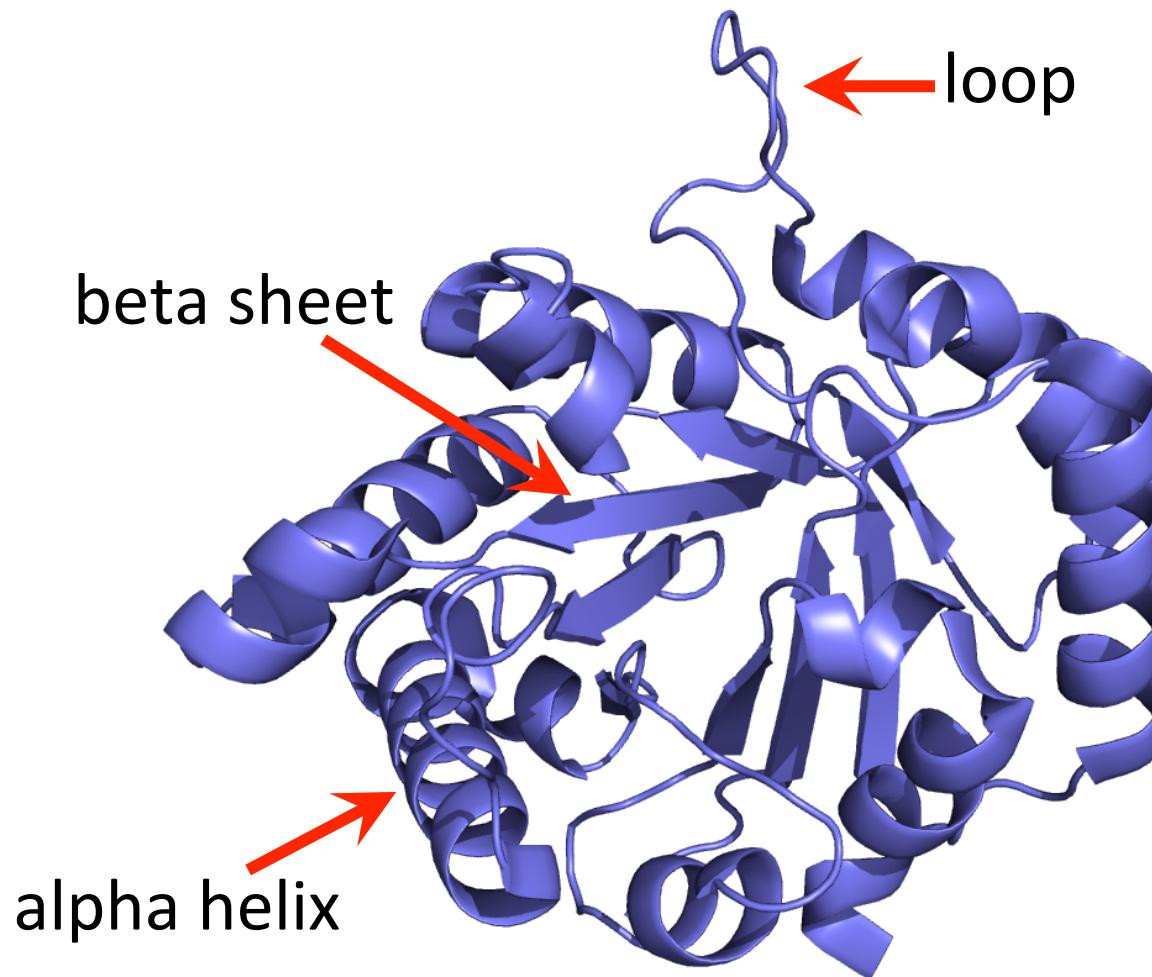


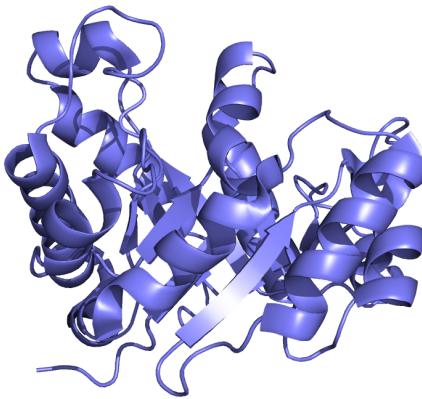
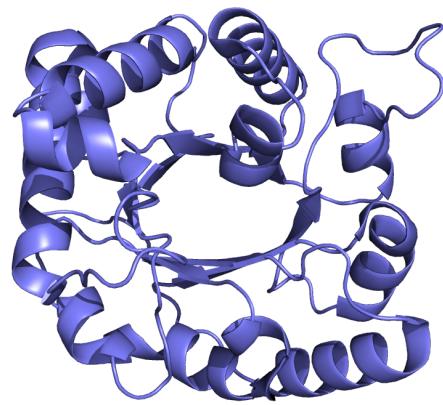
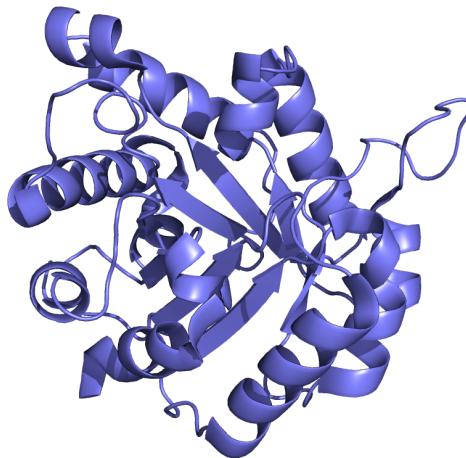
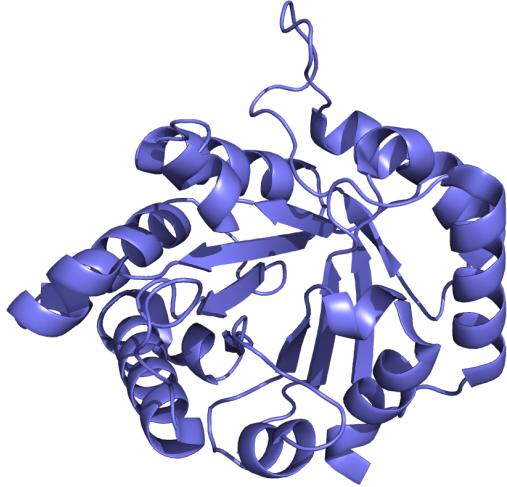
# Working with protein structures / PDB files

