL
REMARK 3 FREE R VALUE TEST SET SELECTION : NULL
REMARK 3 R VALUE (WORKING SET) : 0.186
REMARK 3 FREE R VALUE : 0.249
REMARK 3 FREE R VALUE TEST SET SIZE (%) : NULL
REMARK 3 FREE R VALUE TEST SET COUNT : NULL
REMARK 3 ESTIMATED ERROR OF FREE R VALUE : NULL
REMARK 3
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK 3 TOTAL NUMBER OF BINS USED : NULL
REMARK 3 BIN RESOLUTION RANGE HIGH (A) : NULL
REMARK 3 BIN RESOLUTION RANGE LOW (A) : NULL
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : NULL
REMARK 3 REFLECTIONS IN BIN (WORKING SET) : NULL
REMARK 3 BIN R VALUE (WORKING SET) : NULL
REMARK 3 BIN FREE R VALUE : NULL
REMARK 3 BIN FREE R VALUE TEST SET SIZE (%) : NULL
REMARK 3 BIN FREE R VALUE TEST SET COUNT : NULL
REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : NULL
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 1067
REMARK 3 NUCLEIC ACID ATOMS : 0
REMARK 3 HETEROGEN ATOMS : 5
REMARK 3 SOLVENT ATOMS : 80
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : NULL
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 24.00
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : NULL

REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY BNL.
REMARK 200
REMARK 200 EXPERIMENT DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : NULL
REMARK 200 TEMPERATURE (KELVIN) : NULL
REMARK 200 PH : NULL
REMARK 200 NUMBER OF CRYSTALS USED : NULL
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REMARK 200 SYNCHROTRON (Y/N) : N
REMARK 200 RADIATION SOURCE : NULL
REMARK 200 BEAMLINE : NULL
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A) : 1.5418
REMARK 200 MONOCHROMATOR : NULL
REMARK 200 OPTICS : NULL
REMARK 200
REMARK 200 DETECTOR TYPE : IMAGE PLATE
REMARK 200 DETECTOR MANUFACTURER : RIGAKU RAXIS IIC
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE : NULL
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REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 11214
REMARK 200 RESOLUTION RANGE HIGH (A) : NULL
REMARK 200 RESOLUTION RANGE LOW (A) : NULL
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : 2.000
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REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE (%) : 95.0
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REMARK 200 R MERGE (I) : NULL
REMARK 200 R SYM (T) : NULL
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : NULL ←
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : NULL
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A) : NULL
REMARK 200 COMPLETENESS FOR SHELL (%) : NULL
REMARK 200 DATA REDUNDANCY IN SHELL : NULL
REMARK 200 R MERGE FOR SHELL (I) : NULL
REMARK 200 R SYM FOR SHELL (I) : NULL
REMARK 200 <I/SIGMA(I)> FOR SHELL : NULL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: NULL
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: NULL
REMARK 200 SOFTWARE USED: X-PLOR 3.1
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): 42.24
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 2.13
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: NULL
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 1 21 1
REMARK 290

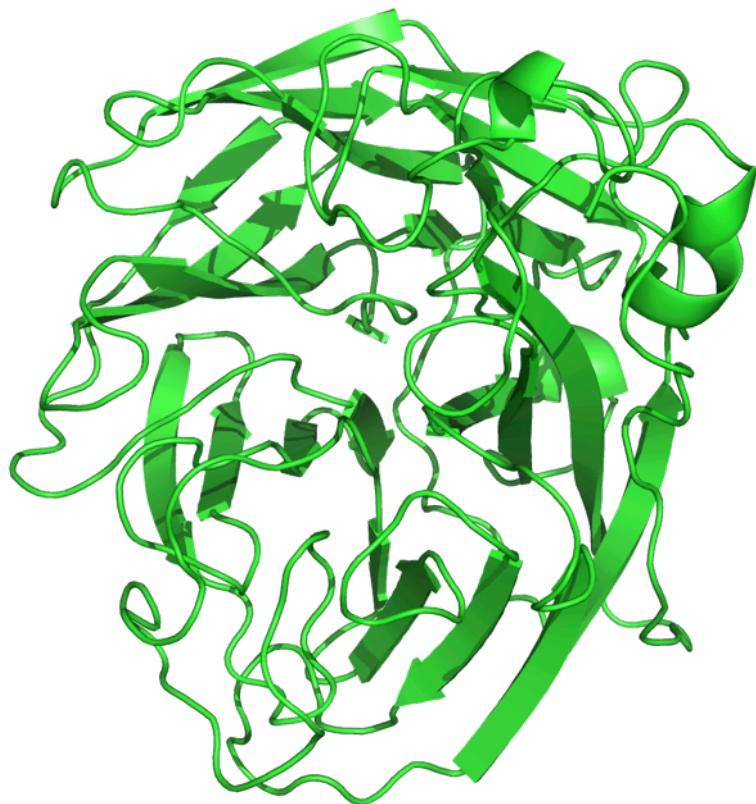
This is a problem these days. Perhaps less so in 1995.



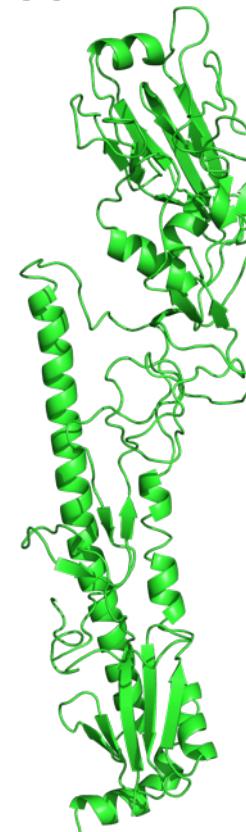
Beyond simple protein biochemistry: How
can PDB/protein structures be useful?

