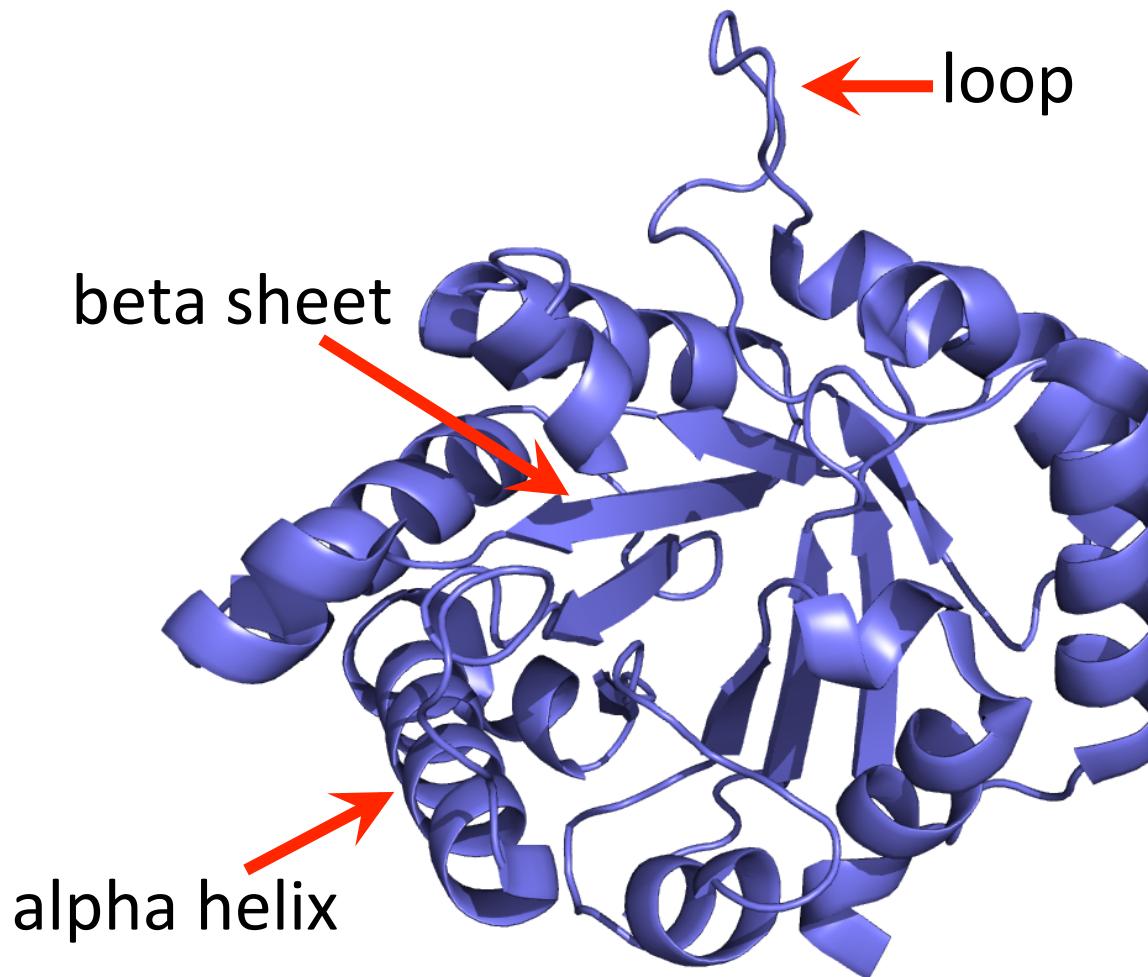


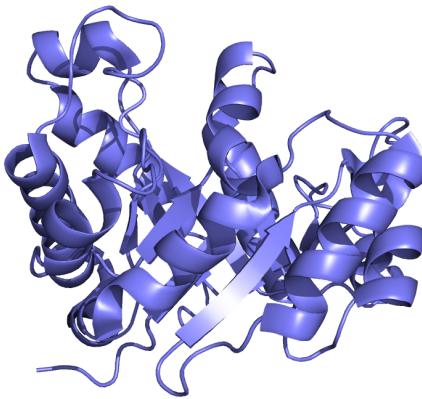
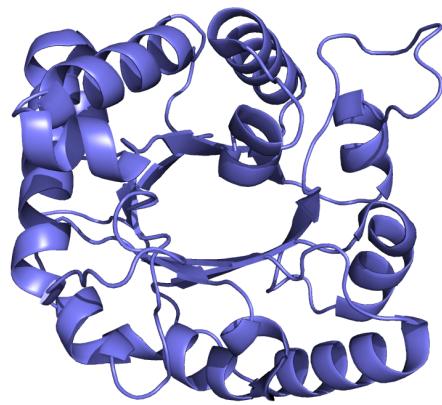
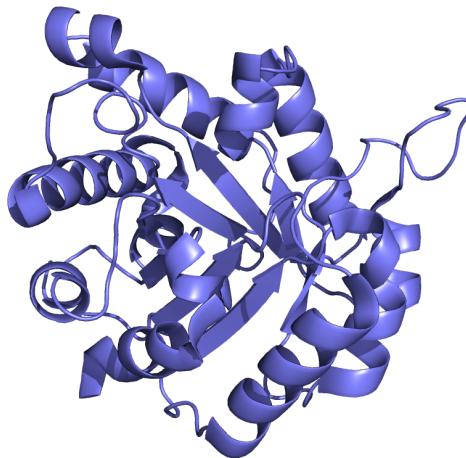
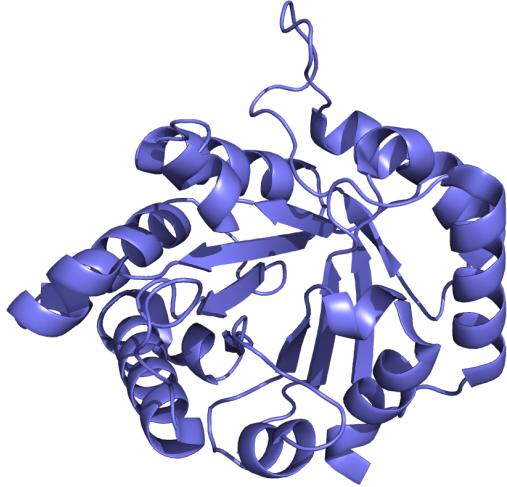
Working with protein structures / PDB files