# Structure of Triosephosphate Isomerase

PDB ID: 1HTI

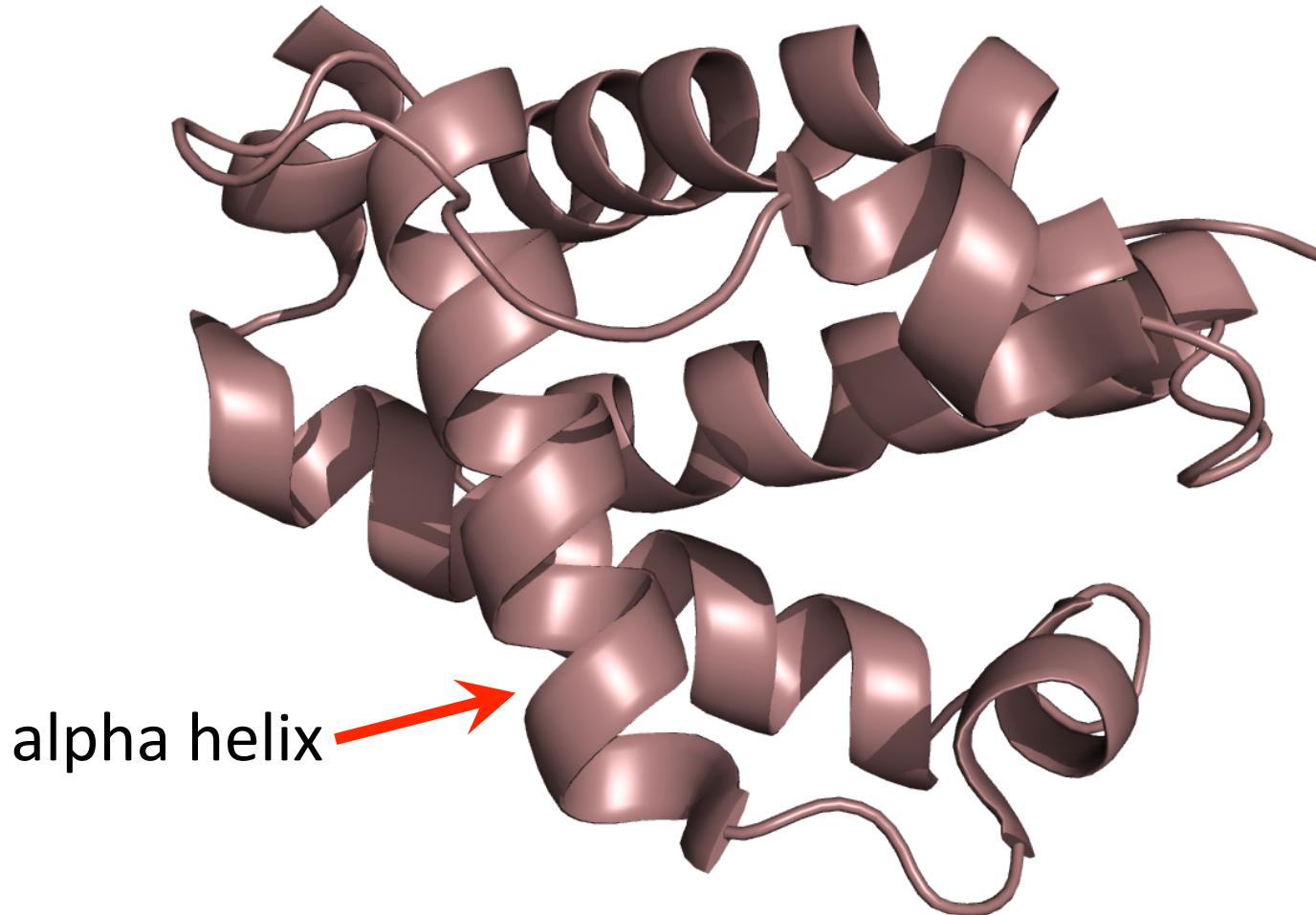


# Different perspectives of the same structure



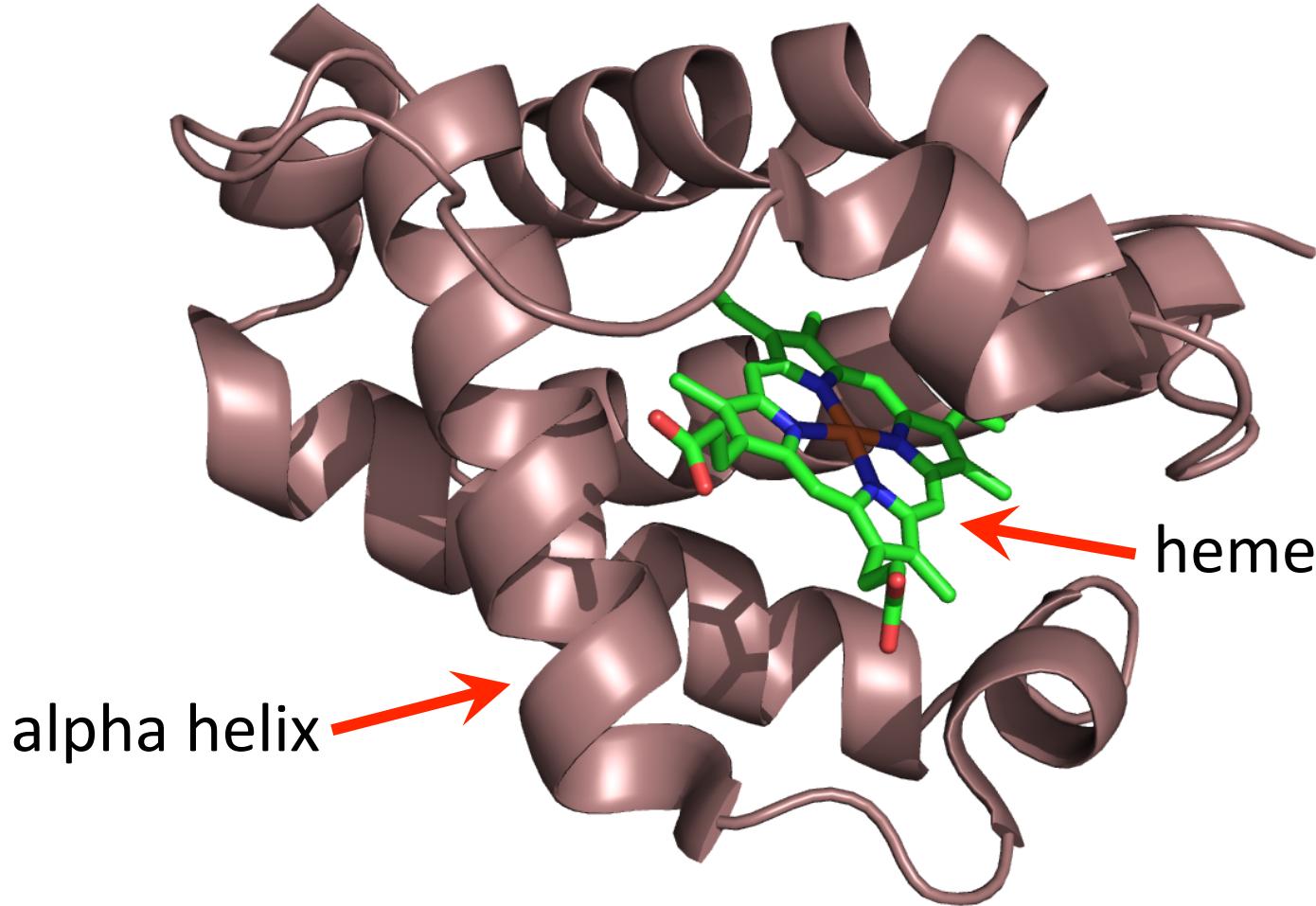
# Structure of Truncated Hemoglobin

PDB ID: 1DLW



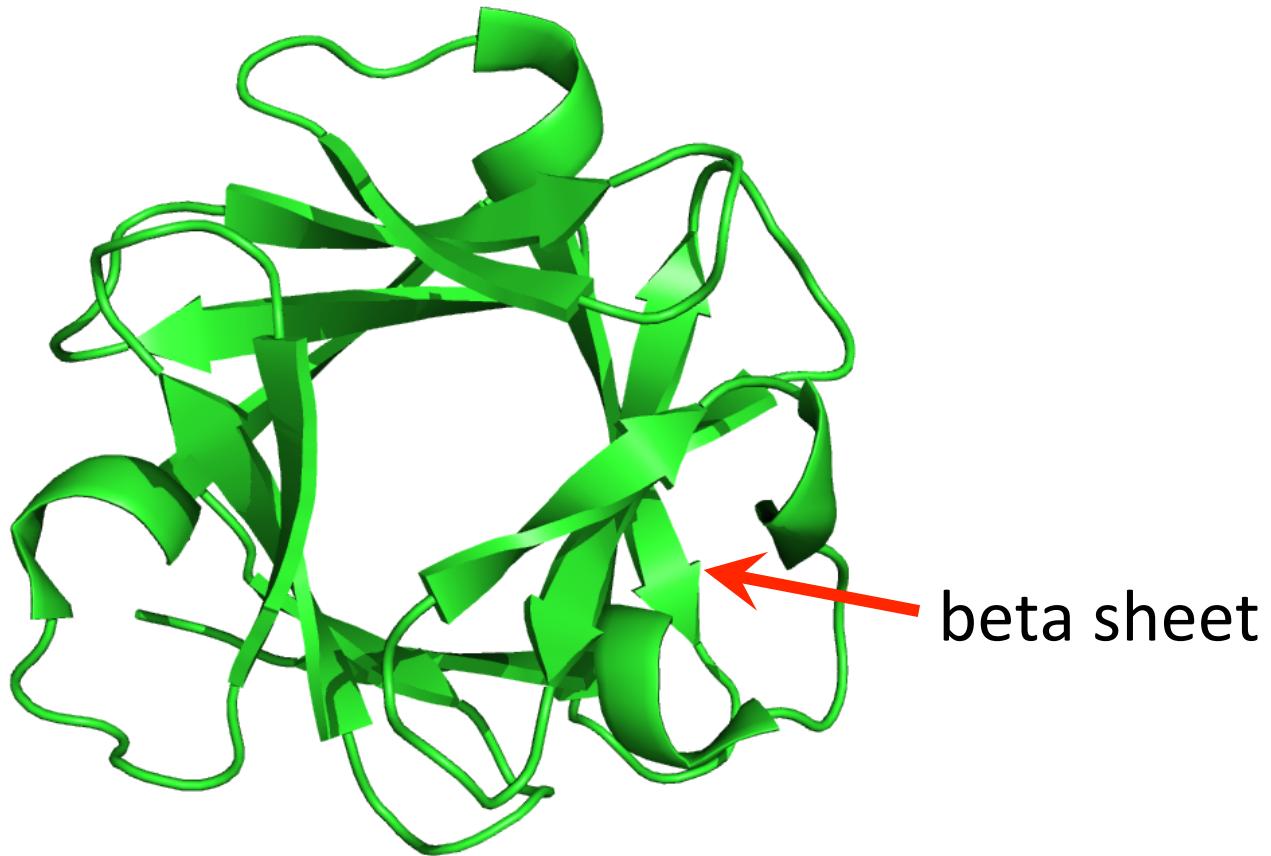
# Structure of Truncated Hemoglobin

PDB ID: 1DLW



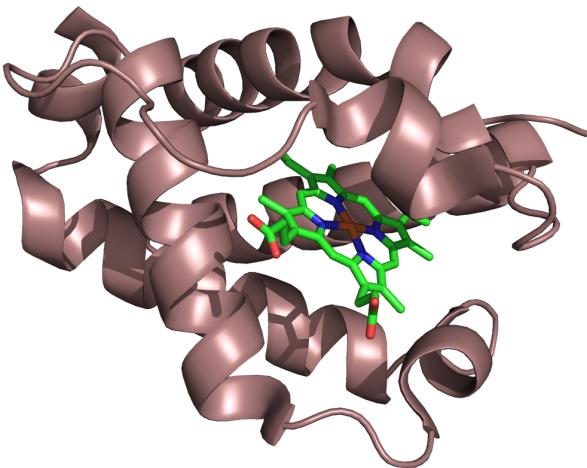
# Structure of Basic Fibroblast Growth Factor