For most proteins, this view is not the functional biological unit

Neuraminidase: 3TI3

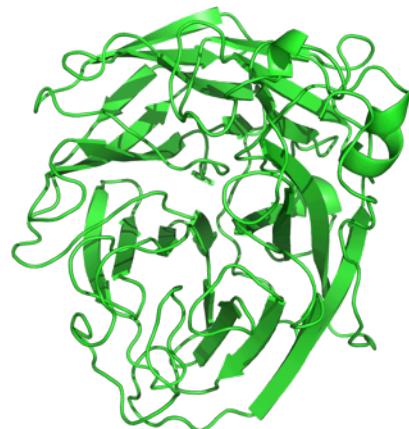


Hemagglutinin: 1RD8

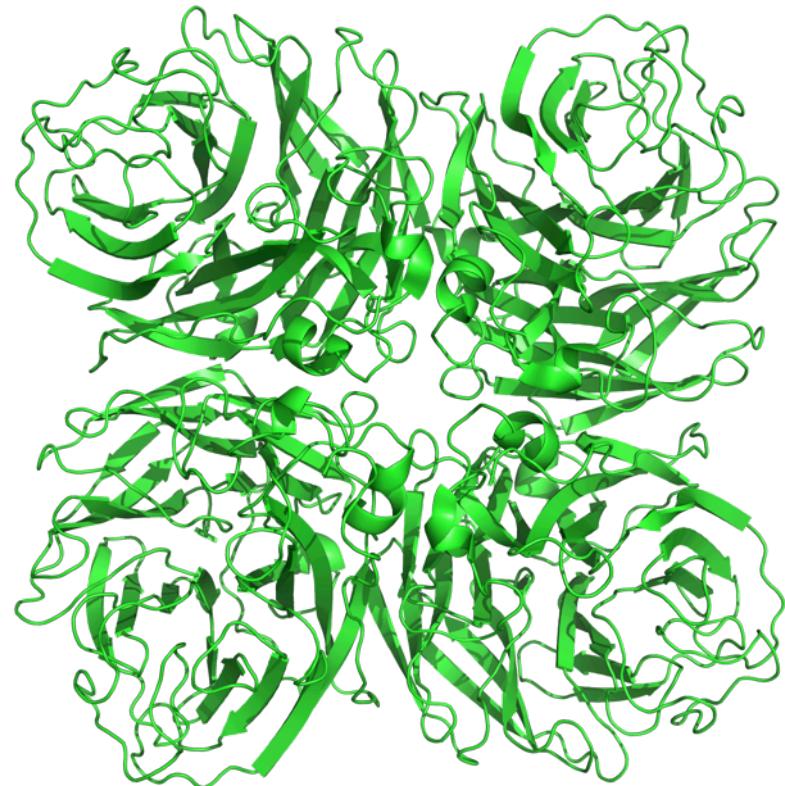


Neuraminidase is only functional as a tetramer

Neuraminidase Monomer

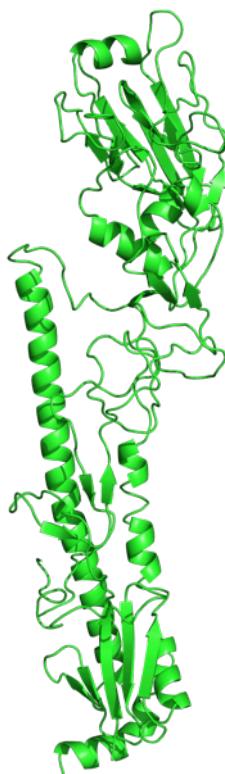


Neuraminidase Tetramer



Hemagglutinin is only functional as a trimer

Hemagglutinin Monomer

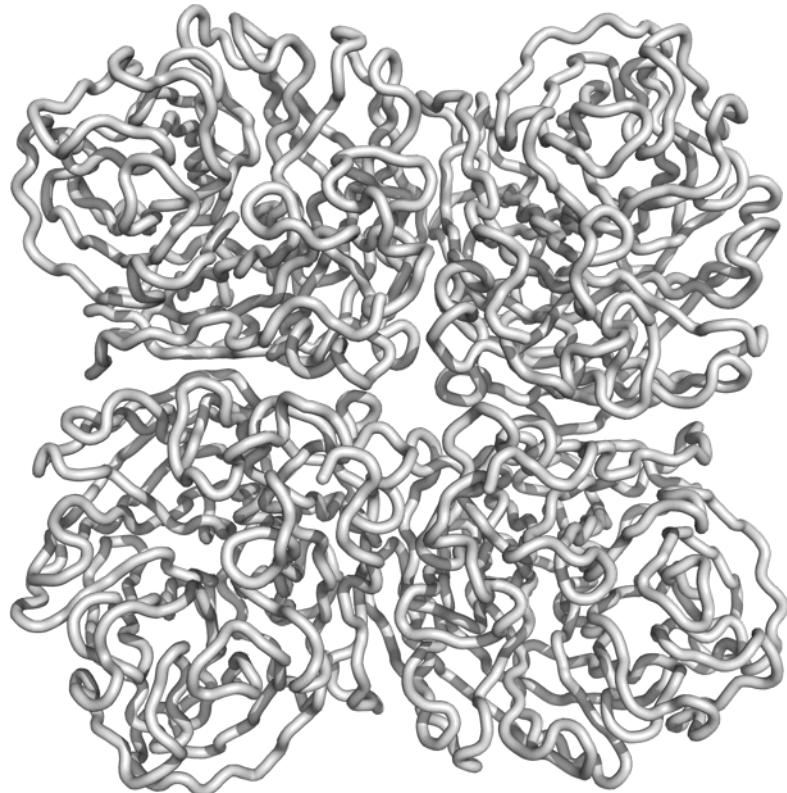


Hemagglutinin Trimer



Basic multimeric state of Influenza proteins

Neuraminidase

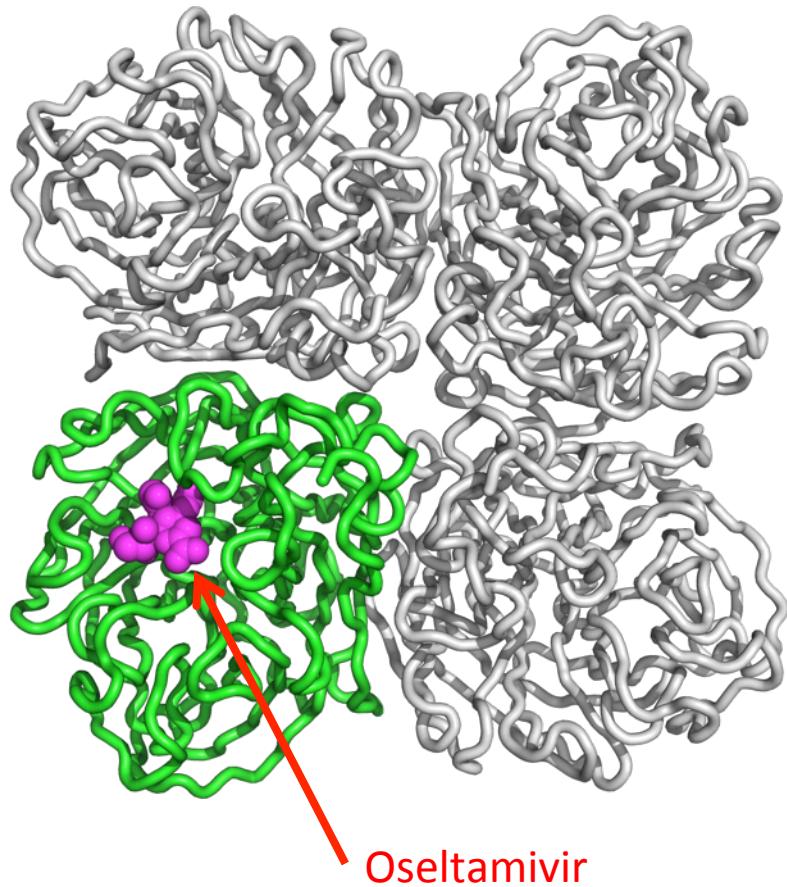


Hemagglutinin

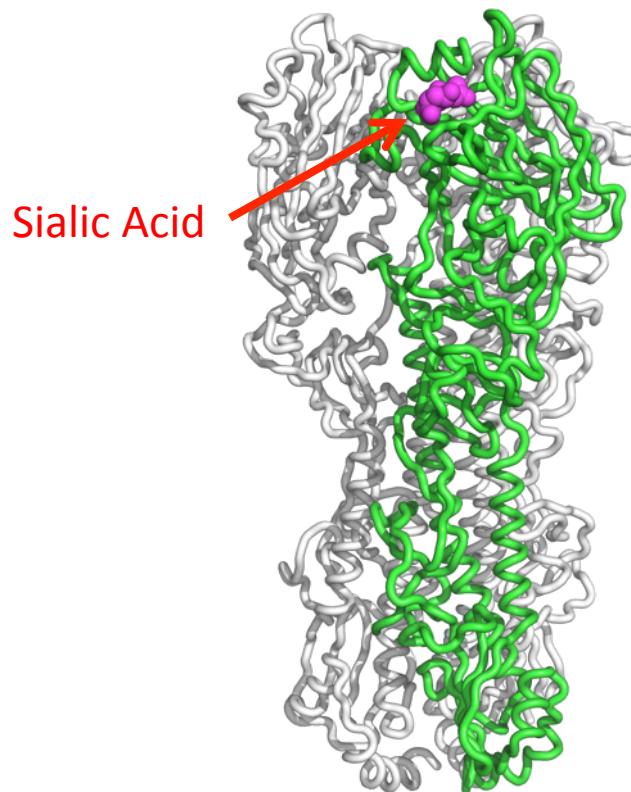


These proteins interact with small non-protein molecules

Neuraminidase w/ 1 Ligand

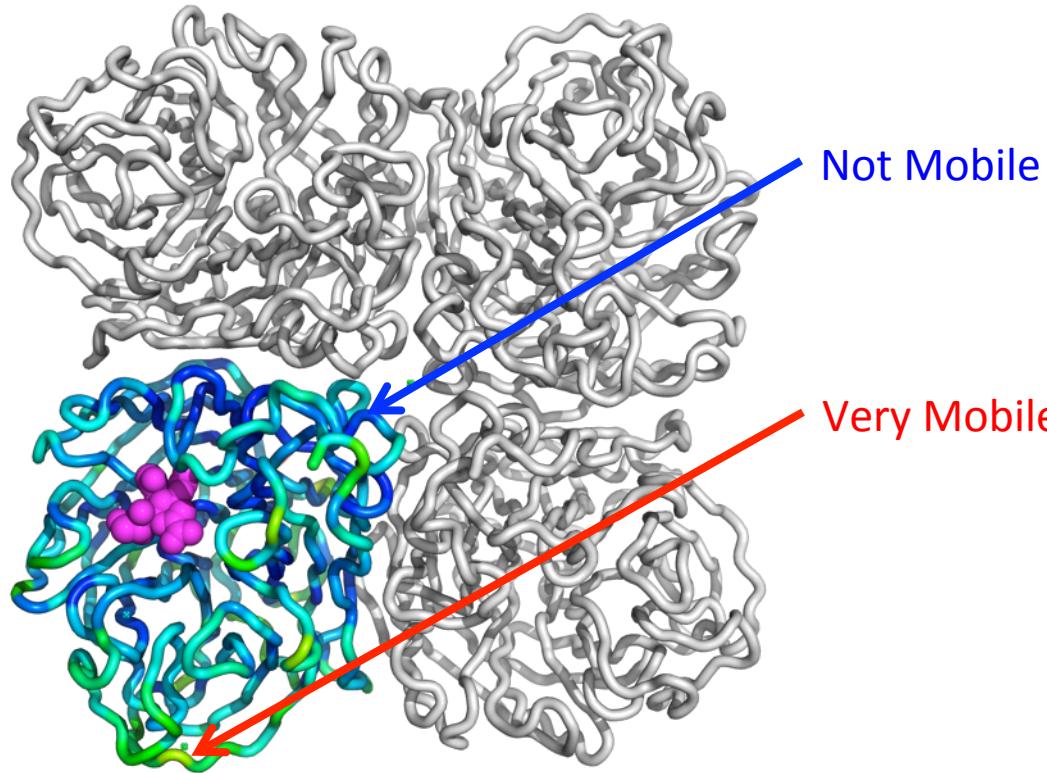


Hemagglutinin w/ 1 Ligand

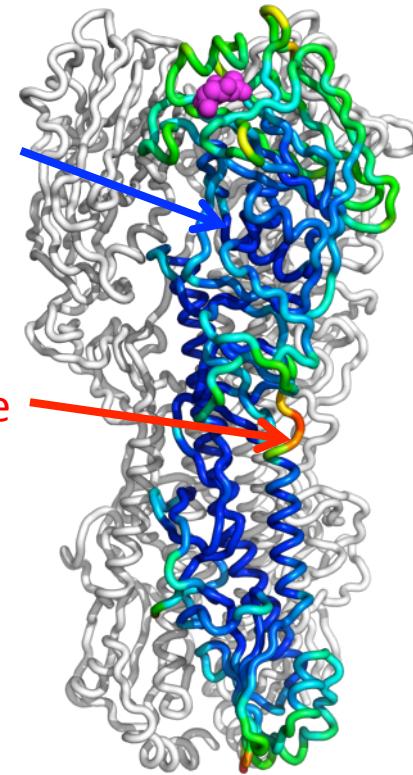


We can display molecular movement (β -factors) as different colors

Neuraminidase