Structure of Triosephosphate Isomerase

PDB ID: 1HTI

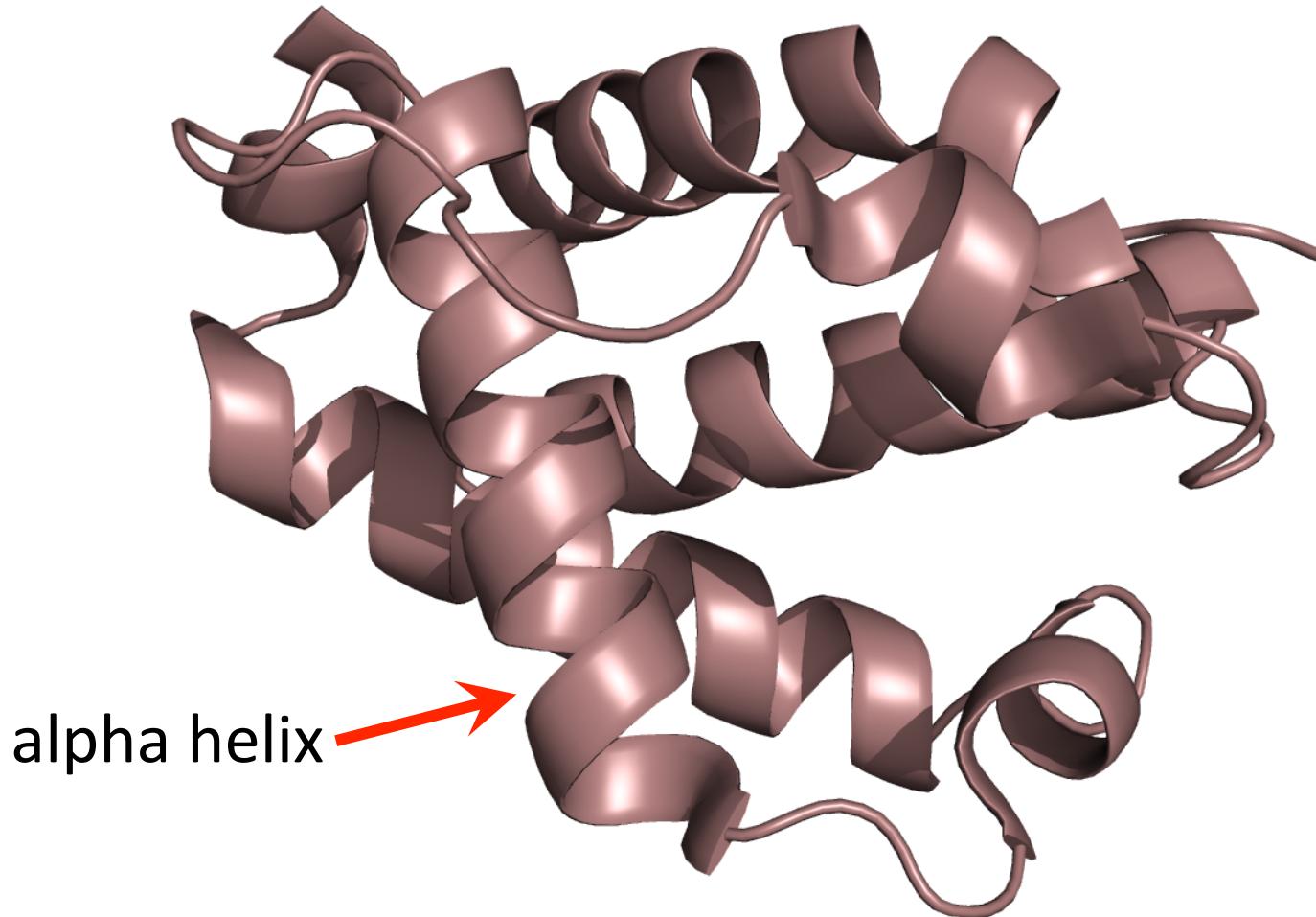


Different perspectives of the same structure



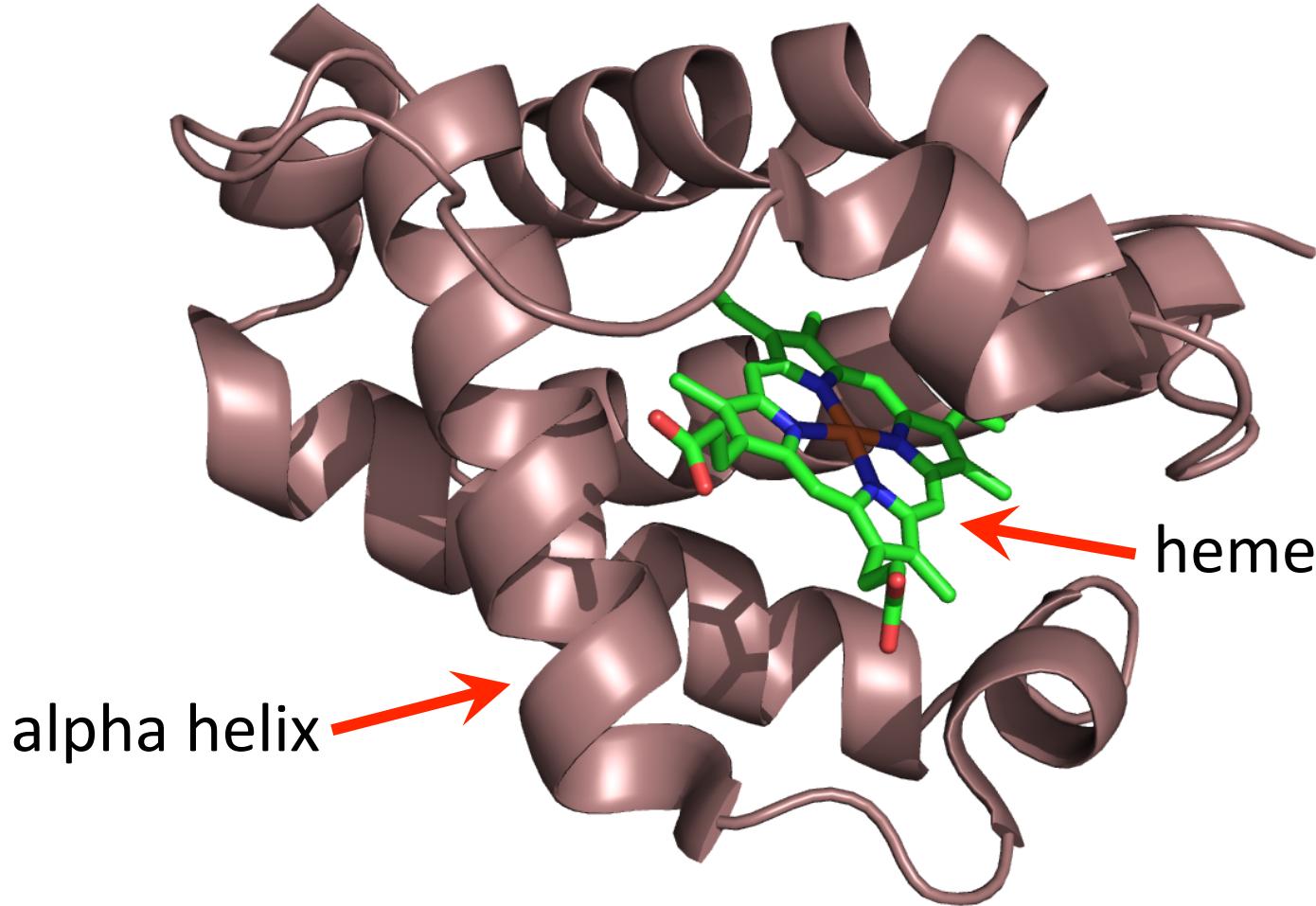
Structure of Truncated Hemoglobin