PDB ID: 1BFG

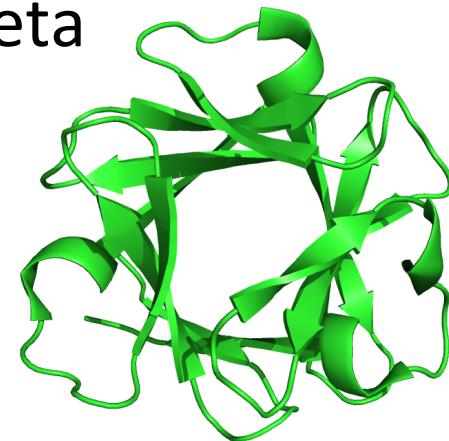


We classify structures by their alpha  
and beta content

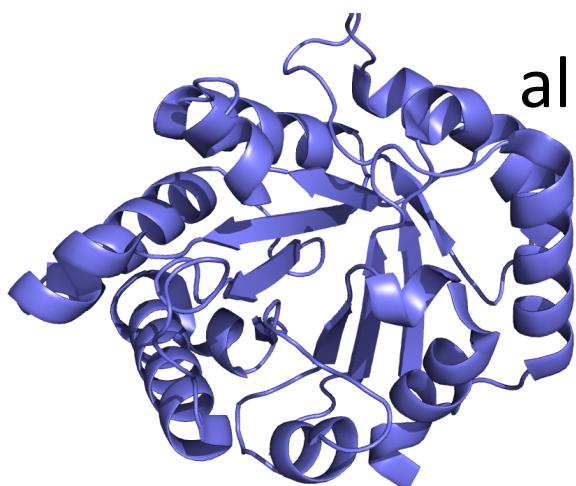
all alpha