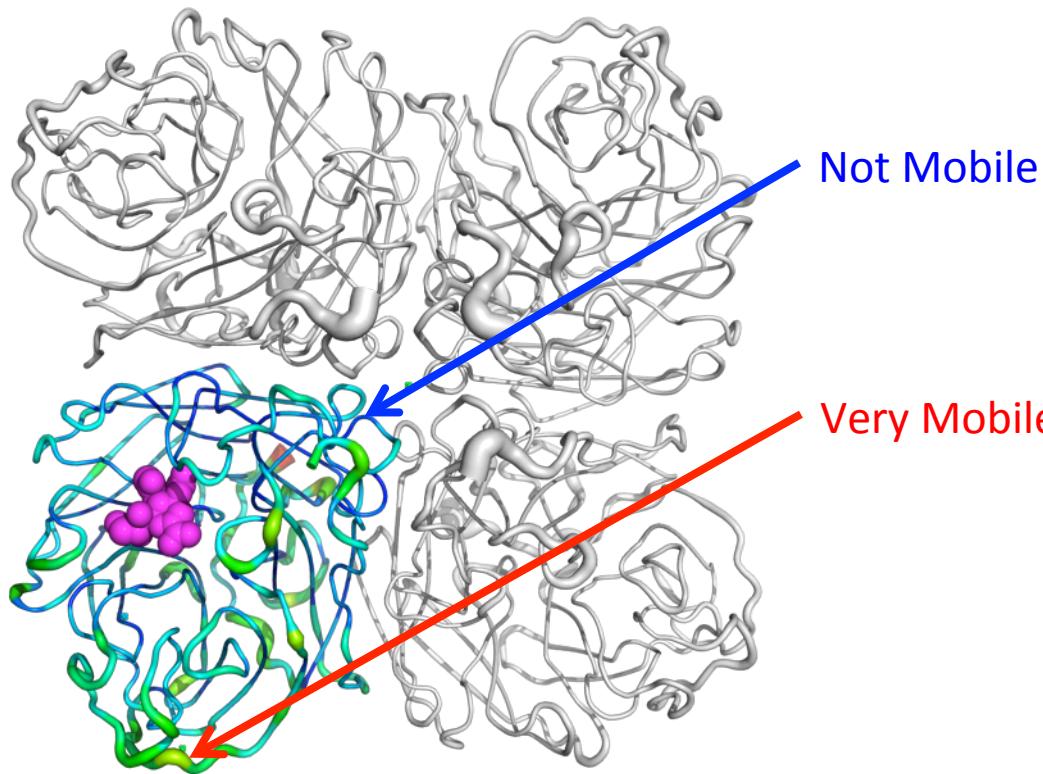


Hemagglutinin

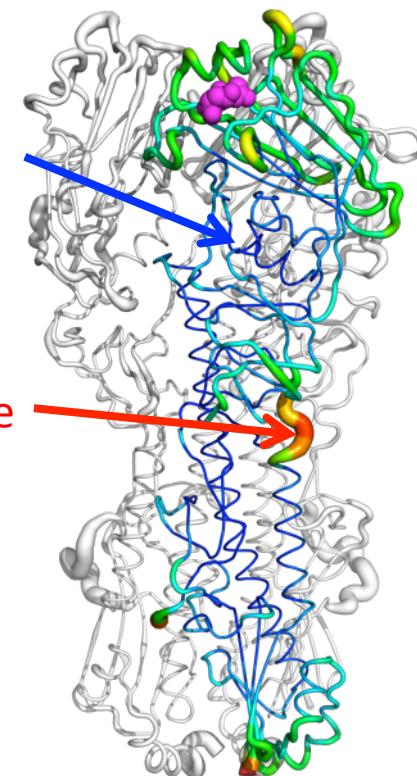


We can display molecular movement as size and color using 'cartoon putty' option

Neuraminidase

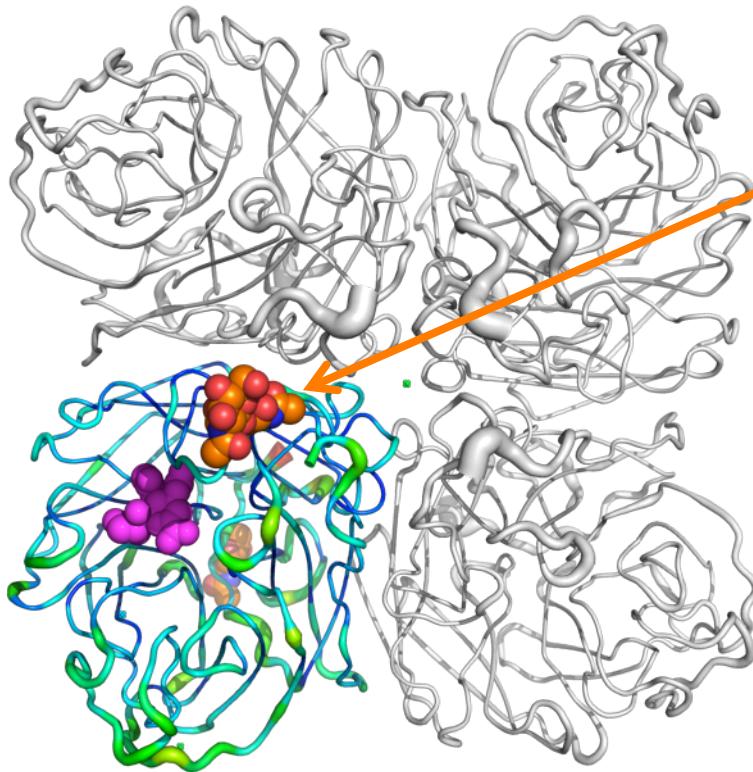


Hemagglutinin

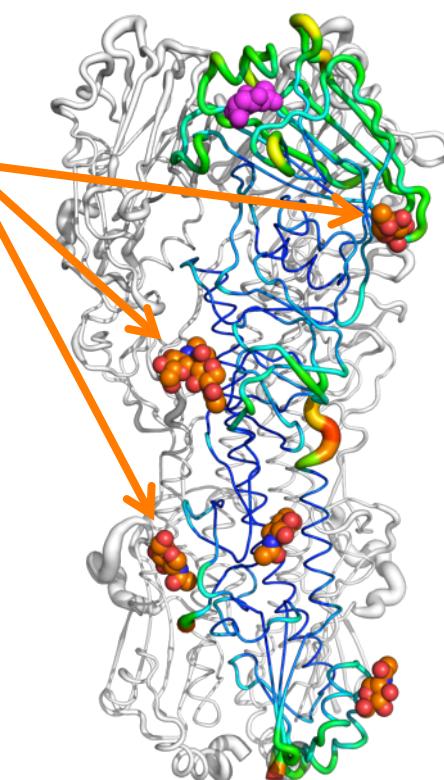


Sugars can also be critical for biological function

Neuraminidase

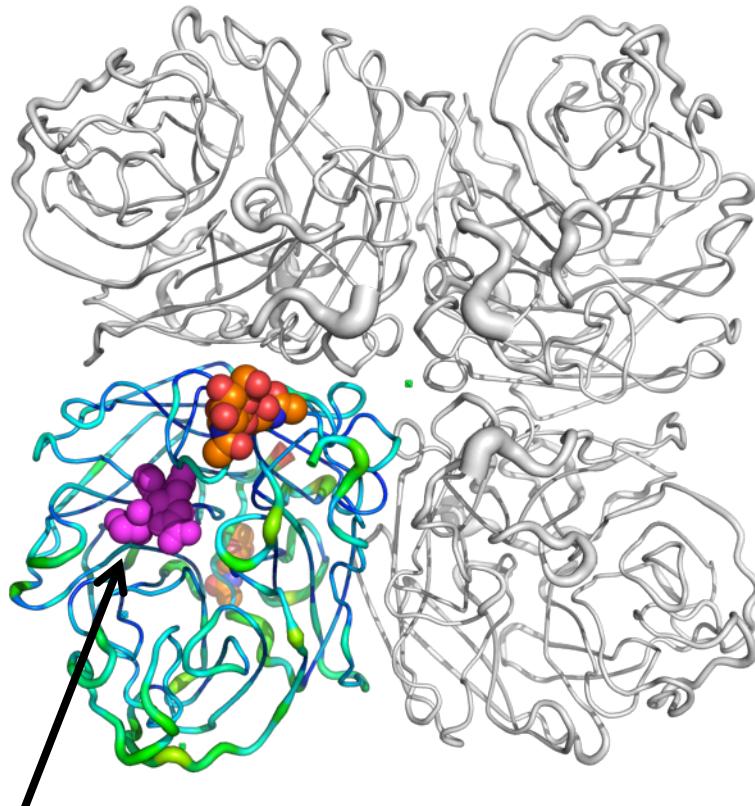


Hemagglutinin



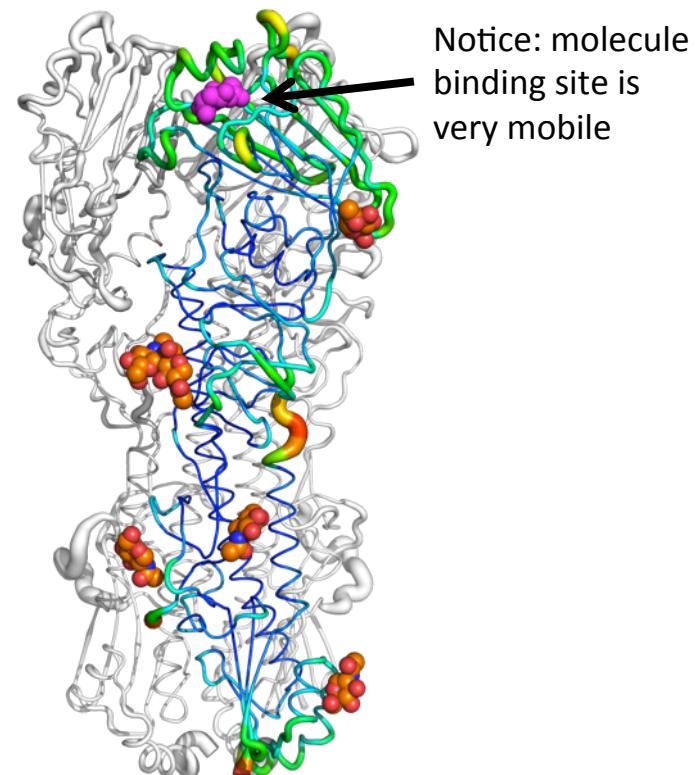
These proteins likely have different functions

Neuraminidase



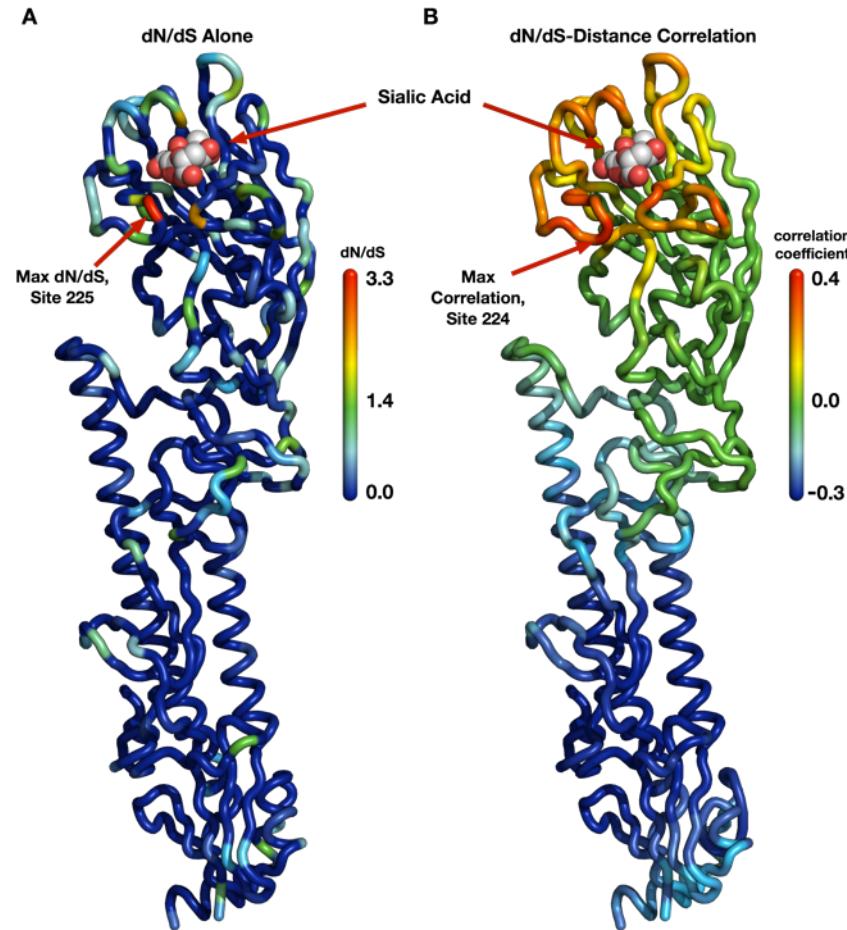
Notice: molecule
binding site is
very immobile

Hemagglutinin



Notice: molecule
binding site is
very mobile

Any site-wise metric can be plotted in place of b-factors



Given multiple time points, we show shifting patterns on the structure: Hemagglutinin



Given multiple time points, we show shifting patterns on the structure: Neuraminidase