PDB ID: 1DLW



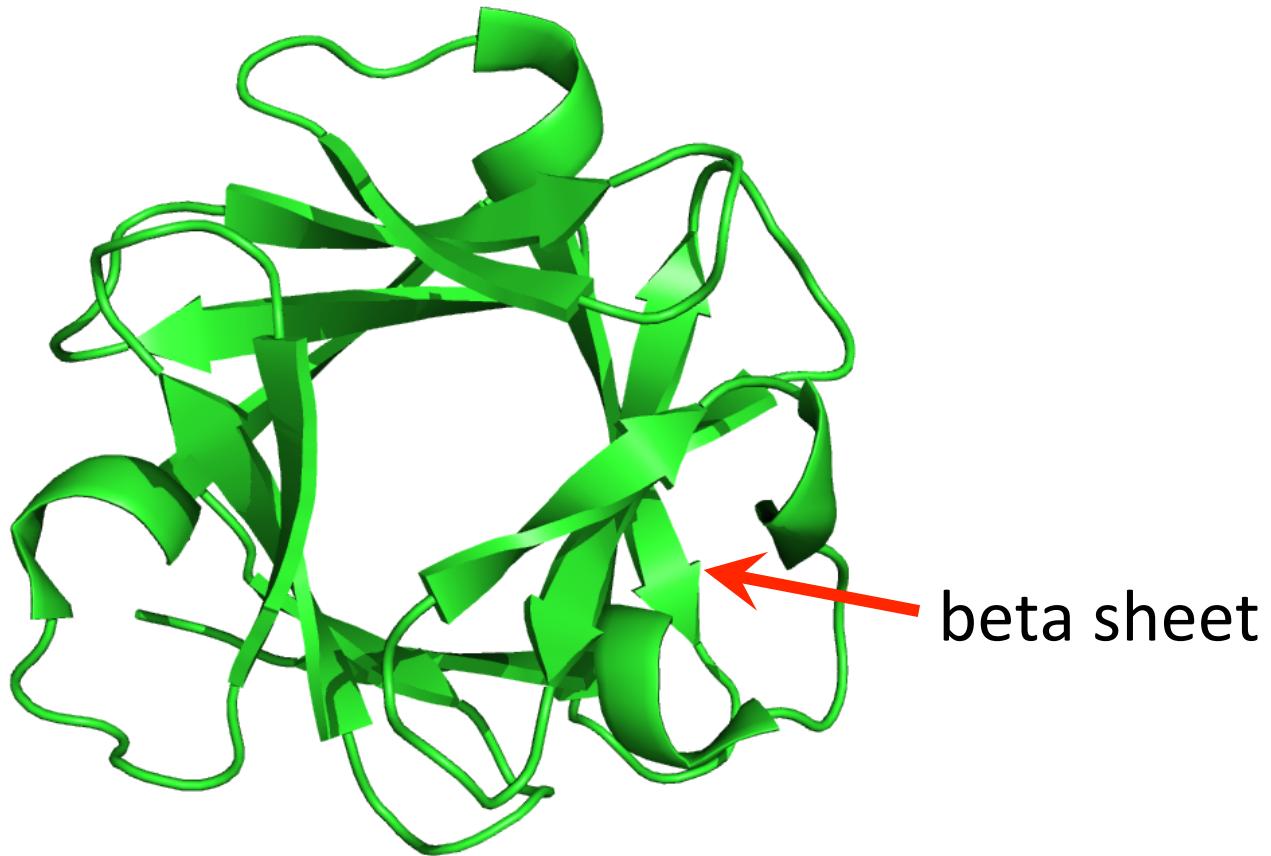
Structure of Truncated Hemoglobin

PDB ID: 1DLW



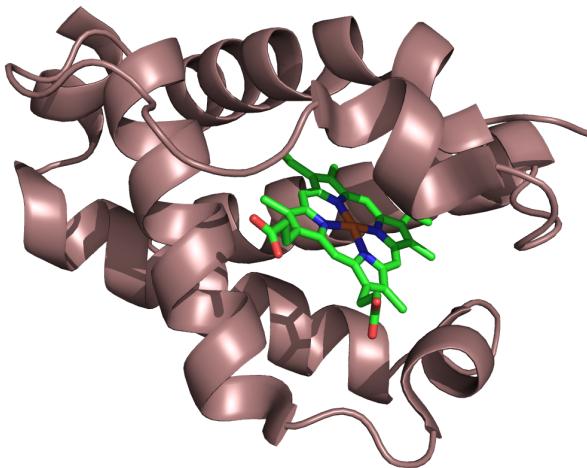
Structure of Basic Fibroblast Growth Factor