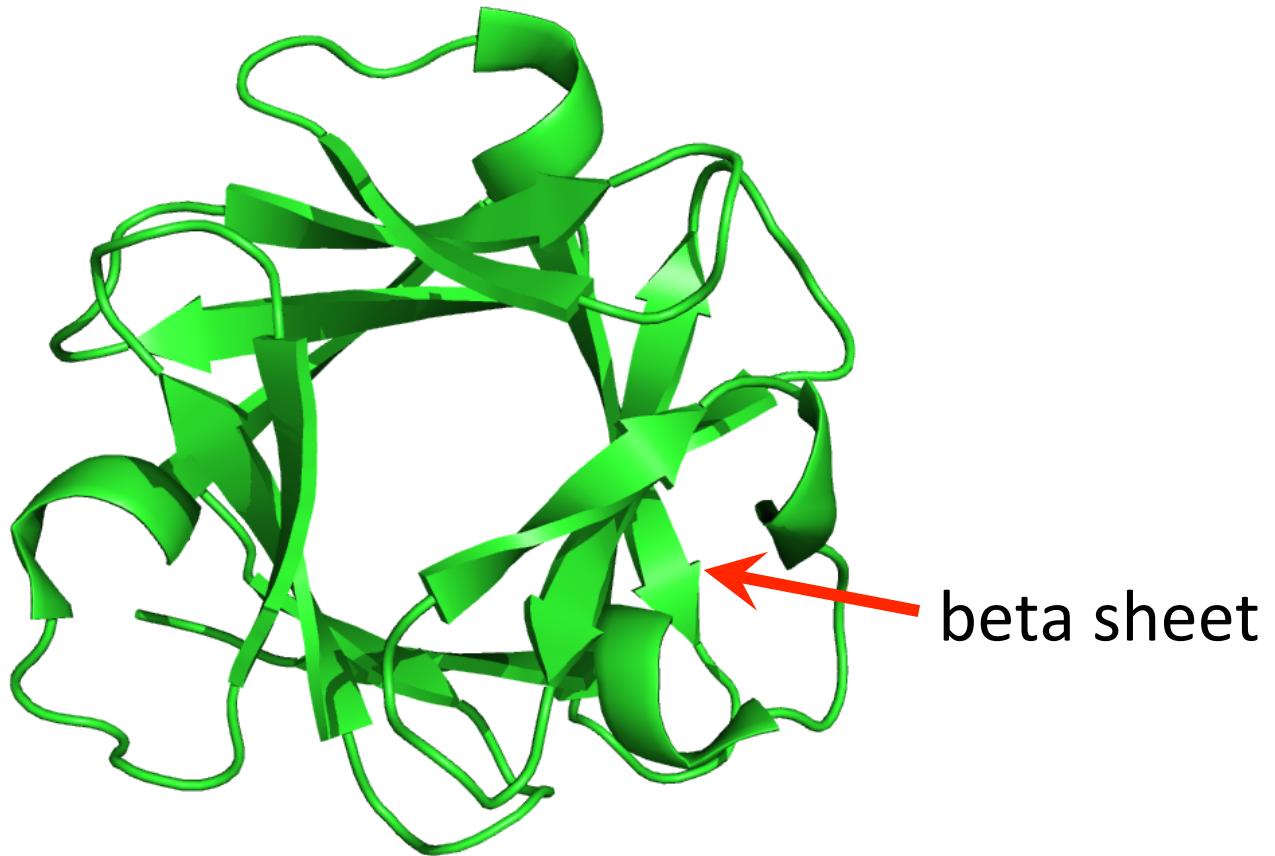
all beta



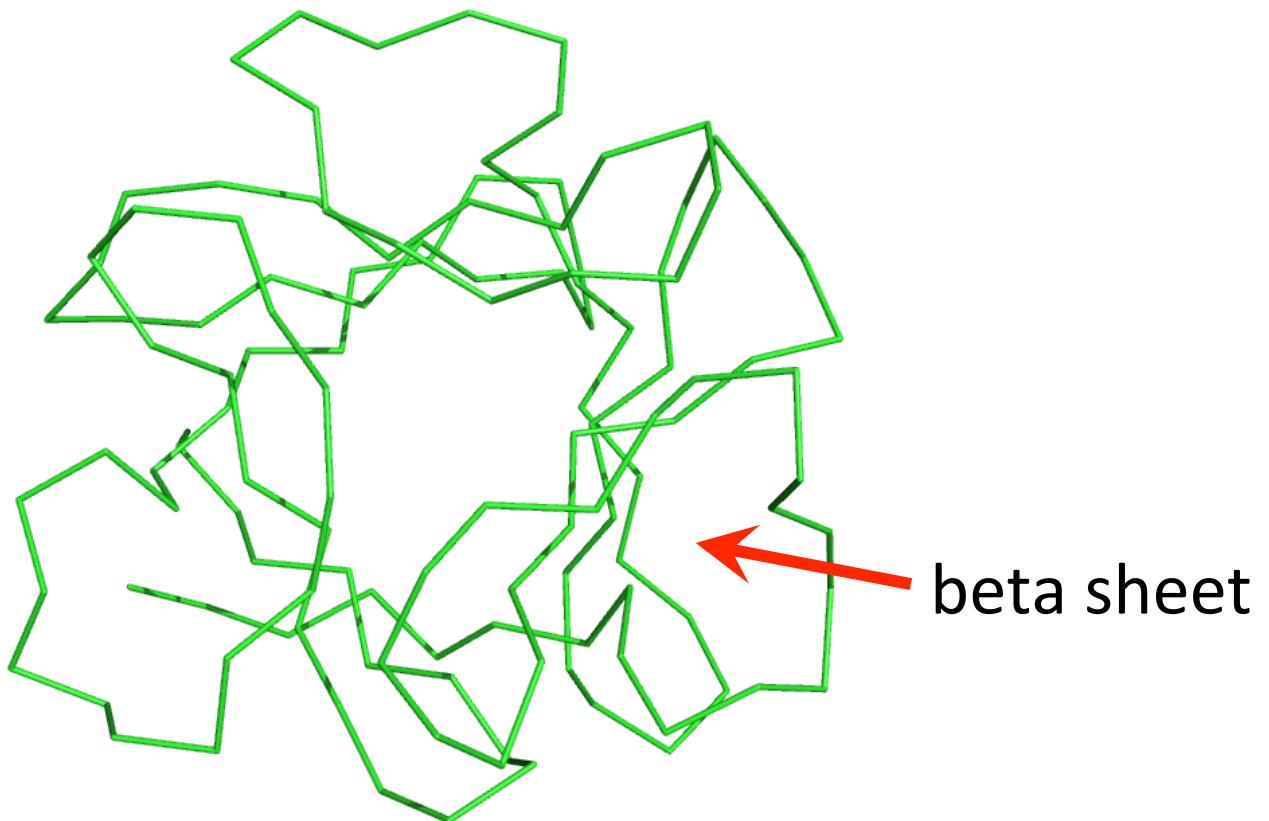
alpha and beta



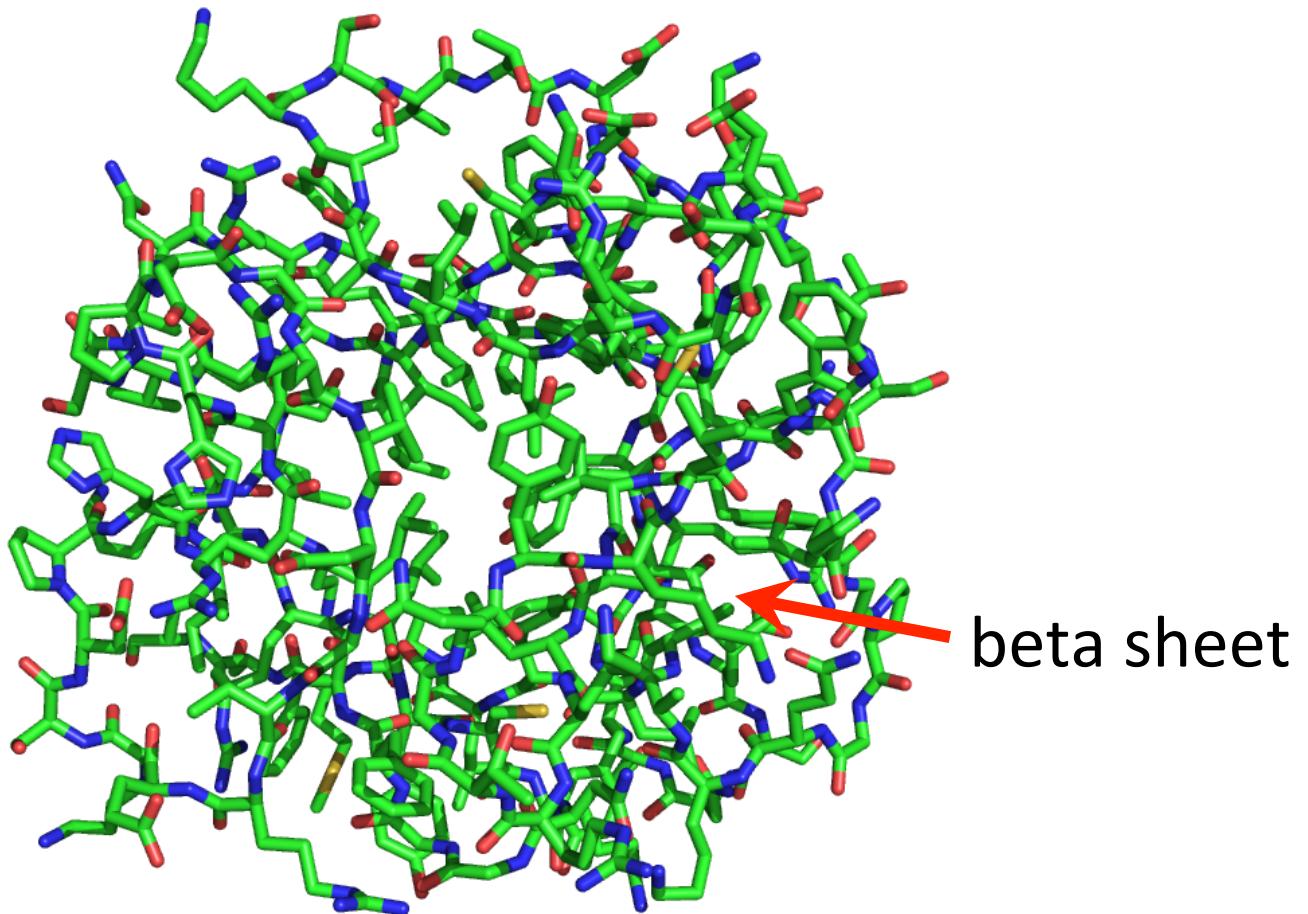
# Different visualizations of a structure: Cartoon