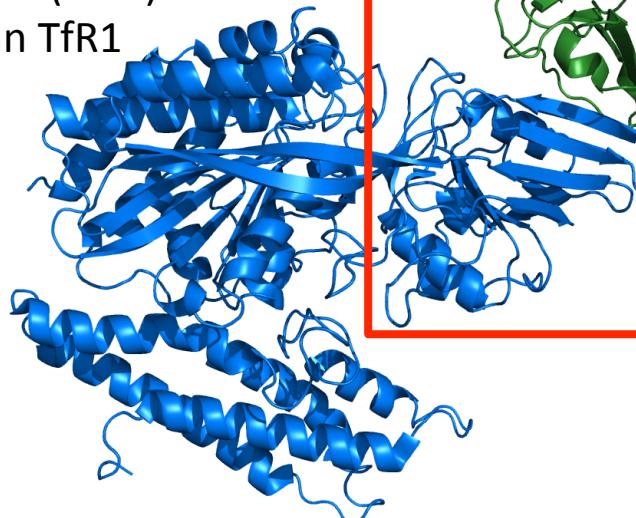
Show how to generate similar structures

Using protein structures as input for other analyses

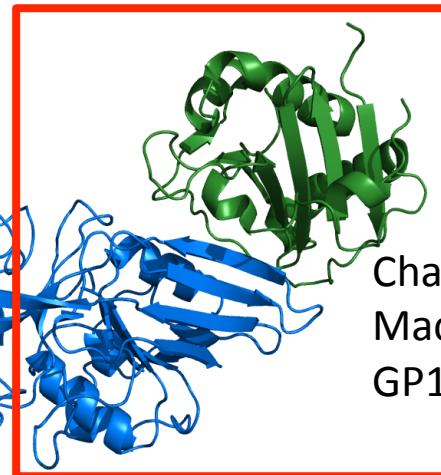
Seen before: the 3kas structure

PDB files can contain multiple chains

Chain A (blue)
human TfR1

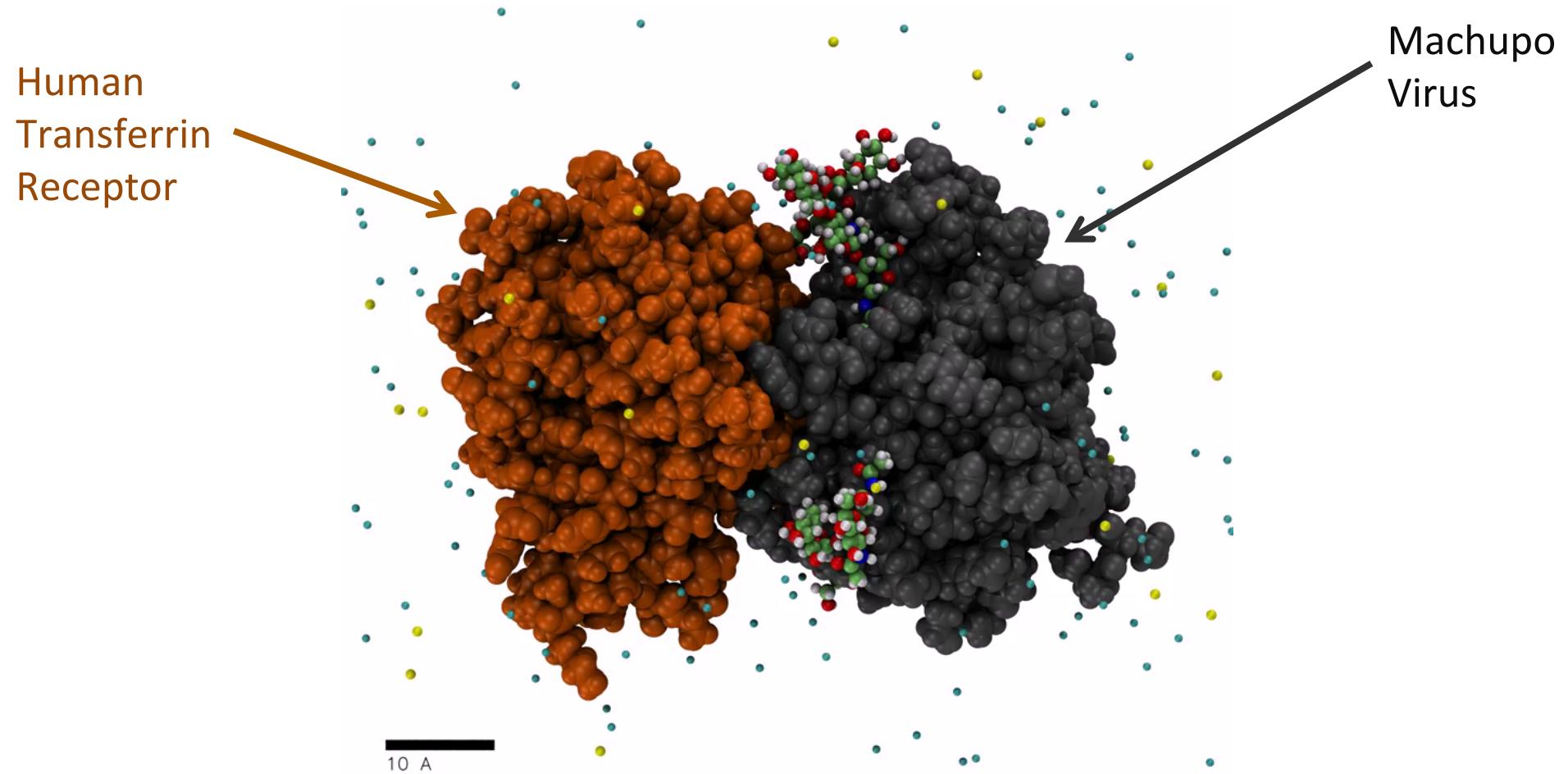


Chain B (green)
Machupo virus
GP1

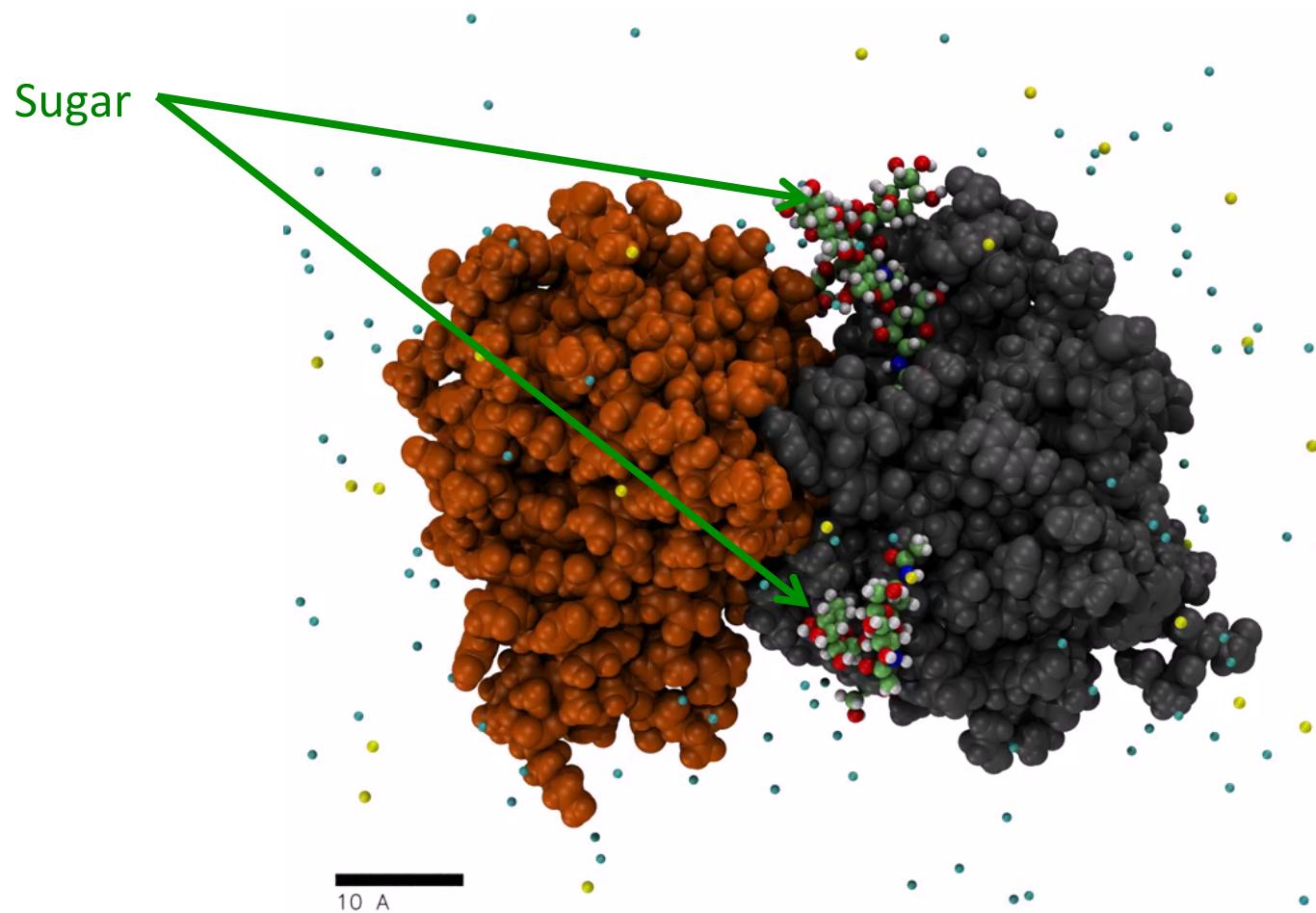


PDB ID: 3KAS

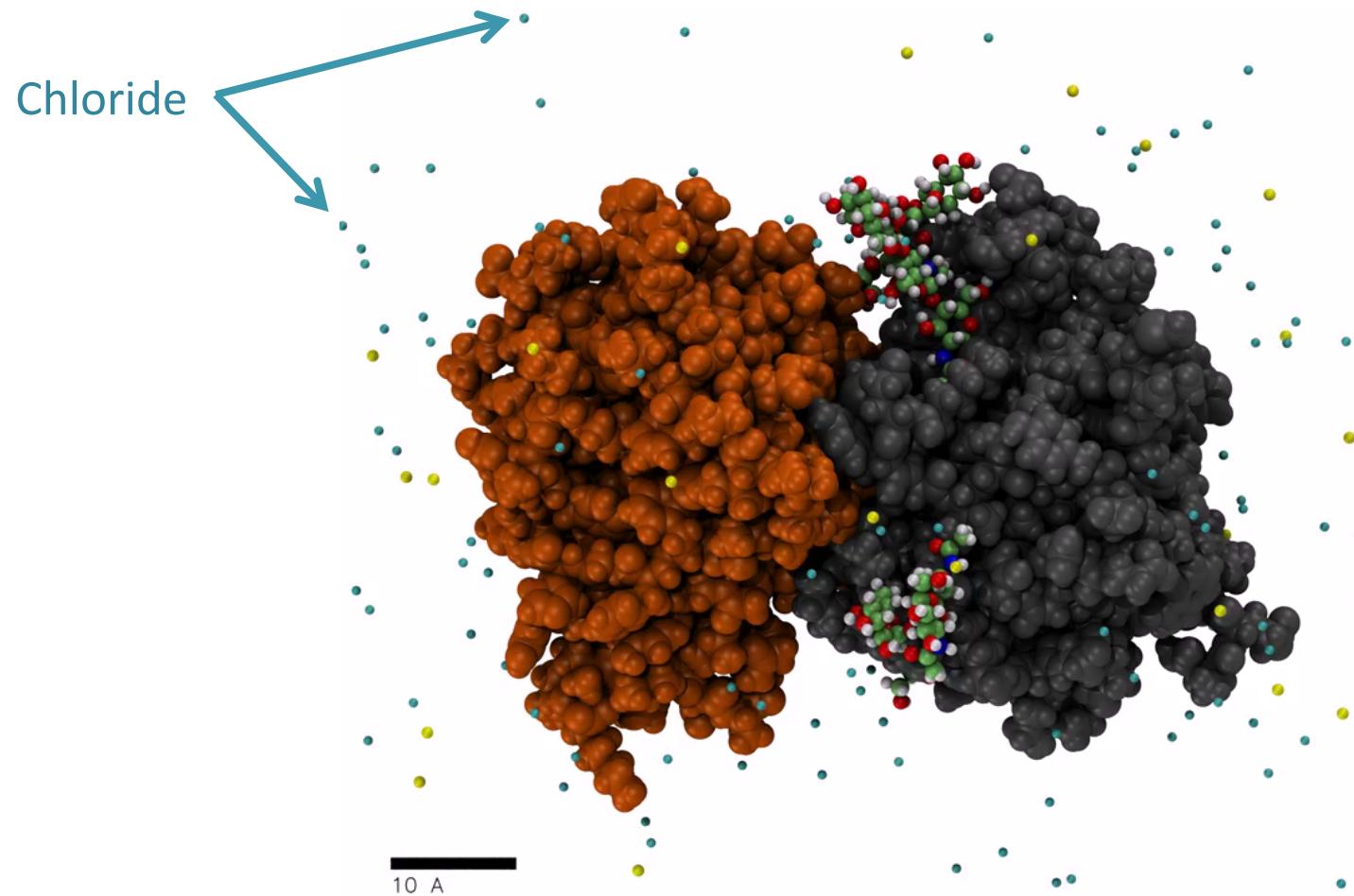
With everything together, we can simulate the protein motions