PDB ID: 1BFG

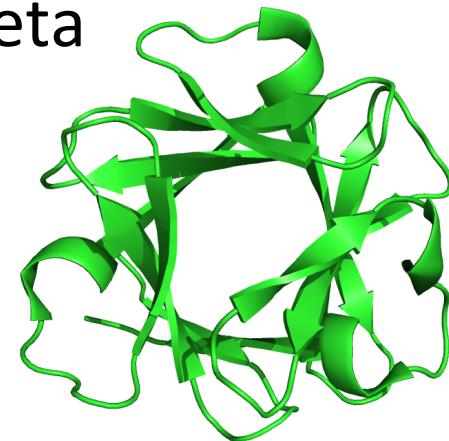


We classify structures by their alpha
and beta content

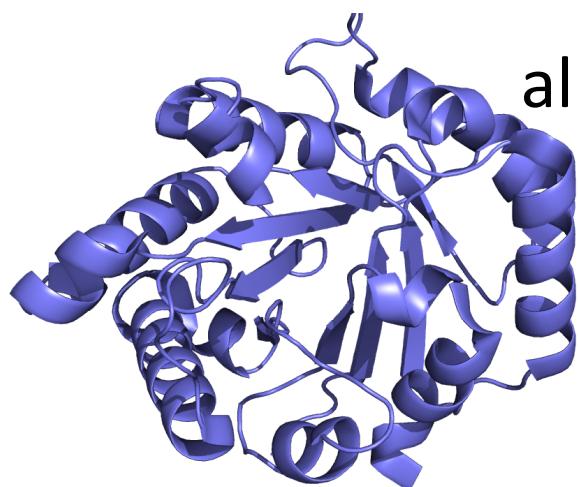
all alpha