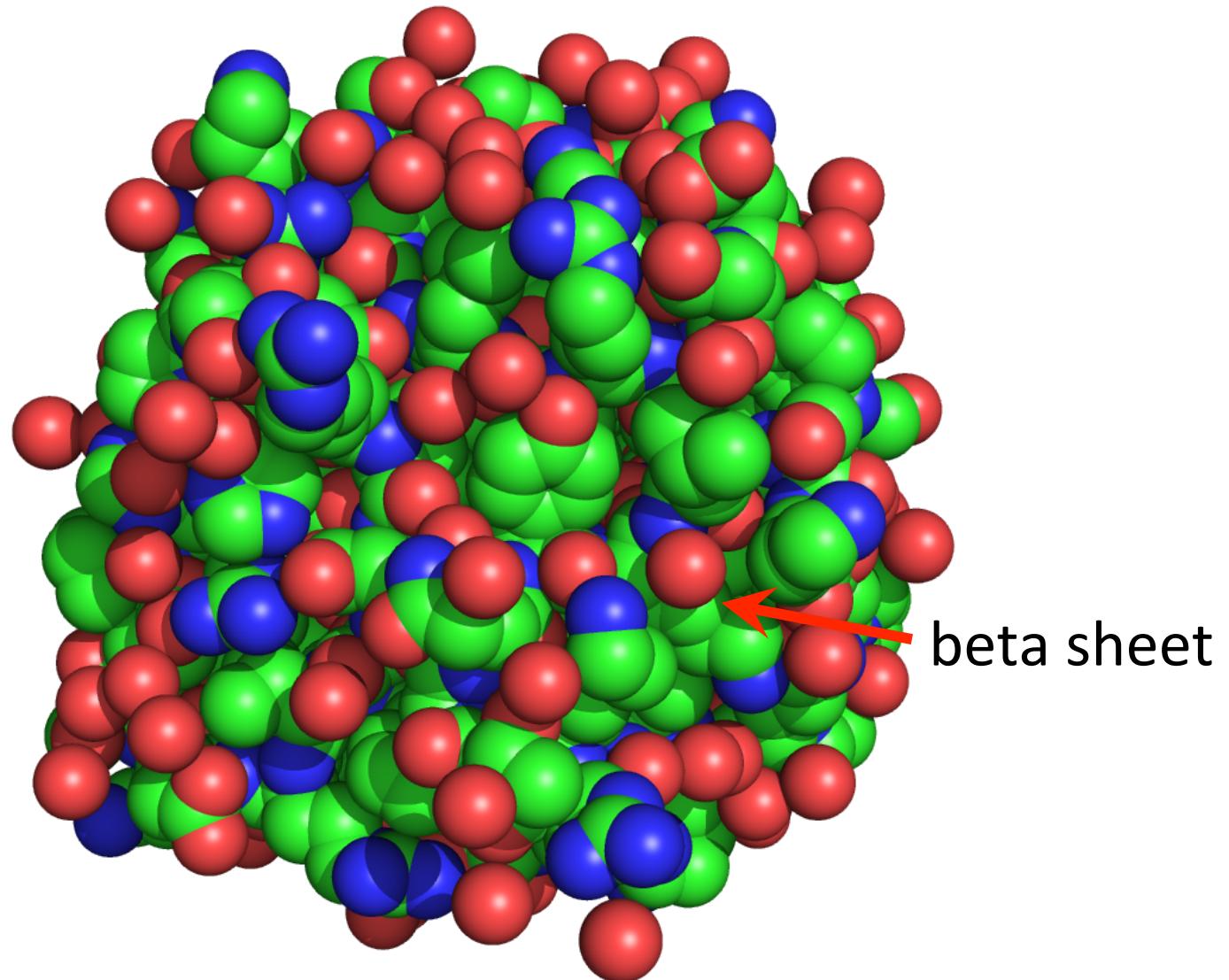
# Different visualizations of a structure: Ribbon



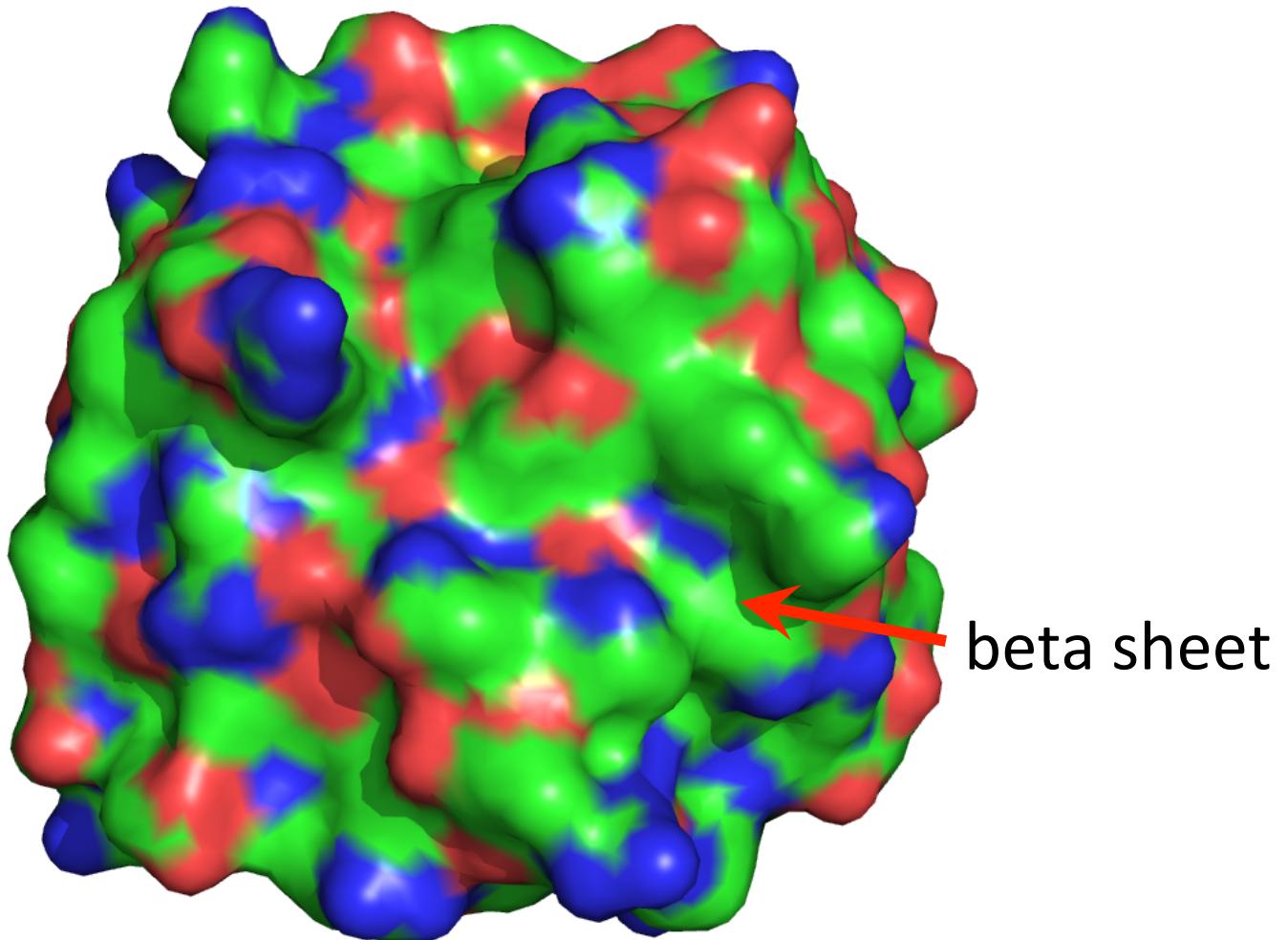
# Different visualizations of a structure: Sticks