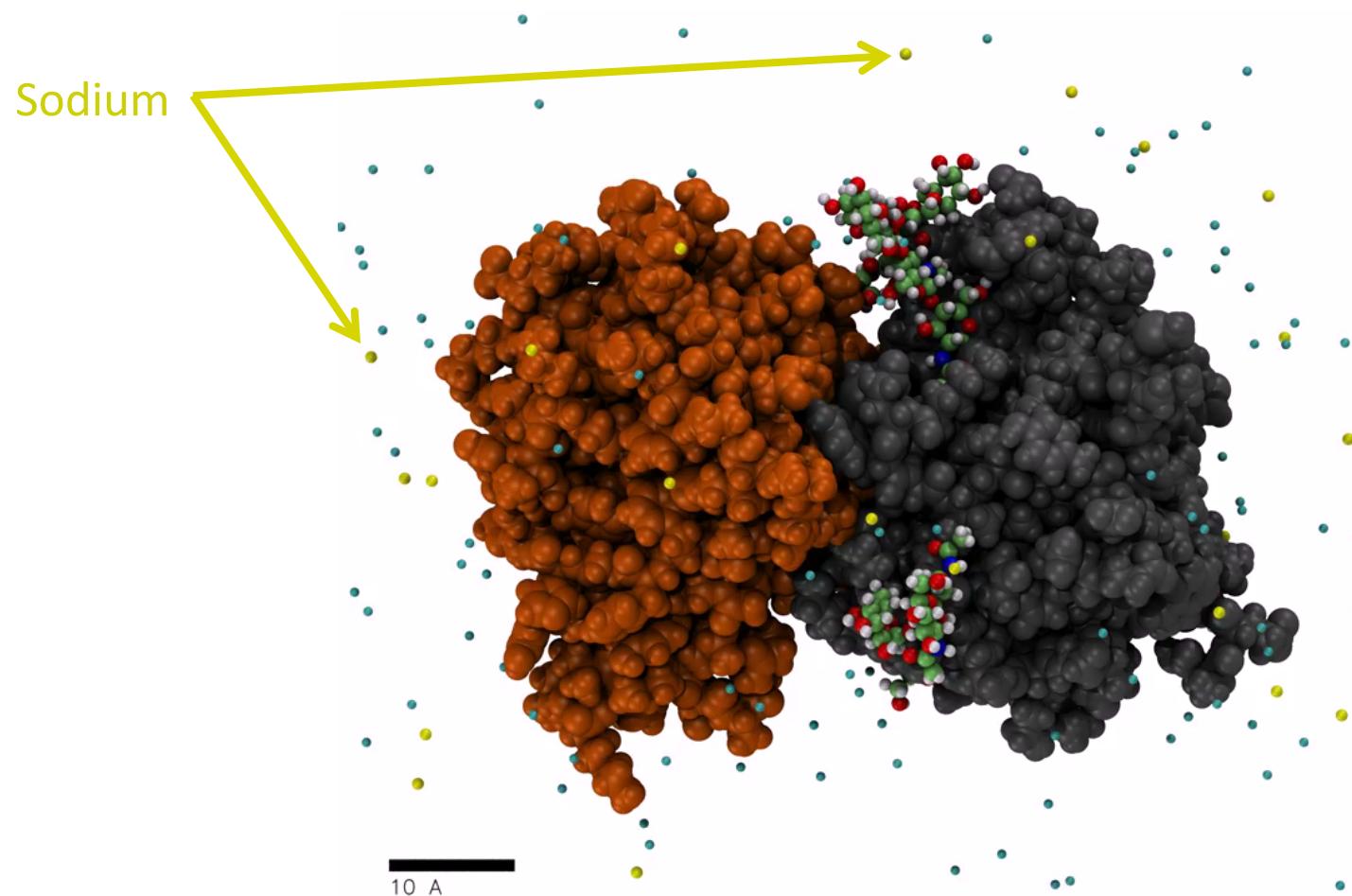
With everything together, we can simulate the protein motions



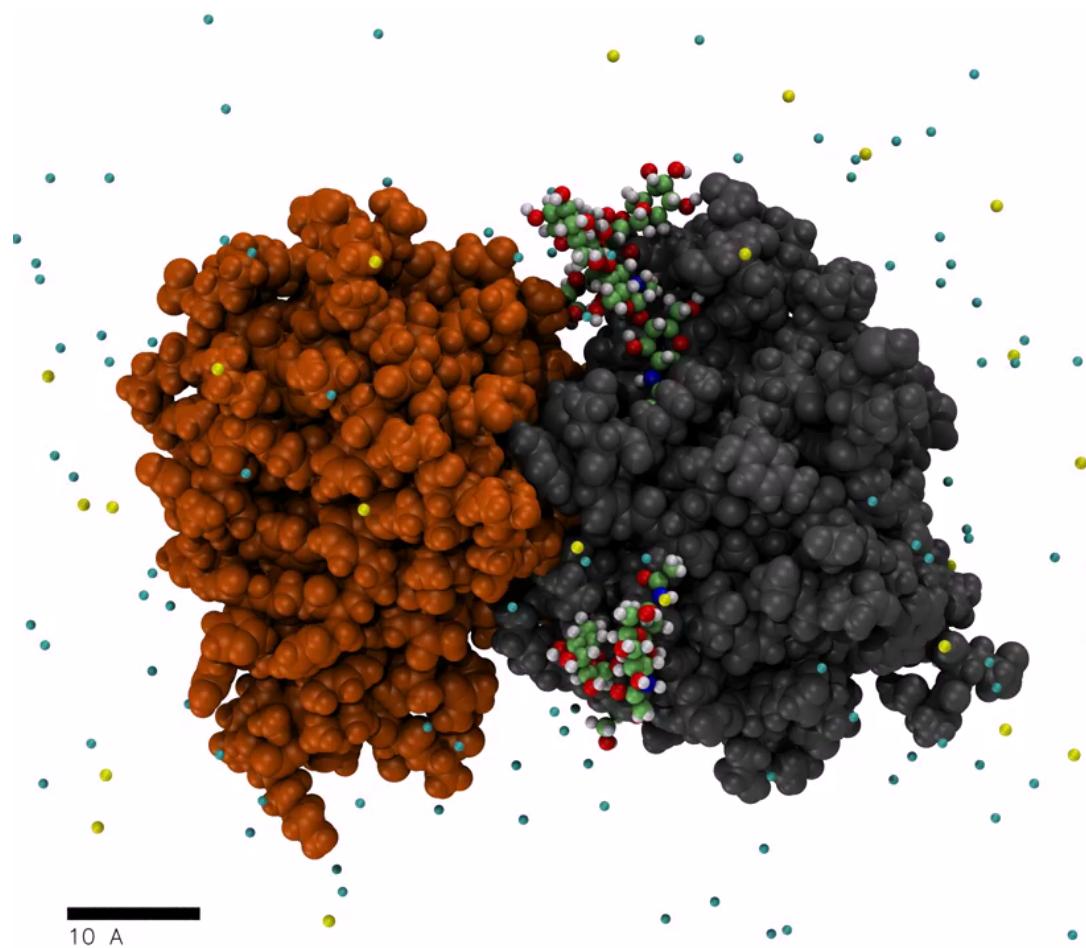
With everything together, we can simulate the protein motions



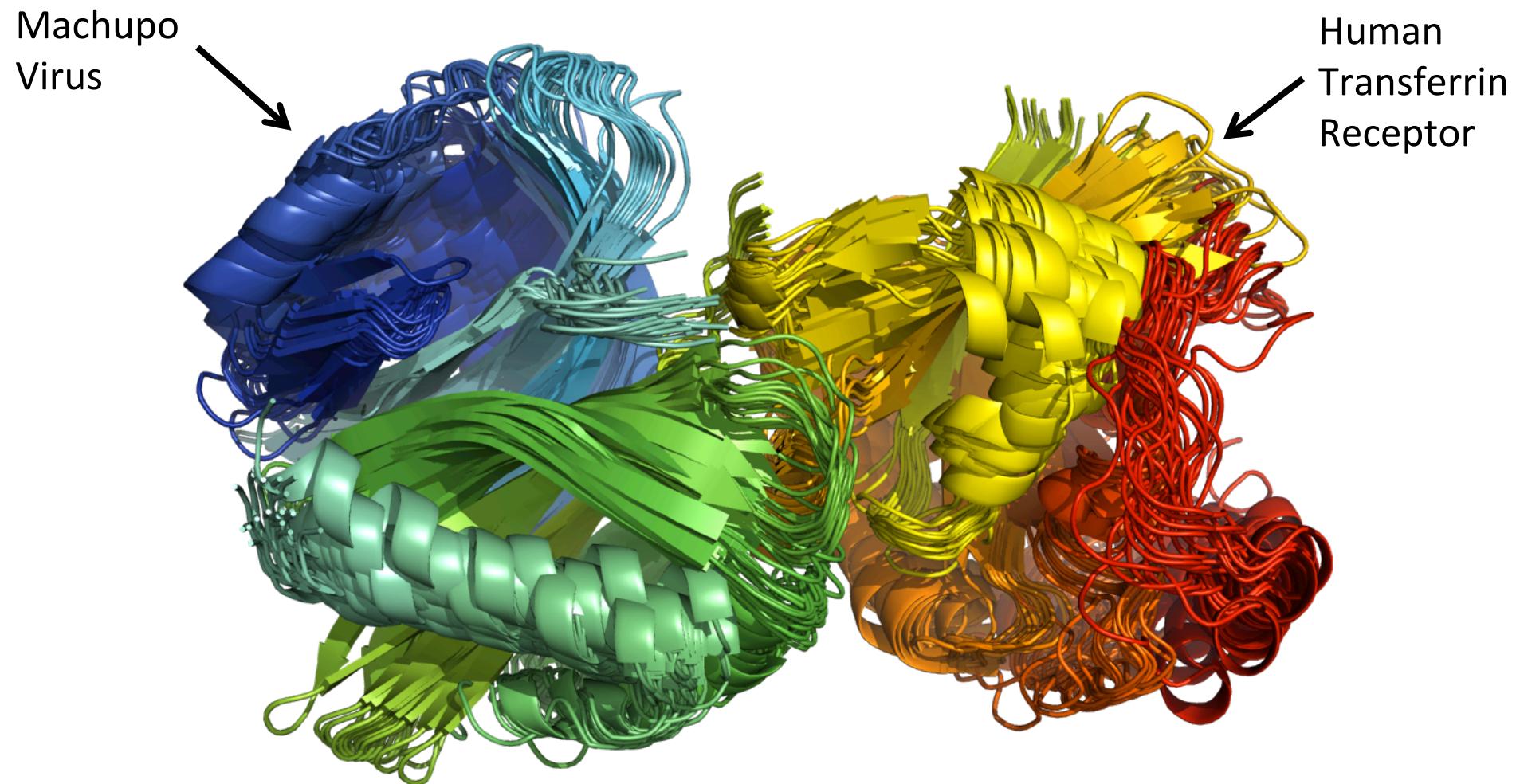
With everything together, we can simulate the protein motions