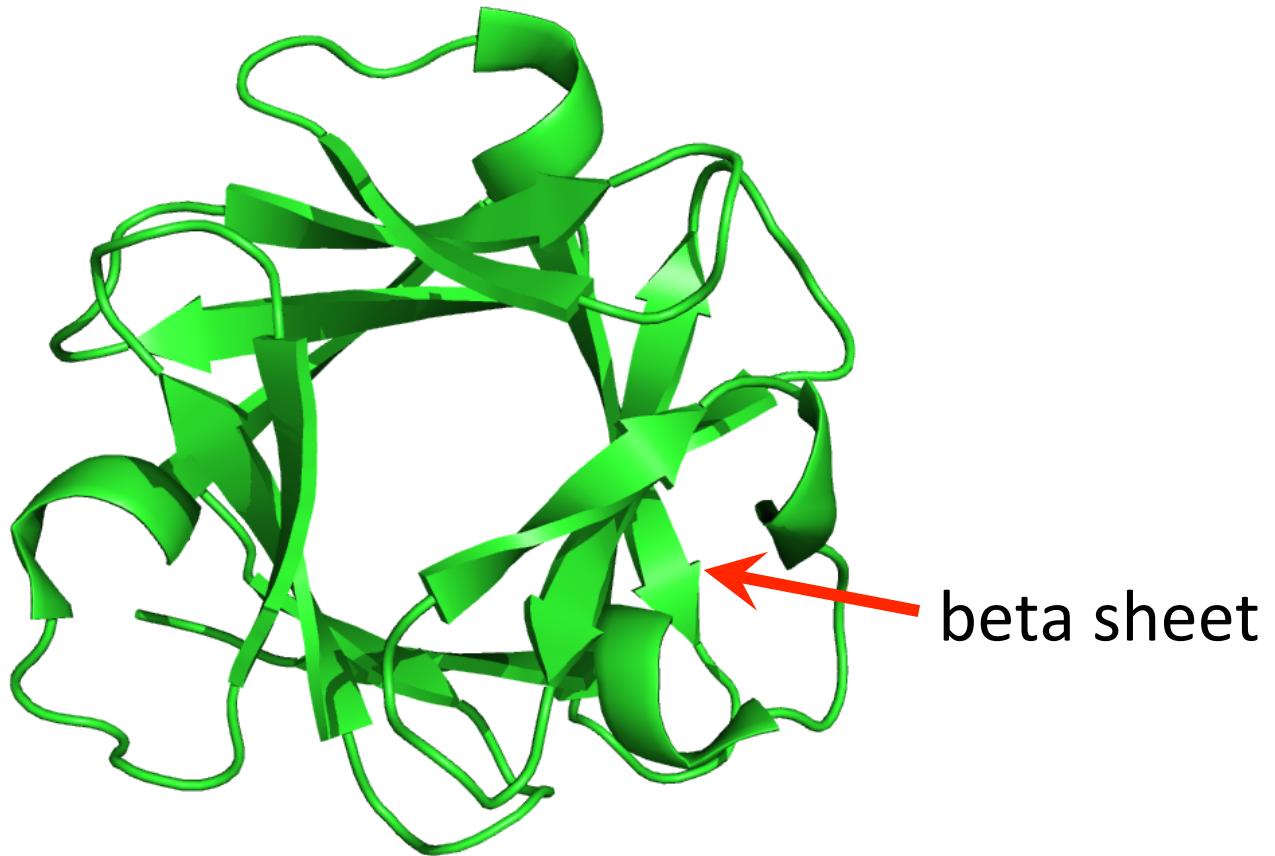
all beta



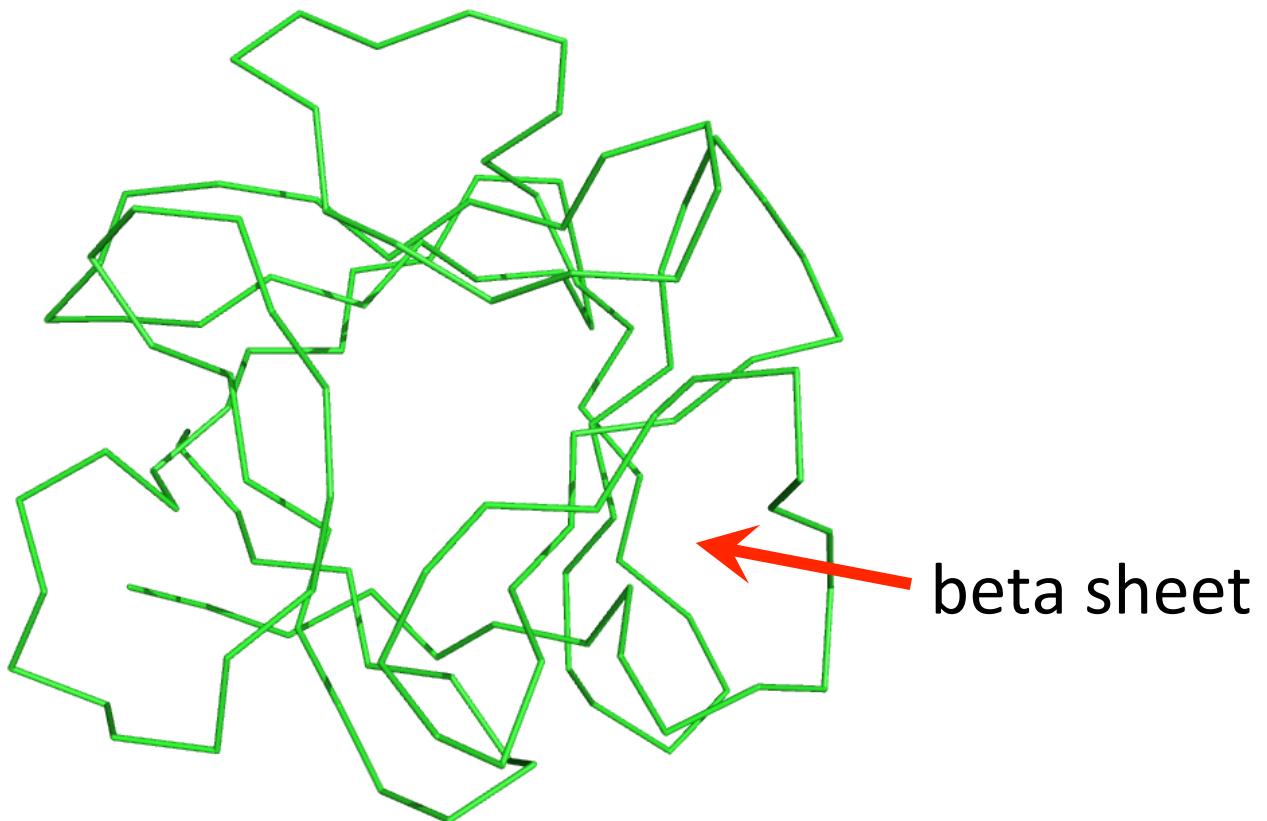
alpha and beta



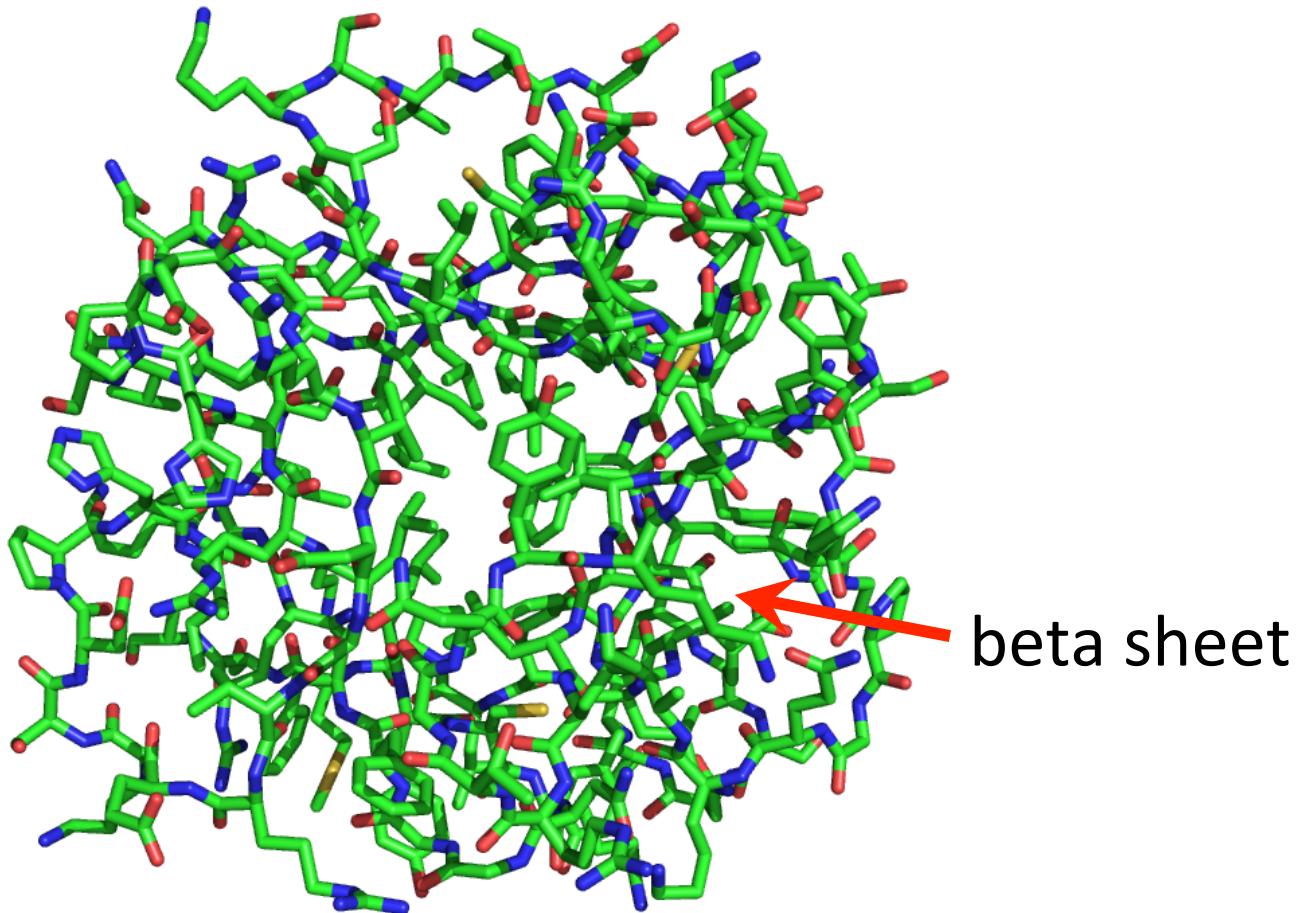
Different visualizations of a structure: Cartoon