# Different visualizations of a structure: Spheres

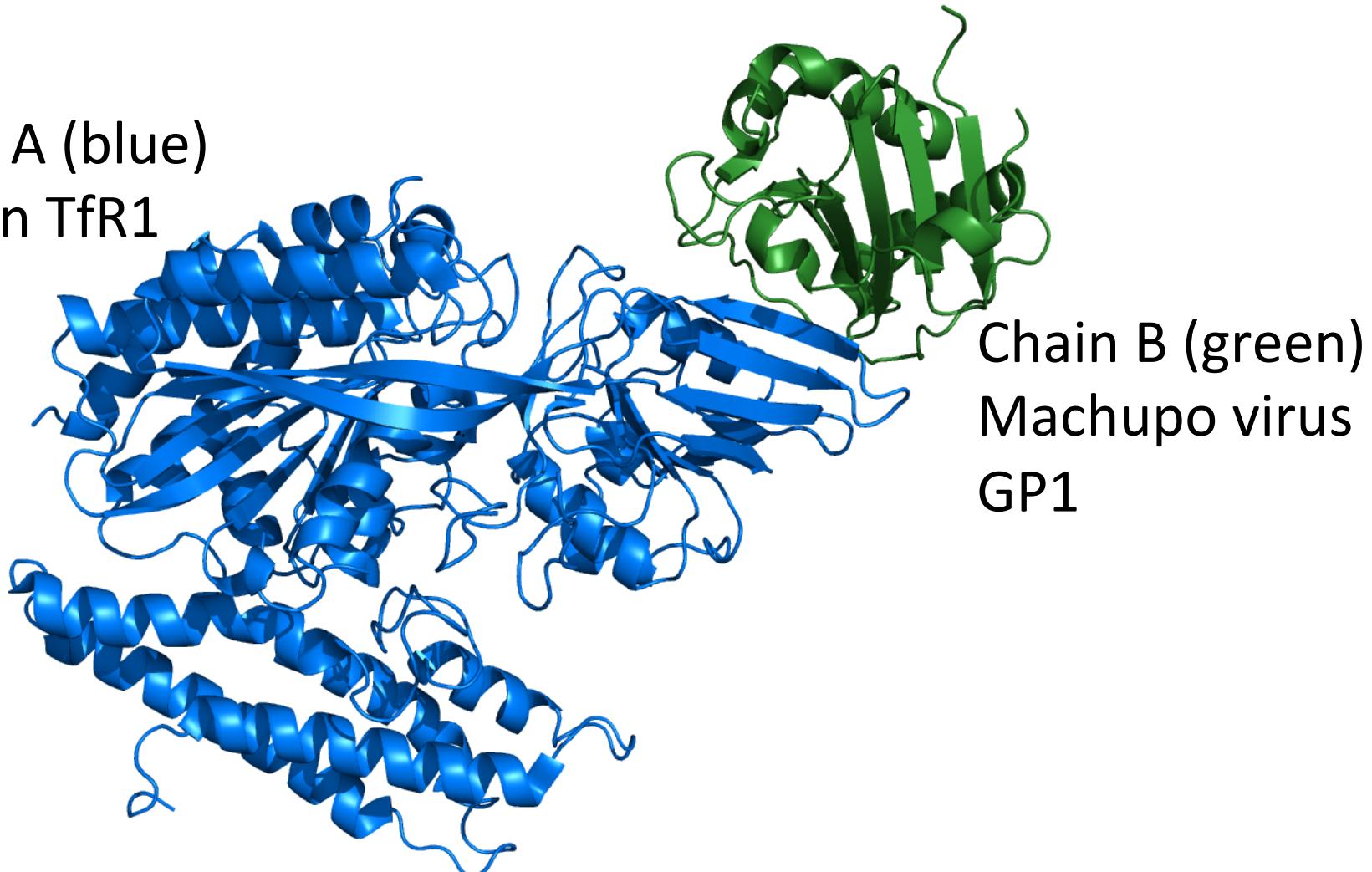


# Different visualizations of a structure: Surface



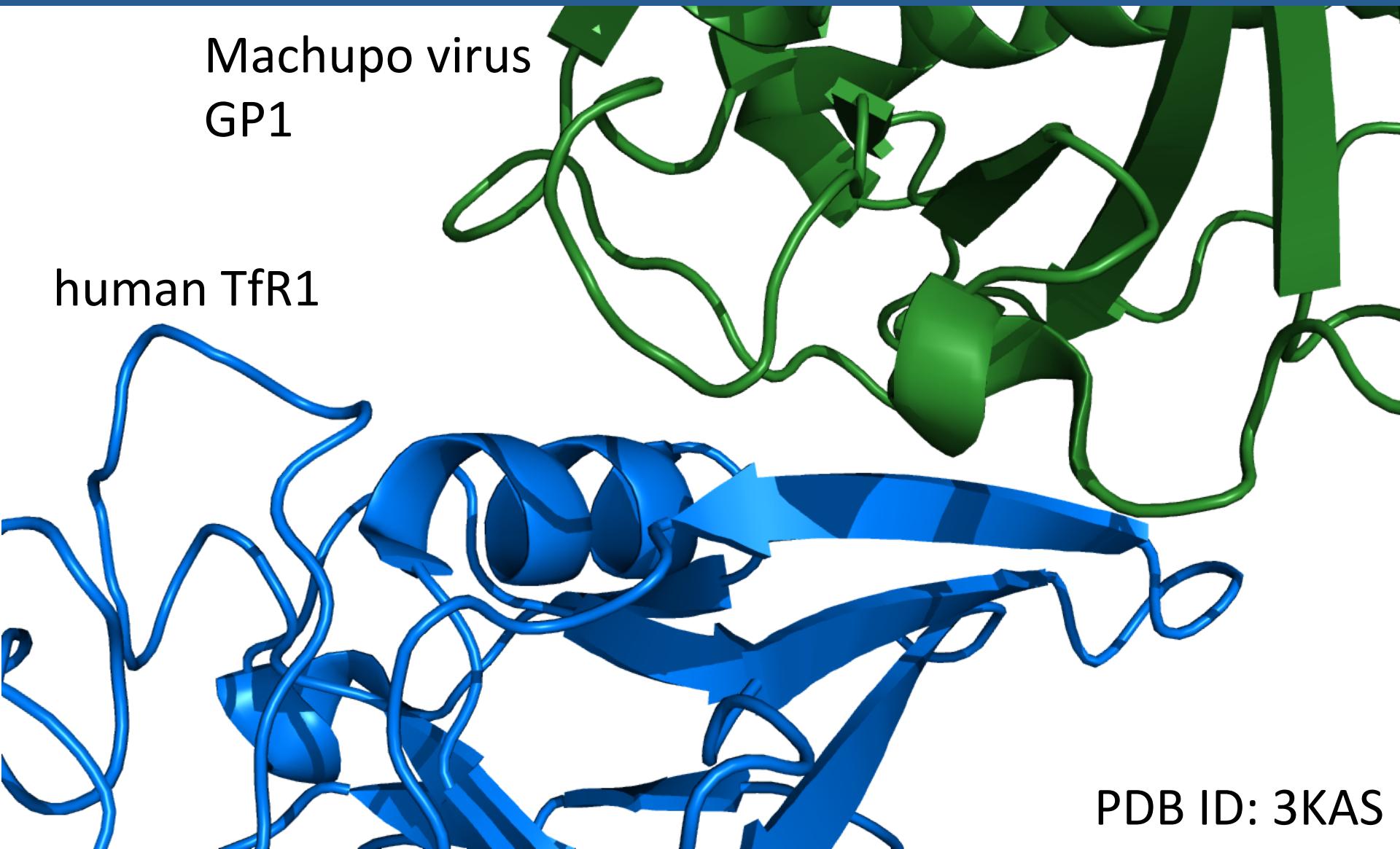
# PDB files can contain multiple chains

Chain A (blue)  
human TfR1



PDB ID: 3KAS

PDB files can contain multiple chains



# Anatomy of a PDB file

HEADER GROWTH FACTOR 15-APR-93 1BFG  
TITLE CRYSTAL STRUCTURE OF BASIC FIBROBLAST GROWTH FACTOR AT 1.6  
TITLE 2 ANGSTROMS RESOLUTION  
COMPND MOL\_ID: 1;  
COMPND 2 MOLECULE: BASIC FIBROBLAST GROWTH FACTOR;  
COMPND 3 CHAIN: A;  
COMPND 4 ENGINEERED: YES  
SOURCE MOL\_ID: 1;  
SOURCE 2 ORGANISM\_SCIENTIFIC: HOMO SAPIENS;  
SOURCE 3 ORGANISM\_COMMON: HUMAN;  
SOURCE 4 ORGANISM\_TAXID: 9606  
KEYWDS GROWTH FACTOR  
EXPDTA X-RAY DIFFRACTION  
AUTHOR Y.KITAGAWA,H.AGO,Y.KATSUBE,A.FUJISHIMA,Y.MATSUURA  
REVDAT 3 24-FEB-09 1BFG 1 VERSN  
REVDAT 2 01-APR-03 1BFG 1 JRNL  
REVDAT 1 31-JAN-94 1BFG 0  
JRNL AUTH H.AGO,Y.KITAGAWA,A.FUJISHIMA,Y.MATSUURA,Y.KATSUBE  
JRNL TITL CRYSTAL STRUCTURE OF BASIC FIBROBLAST GROWTH  
JRNL TITL 2 FACTOR AT 1.6 A RESOLUTION.  
JRNL REF J.BIOCHEM.(TOKYO) V. 110 360 1991  
JRNL REFN ISSN 0021-924X  
JRNL PMID 1769963  
...