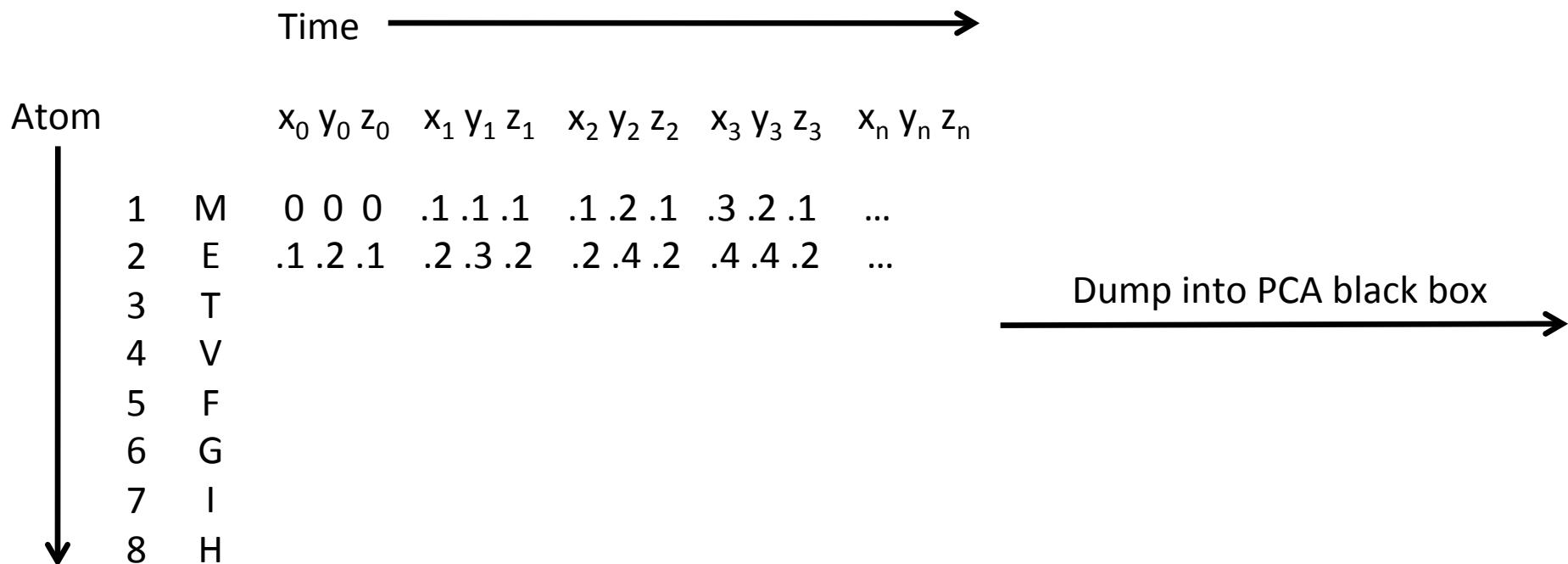
With everything together, we can simulate the protein motions



Instead of playing a movie, the frames can be overlaid on each other

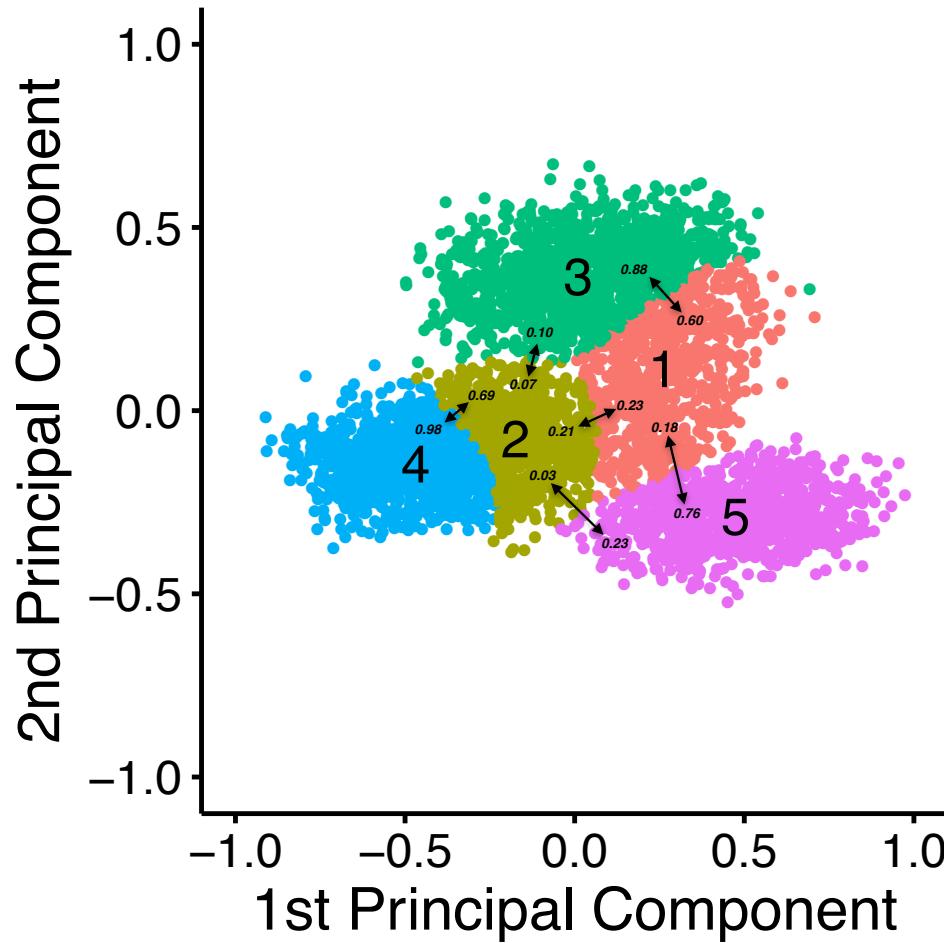


Using those overlaid snapshots, we can do PCA



In this PCA: each dot is one time point, each numbered cluster is a similar protein conformation

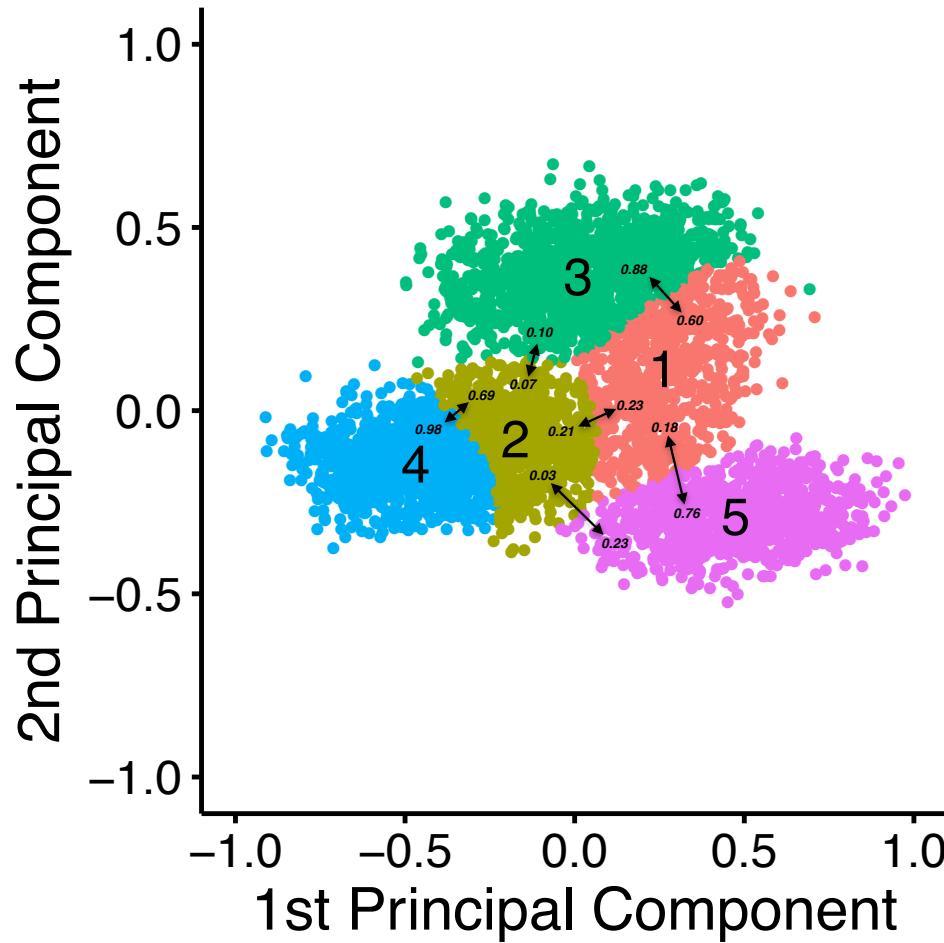
Clustered
by k-means
clustering.