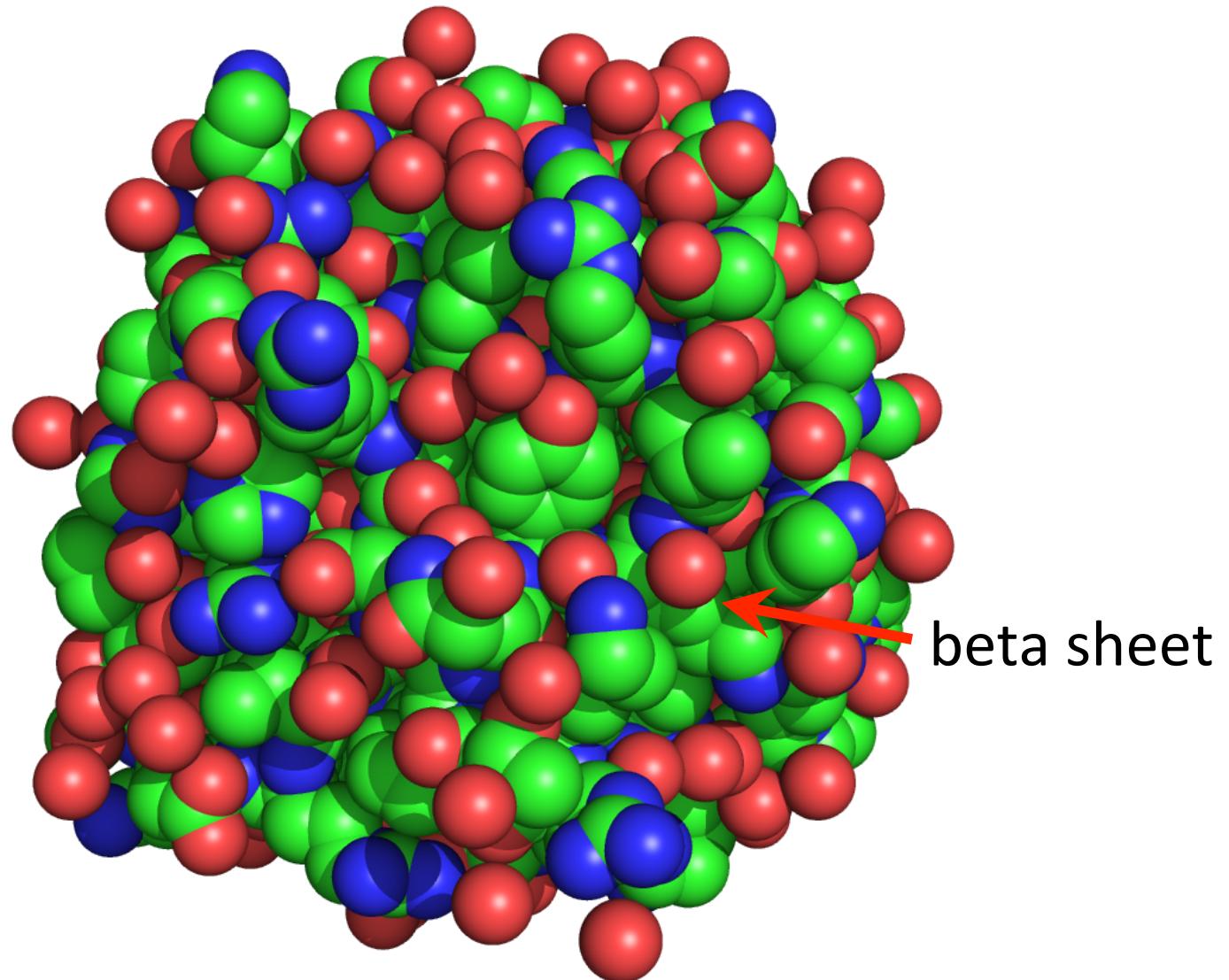
Different visualizations of a structure: Ribbon