# Anatomy of a PDB file

HEADER GROWTH FACTOR 15-APR-93 1BFG  
TITLE CRYSTAL STRUCTURE OF BASIC FIBROBLAST GROWTH FACTOR AT 1.6  
TITLE 2 ANGSTROMS RESOLUTION  
COMPND MOL\_ID: 1;  
COMPND 2 MOLECULE: BASIC FIBROBLAST GROWTH FACTOR;  
COMPND 3 CHAIN: A;  
COMPND 4 ENGINEERED: YES  
SOURCE MOL\_ID: 1;  
SOURCE 2 ORGANISM\_SCIENTIFIC: HOMO SAPIENS;  
SOURCE 3 ORGANISM\_COMMON: HUMAN;  
SOURCE 4 ORGANISM\_TAXID: 9606  
KEYWDS GROWTH FACTOR  
EXPDTA X-RAY DIFFRACTION  
AUTHOR Y.KITAGAWA,H.AGO,Y.KATSUBE,A.FUJISHIMA,Y.MATSUURA  
REVDAT 3 24-FEB-09 1BFG 1 VERSN  
REVDAT 2 01-APR-03 1BFG 1 JRNL  
REVDAT 1 31-JAN-94 1BFG 0  
JRNL AUTH H.AGO,Y.KITAGAWA,A.FUJISHIMA,Y.MATSUURA,Y.KATSUBE  
JRNL TITL CRYSTAL STRUCTURE OF BASIC FIBROBLAST GROWTH  
JRNL TITL 2 FACTOR AT 1.6 A RESOLUTION.  
JRNL REF J.BIOCHEM.(TOKYO) V. 110 360 1991  
JRNL REFN ISSN 0021-924X  
JRNL PMID 1769963  
...

# Anatomy of a PDB file

HEADER	GROWTH FACTOR	15-APR-93	1BFG
TITLE	CRYSTAL STRUCTURE OF BASIC FIBROBLAST GROWTH FACTOR AT 1.6		
TITLE	2 ANGSTROMS RESOLUTION		
COMPND	MOL_ID: 1;		
COMPND	2 MOLECULE: BASIC FIBROBLAST GROWTH FACTOR;		
COMPND	3 CHAIN: A;		
COMPND	4 ENGINEERED: YES		
SOURCE	MOL_ID: 1;		
SOURCE	2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;		
SOURCE	3 ORGANISM_COMMON: HUMAN;		
SOURCE	4 ORGANISM_TAXID: 9606		
KEYWDS	GROWTH FACTOR		
EXPDTA	X-RAY DIFFRACTION		
AUTHOR	Y.KITAGAWA, H.AGO, Y.KATSUBE, A.FUJISHIMA, Y.MATSUURA		
REVDAT	3	24-FEB-09 1BFG	1 VERSN
REVDAT	2	01-APR-03 1BFG	1 JRNL
REVDAT	1	31-JAN-94 1BFG	0
JRNL	AUTH H.AGO, Y.KITAGAWA, A.FUJISHIMA, Y.MATSUURA, Y.KATSUBE		
JRNL	TITL CRYSTAL STRUCTURE OF BASIC FIBROBLAST GROWTH		
JRNL	TITL 2 FACTOR AT 1.6 A RESOLUTION.		
JRNL	REF	J.BIOCHEM.(TOKYO)	V. 110 360 1991
JRNL	REFN	ISSN 0021-924X	
JRNL	PMID	1769963	
...			

# Anatomy of a PDB file

HEADER GROWTH FACTOR 15-APR-93 1BFG  
TITLE CRYSTAL STRUCTURE OF BASIC FIBROBLAST GROWTH FACTOR AT 1.6  
TITLE 2 ANGSTROMS RESOLUTION  
COMPND MOL\_ID: 1;  
COMPND 2 MOLECULE: BASIC FIBROBLAST GROWTH FACTOR;  
COMPND 3 CHAIN: A;  
COMPND 4 ENGINEERED: YES  
SOURCE MOL\_ID: 1;  
SOURCE 2 ORGANISM\_SCIENTIFIC: HOMO SAPIENS;  
SOURCE 3 ORGANISM\_COMMON: HUMAN;  
SOURCE 4 ORGANISM\_TAXID: 9606  
KEYWDS GROWTH FACTOR  
EXPDTA X-RAY DIFFRACTION  
AUTHOR Y.KITAGAWA,H.AGO,Y.KATSUKE,A.FUJISHIMA,Y.MATSUURA  
REVDAT 3 24-FEB-09 1BFG 1 VERSN  
REVDAT 2 01-APR-03 1BFG 1 JRNL  
REVDAT 1 31-JAN-94 1BFG 0  
JRNL AUTH H.AGO,Y.KITAGAWA,A.FUJISHIMA,Y.MATSUURA,Y.KATSUKE  
JRNL TITL CRYSTAL STRUCTURE OF BASIC FIBROBLAST GROWTH  
JRNL TITL 2 FACTOR AT 1.6 A RESOLUTION.  
JRNL REF J.BIOCHEM.(TOKYO) V. 110 360 1991  
JRNL REFN ISSN 0021-924X  
JRNL PMID 1769963  
...

# Anatomy of a PDB file

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ATOM	1	N	ASP	A	19	6.864	13.397	-2.220	1.00	40.02	N
ATOM	2	CA	ASP	A	19	6.806	14.455	-1.186	1.00	38.62	C
ATOM	3	C	ASP	A	19	7.688	14.002	-0.016	1.00	36.01	C
ATOM	4	O	ASP	A	19	8.837	14.477	0.052	1.00	35.96	O
ATOM	5	CB	ASP	A	19	5.372	14.834	-0.851	1.00	43.28	C
ATOM	6	CG	ASP	A	19	5.264	16.239	-0.268	1.00	46.36	C
ATOM	7	OD1	ASP	A	19	5.447	16.322	0.978	1.00	48.00	O
ATOM	8	OD2	ASP	A	19	5.015	17.239	-0.970	1.00	48.45	O
ATOM	9	N	PRO	A	20	7.165	13.125	0.822	1.00	33.63	N
ATOM	10	CA	PRO	A	20	7.888	12.572	1.982	1.00	30.69	C
ATOM	11	C	PRO	A	20	9.049	11.697	1.528	1.00	27.78	C

...

# Anatomy of a PDB file

atom number



ATOM	1	N	ASP	A	19	6.864	13.397	-2.220	1.00	40.02	N
ATOM	2	CA	ASP	A	19	6.806	14.455	-1.186	1.00	38.62	C
ATOM	3	C	ASP	A	19	7.688	14.002	-0.016	1.00	36.01	C
ATOM	4	O	ASP	A	19	8.837	14.477	0.052	1.00	35.96	O
ATOM	5	CB	ASP	A	19	5.372	14.834	-0.851	1.00	43.28	C
ATOM	6	CG	ASP	A	19	5.264	16.239	-0.268	1.00	46.36	C
ATOM	7	OD1	ASP	A	19	5.447	16.322	0.978	1.00	48.00	O
ATOM	8	OD2	ASP	A	19	5.015	17.239	-0.970	1.00	48.45	O
ATOM	9	N	PRO	A	20	7.165	13.125	0.822	1.00	33.63	N
ATOM	10	CA	PRO	A	20	7.888	12.572	1.982	1.00	30.69	C
ATOM	11	C	PRO	A	20	9.049	11.697	1.528	1.00	27.78	C

...