In this PCA: each dot is one time point, each numbered cluster is a similar protein conformation

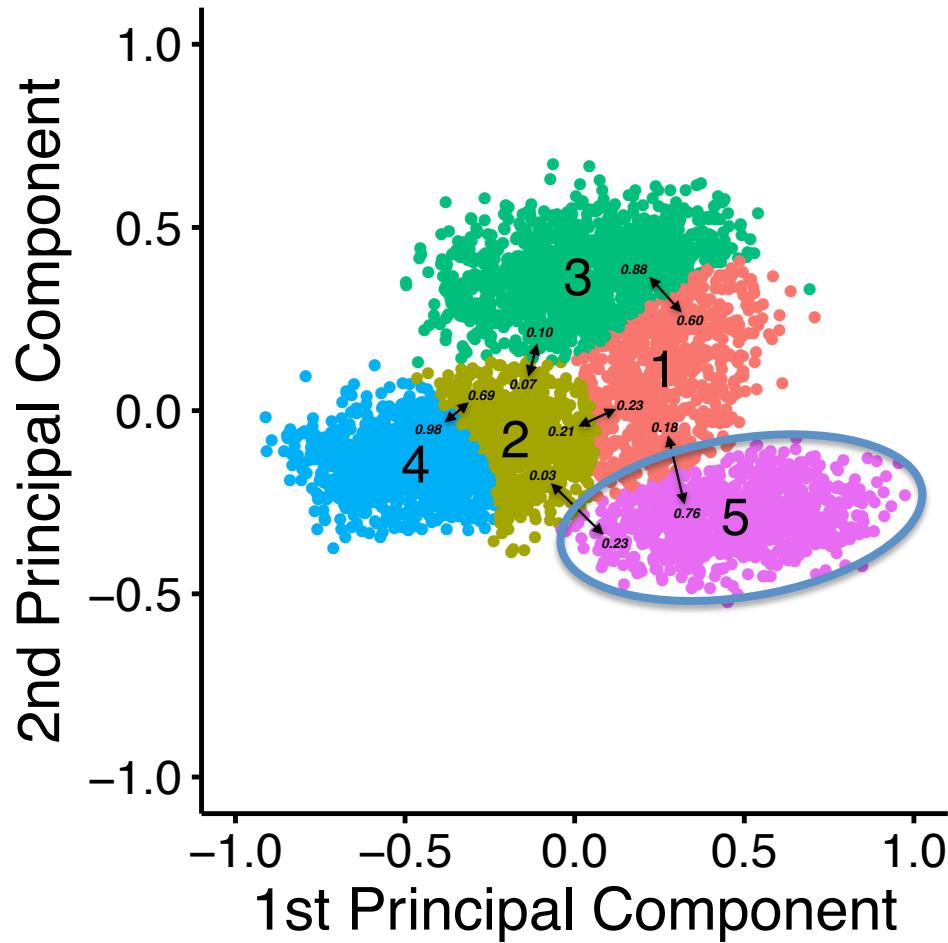
Clustered
by k-means
clustering.

Arrows
show
transition
probability.



In this PCA: each dot is one time point, each numbered cluster is a similar protein conformation

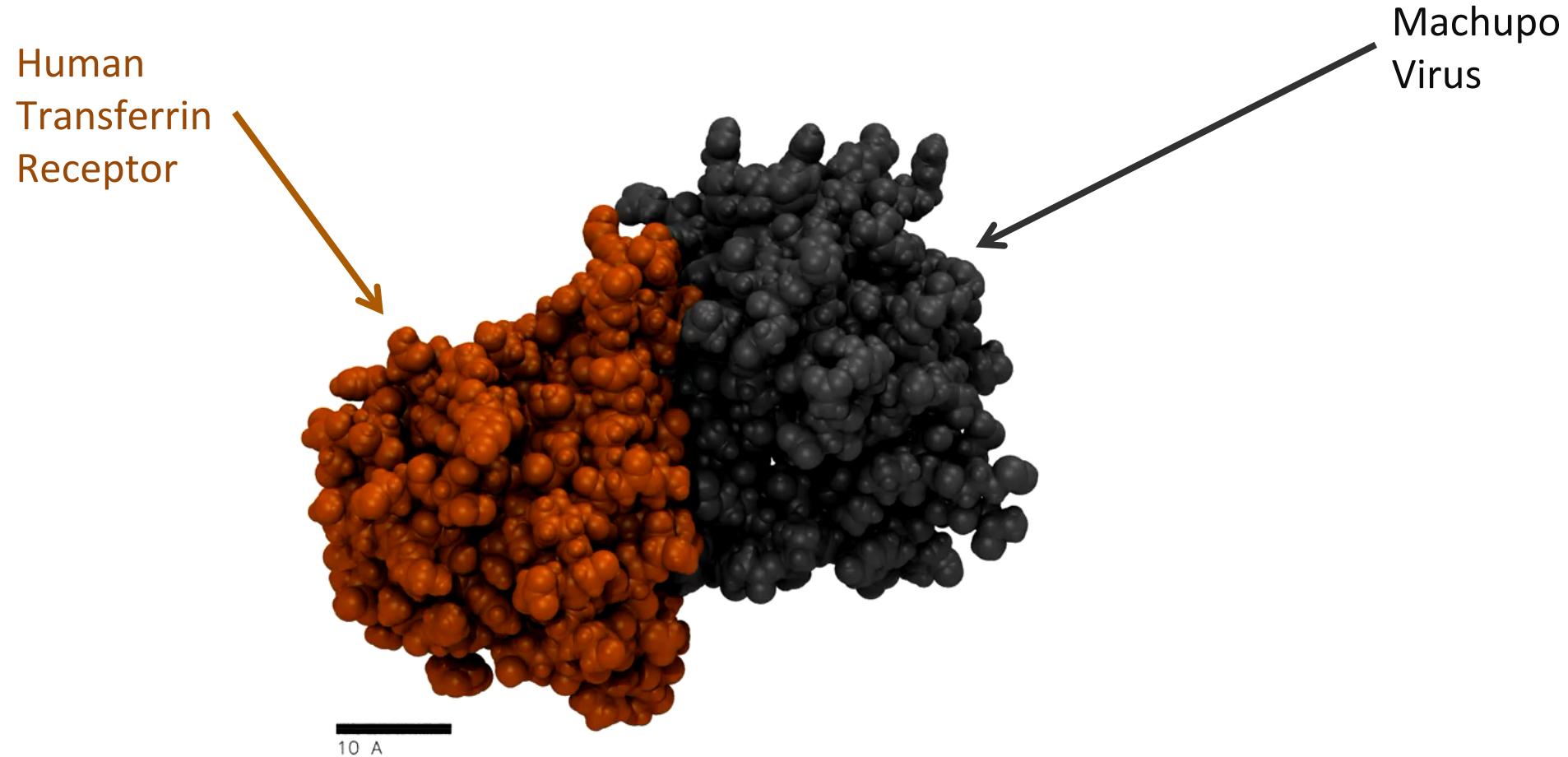
Clustered
by k-means
clustering.



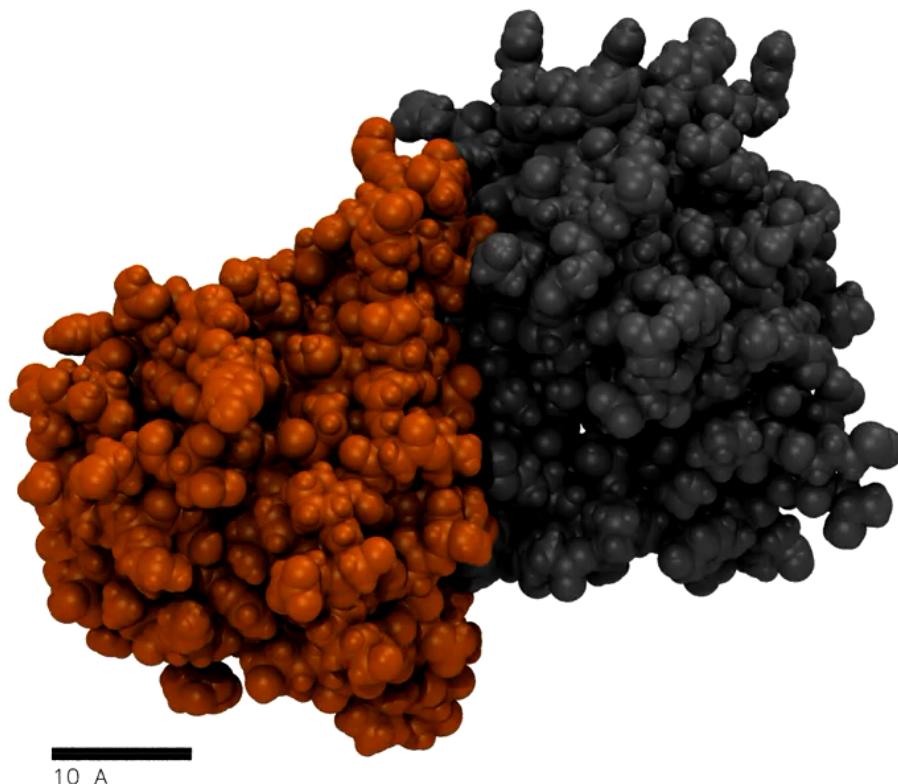
Arrows
show
transition
probability.

Sum of
arrows
exiting one
cluster
equals ~ 1 .

You can also apply and measure forces in these simulations if that is useful



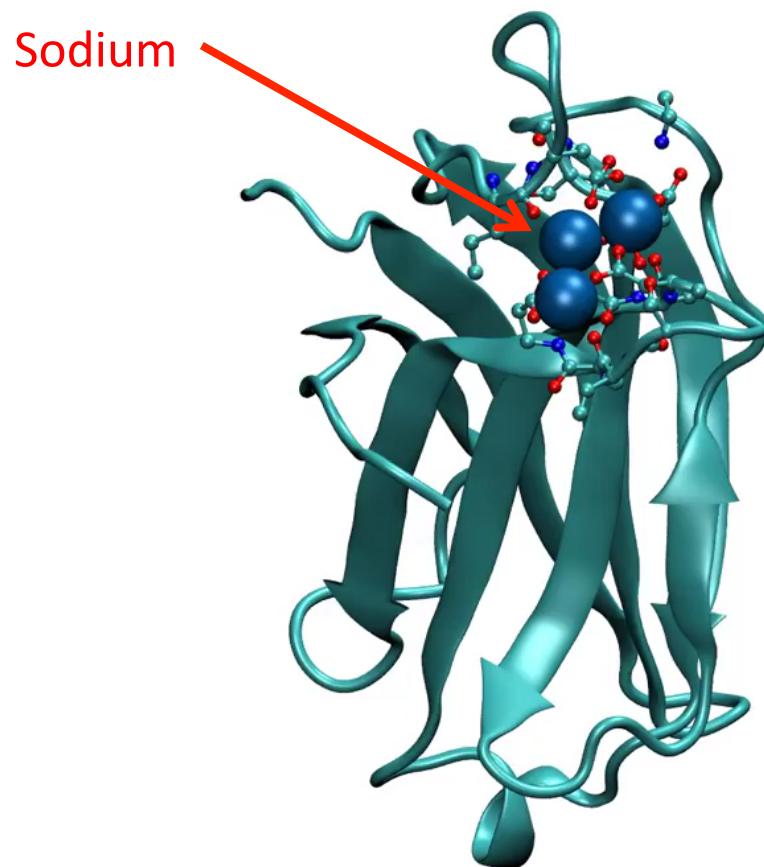
You can also apply and measure forces in these simulations if that is useful