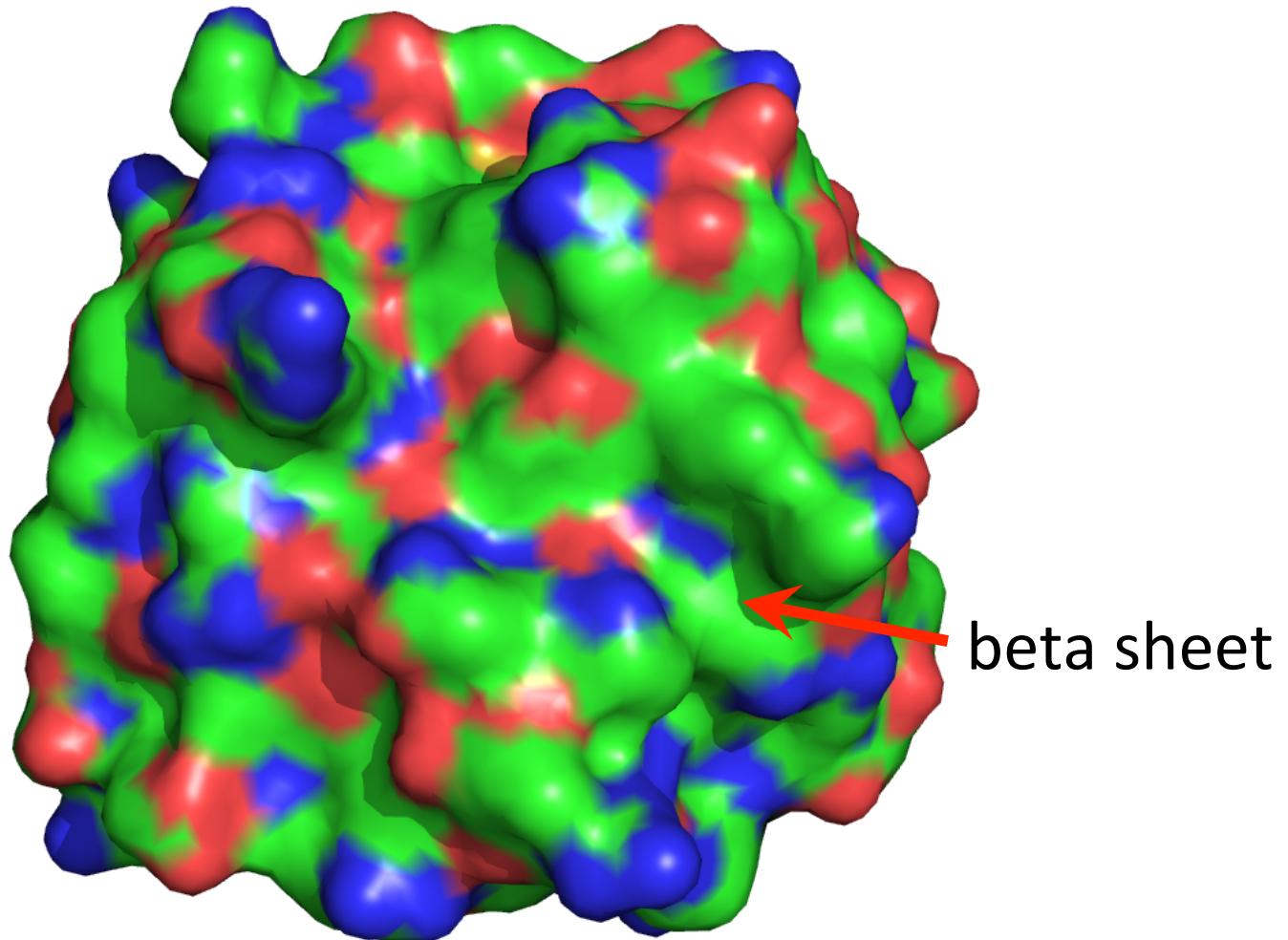
Different visualizations of a structure: Sticks