# Anatomy of a PDB file

atom name



ATOM	1	N	ASP	A	19	6.864	13.397	-2.220	1.00	40.02	N
ATOM	2	CA	ASP	A	19	6.806	14.455	-1.186	1.00	38.62	C
ATOM	3	C	ASP	A	19	7.688	14.002	-0.016	1.00	36.01	C
ATOM	4	O	ASP	A	19	8.837	14.477	0.052	1.00	35.96	O
ATOM	5	CB	ASP	A	19	5.372	14.834	-0.851	1.00	43.28	C
ATOM	6	CG	ASP	A	19	5.264	16.239	-0.268	1.00	46.36	C
ATOM	7	OD1	ASP	A	19	5.447	16.322	0.978	1.00	48.00	O
ATOM	8	OD2	ASP	A	19	5.015	17.239	-0.970	1.00	48.45	O
ATOM	9	N	PRO	A	20	7.165	13.125	0.822	1.00	33.63	N
ATOM	10	CA	PRO	A	20	7.888	12.572	1.982	1.00	30.69	C
ATOM	11	C	PRO	A	20	9.049	11.697	1.528	1.00	27.78	C

...

# Anatomy of a PDB file

residue name



ATOM	1	N	ASP	A	19	6.864	13.397	-2.220	1.00	40.02	N
ATOM	2	CA	ASP	A	19	6.806	14.455	-1.186	1.00	38.62	C
ATOM	3	C	ASP	A	19	7.688	14.002	-0.016	1.00	36.01	C
ATOM	4	O	ASP	A	19	8.837	14.477	0.052	1.00	35.96	O
ATOM	5	CB	ASP	A	19	5.372	14.834	-0.851	1.00	43.28	C
ATOM	6	CG	ASP	A	19	5.264	16.239	-0.268	1.00	46.36	C
ATOM	7	OD1	ASP	A	19	5.447	16.322	0.978	1.00	48.00	O
ATOM	8	OD2	ASP	A	19	5.015	17.239	-0.970	1.00	48.45	O
ATOM	9	N	PRO	A	20	7.165	13.125	0.822	1.00	33.63	N
ATOM	10	CA	PRO	A	20	7.888	12.572	1.982	1.00	30.69	C
ATOM	11	C	PRO	A	20	9.049	11.697	1.528	1.00	27.78	C

# Anatomy of a PDB file

chain



ATOM	1	N	ASP	A	19	6.864	13.397	-2.220	1.00	40.02	N
ATOM	2	CA	ASP	A	19	6.806	14.455	-1.186	1.00	38.62	C
ATOM	3	C	ASP	A	19	7.688	14.002	-0.016	1.00	36.01	C
ATOM	4	O	ASP	A	19	8.837	14.477	0.052	1.00	35.96	O
ATOM	5	CB	ASP	A	19	5.372	14.834	-0.851	1.00	43.28	C
ATOM	6	CG	ASP	A	19	5.264	16.239	-0.268	1.00	46.36	C
ATOM	7	OD1	ASP	A	19	5.447	16.322	0.978	1.00	48.00	O
ATOM	8	OD2	ASP	A	19	5.015	17.239	-0.970	1.00	48.45	O
ATOM	9	N	PRO	A	20	7.165	13.125	0.822	1.00	33.63	N
ATOM	10	CA	PRO	A	20	7.888	12.572	1.982	1.00	30.69	C
ATOM	11	C	PRO	A	20	9.049	11.697	1.528	1.00	27.78	C

# Anatomy of a PDB file

residue number



ATOM	1	N	ASP	A	19	6.864	13.397	-2.220	1.00	40.02	N
ATOM	2	CA	ASP	A	19	6.806	14.455	-1.186	1.00	38.62	C
ATOM	3	C	ASP	A	19	7.688	14.002	-0.016	1.00	36.01	C
ATOM	4	O	ASP	A	19	8.837	14.477	0.052	1.00	35.96	O
ATOM	5	CB	ASP	A	19	5.372	14.834	-0.851	1.00	43.28	C
ATOM	6	CG	ASP	A	19	5.264	16.239	-0.268	1.00	46.36	C
ATOM	7	OD1	ASP	A	19	5.447	16.322	0.978	1.00	48.00	O
ATOM	8	OD2	ASP	A	19	5.015	17.239	-0.970	1.00	48.45	O
ATOM	9	N	PRO	A	20	7.165	13.125	0.822	1.00	33.63	N
ATOM	10	CA	PRO	A	20	7.888	12.572	1.982	1.00	30.69	C
ATOM	11	C	PRO	A	20	9.049	11.697	1.528	1.00	27.78	C

# Anatomy of a PDB file

*x, y, z coordinates*



ATOM	1	N	ASP	A	19	6.864	13.397	-2.220	1.00	40.02	N
ATOM	2	CA	ASP	A	19	6.806	14.455	-1.186	1.00	38.62	C
ATOM	3	C	ASP	A	19	7.688	14.002	-0.016	1.00	36.01	C
ATOM	4	O	ASP	A	19	8.837	14.477	0.052	1.00	35.96	O
ATOM	5	CB	ASP	A	19	5.372	14.834	-0.851	1.00	43.28	C
ATOM	6	CG	ASP	A	19	5.264	16.239	-0.268	1.00	46.36	C
ATOM	7	OD1	ASP	A	19	5.447	16.322	0.978	1.00	48.00	O
ATOM	8	OD2	ASP	A	19	5.015	17.239	-0.970	1.00	48.45	O
ATOM	9	N	PRO	A	20	7.165	13.125	0.822	1.00	33.63	N
ATOM	10	CA	PRO	A	20	7.888	12.572	1.982	1.00	30.69	C
ATOM	11	C	PRO	A	20	9.049	11.697	1.528	1.00	27.78	C

# Anatomy of a PDB file

occupancy



ATOM	1	N	ASP	A	19	6.864	13.397	-2.220	1.00	40.02	N
ATOM	2	CA	ASP	A	19	6.806	14.455	-1.186	1.00	38.62	C
ATOM	3	C	ASP	A	19	7.688	14.002	-0.016	1.00	36.01	C
ATOM	4	O	ASP	A	19	8.837	14.477	0.052	1.00	35.96	O
ATOM	5	CB	ASP	A	19	5.372	14.834	-0.851	1.00	43.28	C
ATOM	6	CG	ASP	A	19	5.264	16.239	-0.268	1.00	46.36	C
ATOM	7	OD1	ASP	A	19	5.447	16.322	0.978	1.00	48.00	O
ATOM	8	OD2	ASP	A	19	5.015	17.239	-0.970	1.00	48.45	O
ATOM	9	N	PRO	A	20	7.165	13.125	0.822	1.00	33.63	N
ATOM	10	CA	PRO	A	20	7.888	12.572	1.982	1.00	30.69	C
ATOM	11	C	PRO	A	20	9.049	11.697	1.528	1.00	27.78	C

# Anatomy of a PDB file

B factor										
ATOM	1	N	ASP	A	19	6.864	13.397	-2.220	1.00 40.02	N
ATOM	2	CA	ASP	A	19	6.806	14.455	-1.186	1.00 38.62	C
ATOM	3	C	ASP	A	19	7.688	14.002	-0.016	1.00 36.01	C
ATOM	4	O	ASP	A	19	8.837	14.477	0.052	1.00 35.96	O
ATOM	5	CB	ASP	A	19	5.372	14.834	-0.851	1.00 43.28	C
ATOM	6	CG	ASP	A	19	5.264	16.239	-0.268	1.00 46.36	C
ATOM	7	OD1	ASP	A	19	5.447	16.322	0.978	1.00 48.00	O
ATOM	8	OD2	ASP	A	19	5.015	17.239	-0.970	1.00 48.45	O
ATOM	9	N	PRO	A	20	7.165	13.125	0.822	1.00 33.63	N
ATOM	10	CA	PRO	A	20	7.888	12.572	1.982	1.00 30.69	C
ATOM	11	C	PRO	A	20	9.049	11.697	1.528	1.00 27.78	C

# PyMOL exercises

1. Download & open structure 3KAS:  
`fetch 3KAS`
  - Display in various forms (cartoon, stick, spheres, ...)
  - Color different chains
  - Zoom in to display protein-protein interface
  
2. Download & open structure 1DLW
  - Display as cartoon
  - Show heme as sticks