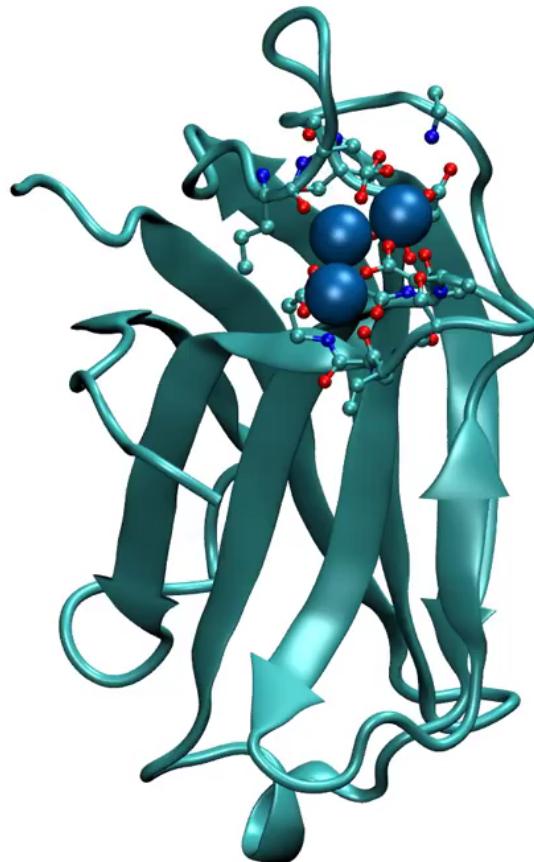
Imagine a weak force pulling the Machupo virus away from the human receptor

A few additional videos

Synaptotagmin unbinding from calcium ions

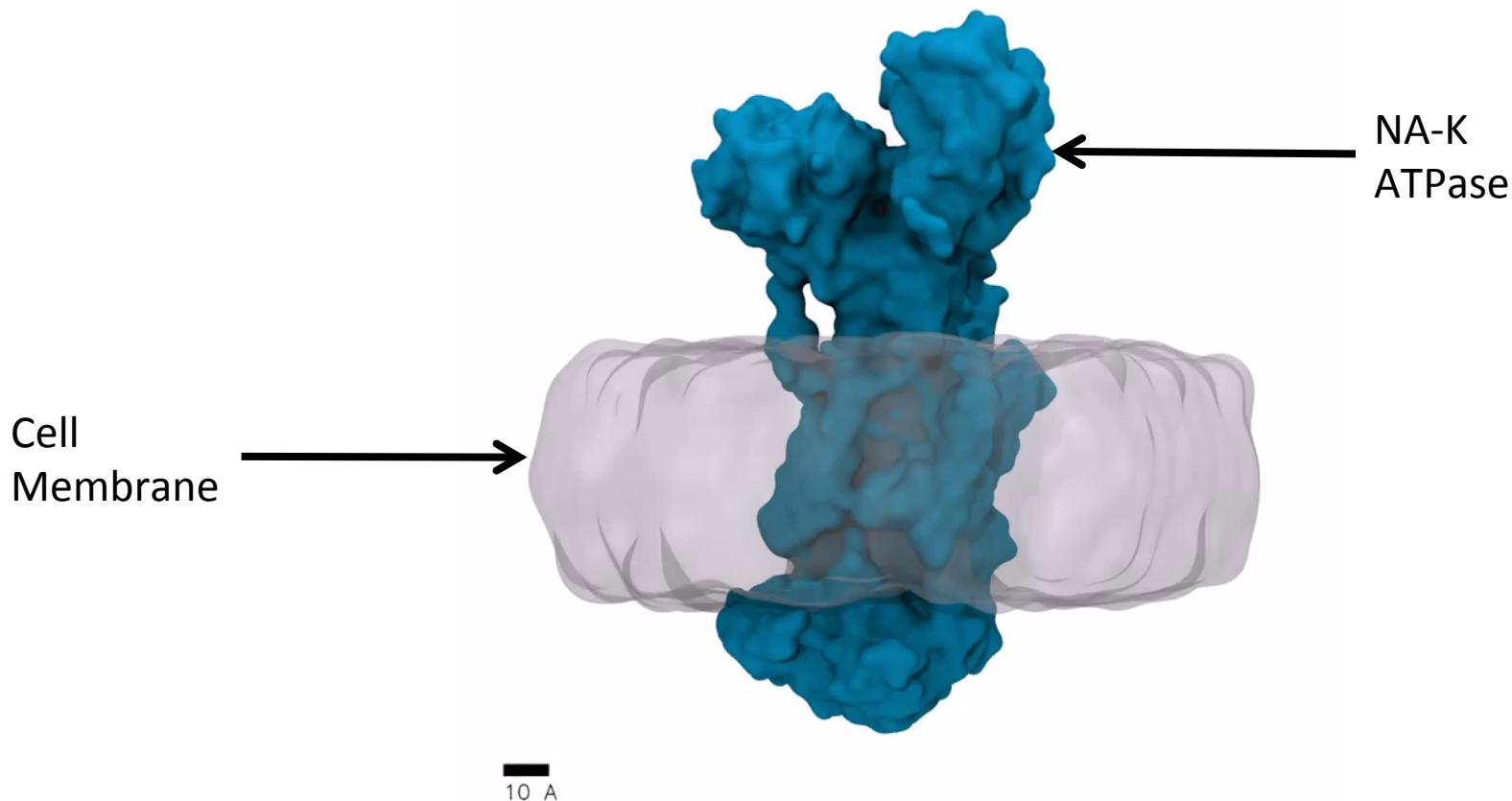


Synaptotagmin unbinding from calcium ions

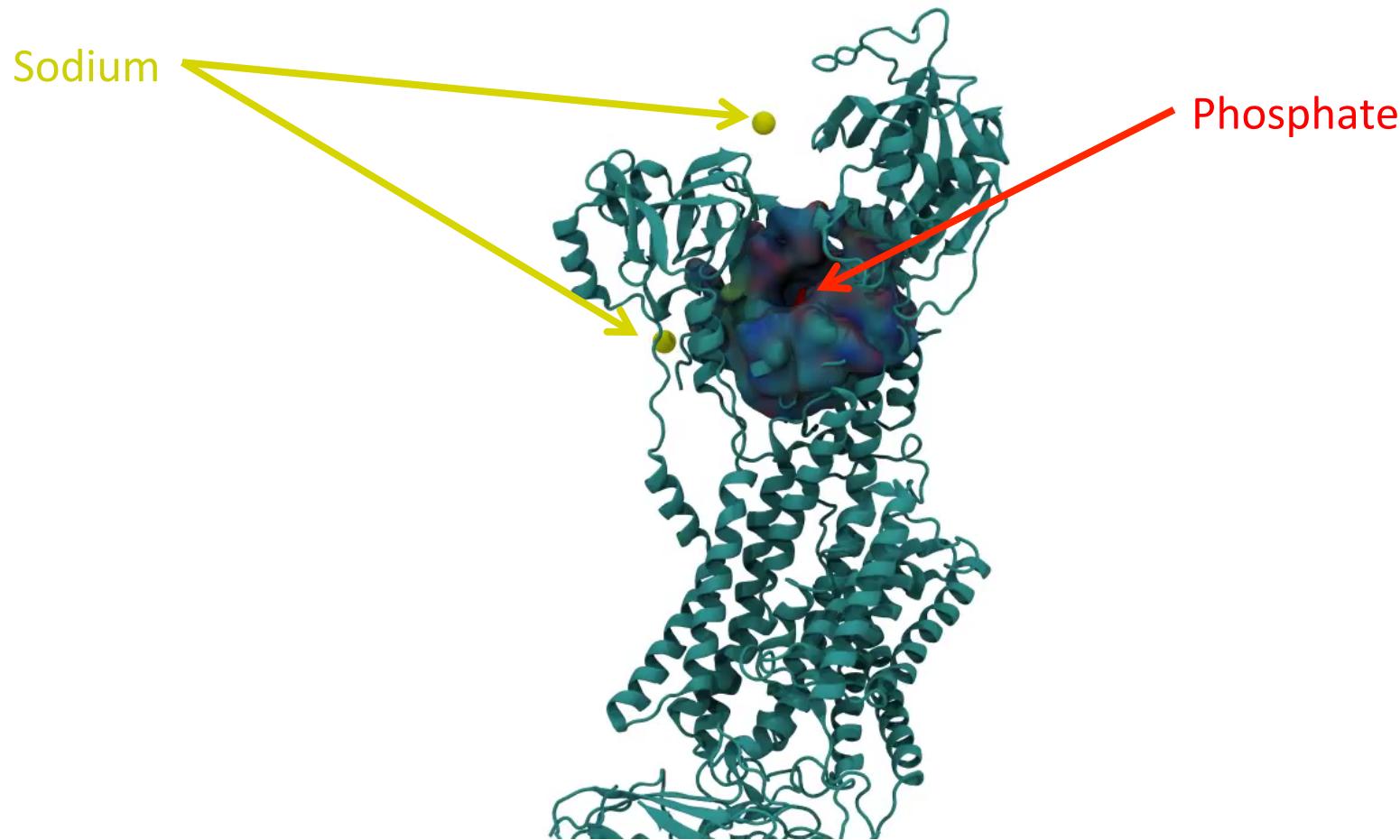


Any atom that is shown explicitly is within 5 Angstroms of a calcium atom.

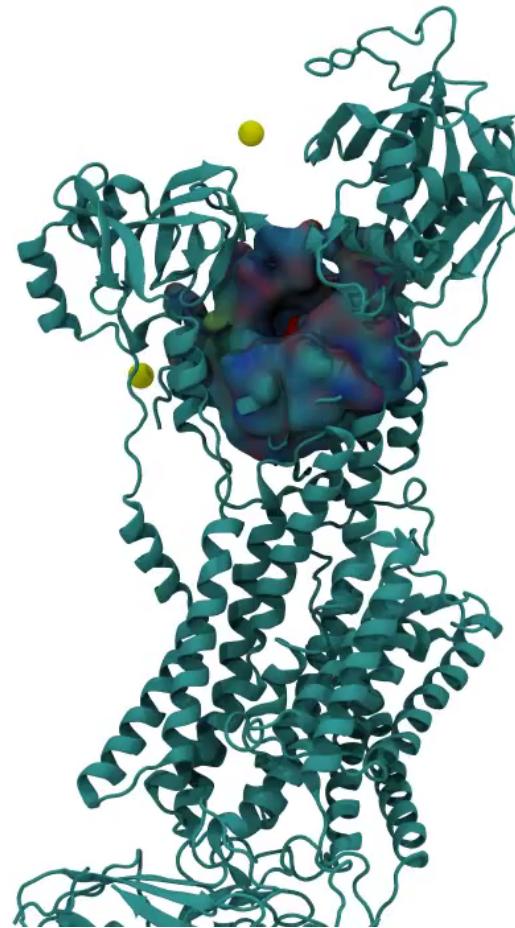
Na-K ATPase is the primary power user in any cell



Na-K ATPase binding 3 sodium ions



Na-K ATPase binding 3 sodium ions



Any surface that is shown explicitly is within 5 Angstroms of a sodium atom at the end of the simulation.