Different visualizations of a structure: Spheres

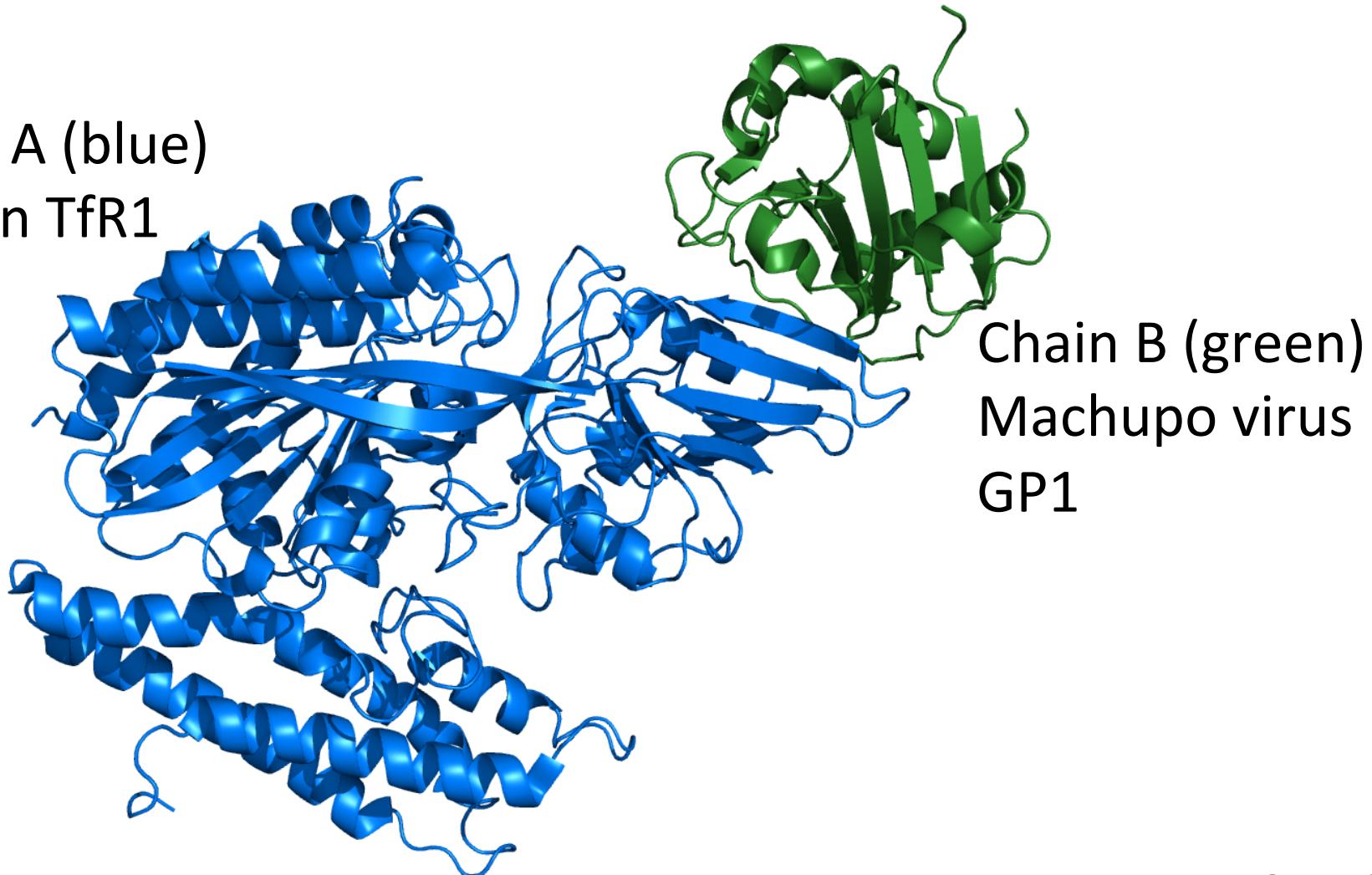


Different visualizations of a structure: Surface



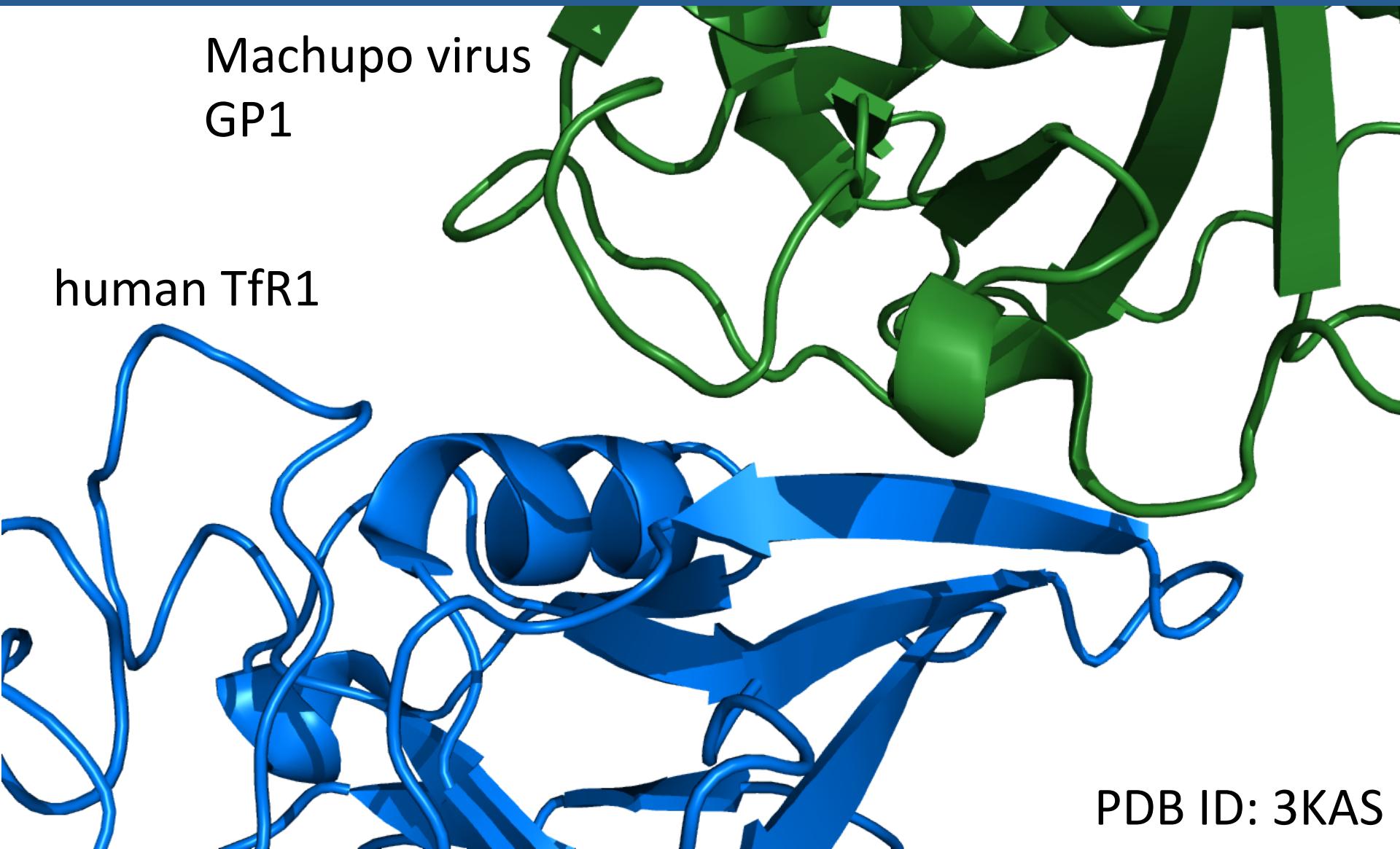
PDB files can contain multiple chains

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;
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SOURCE MOL_ID: 1;
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JRNL REFN ISSN 0021-924X
JRNL PMID 1769963
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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	
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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;
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COMPND 3 CHAIN: A;
COMPND 4 ENGINEERED: YES
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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
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JRNL REF J.BIOCHEM.(TOKYO) V. 110 360 1991
JRNL REFN ISSN 0021-924X
JRNL PMID 1769963
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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

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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

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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
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Anatomy of a PDB file

residue name



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



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