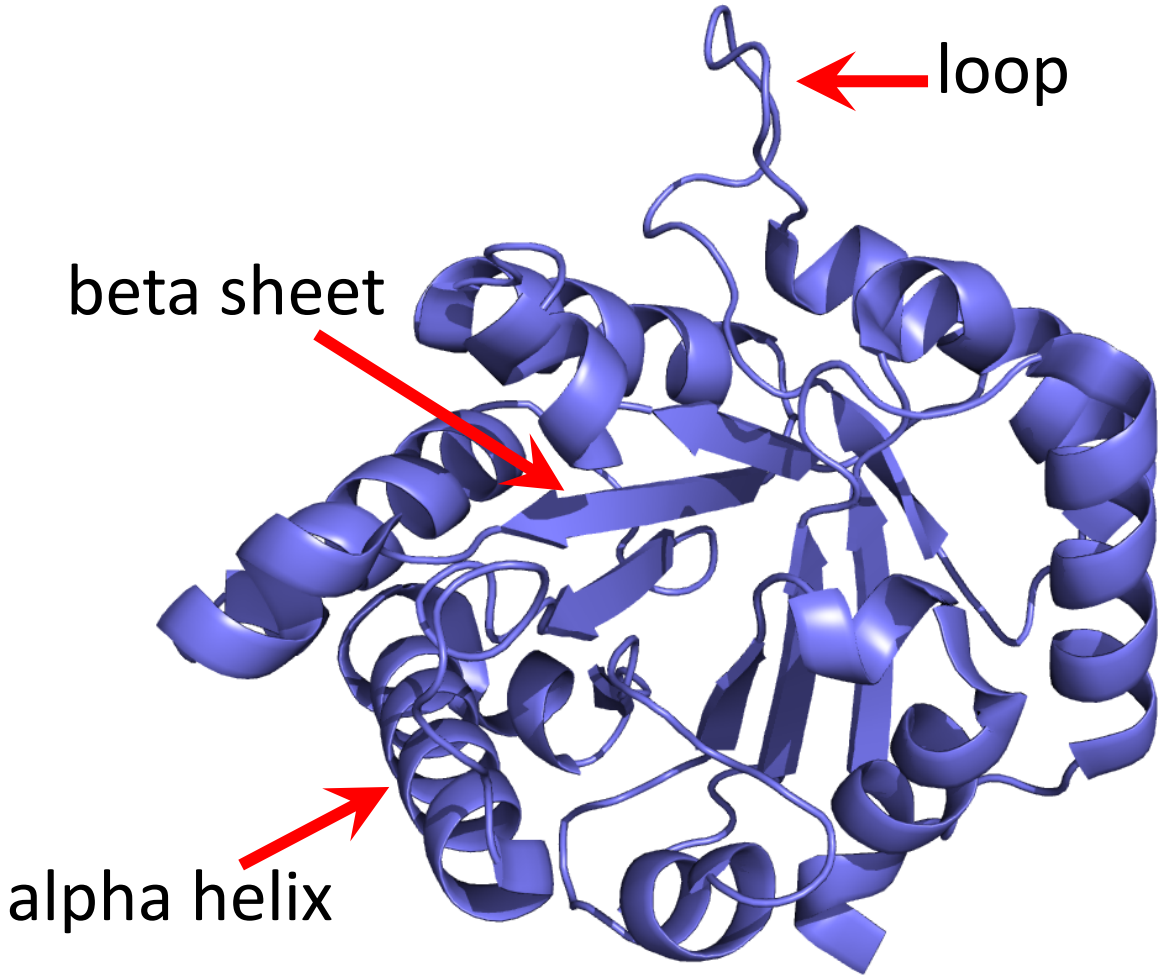
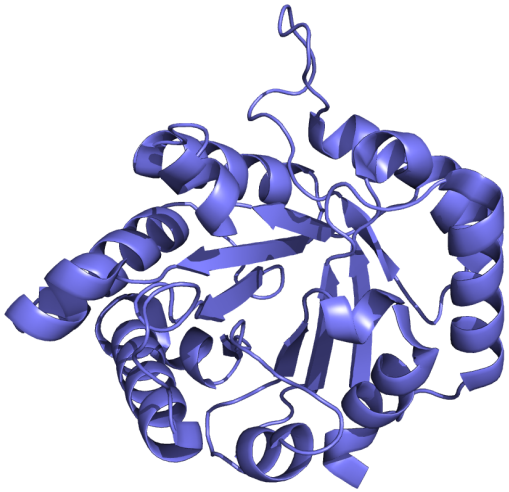
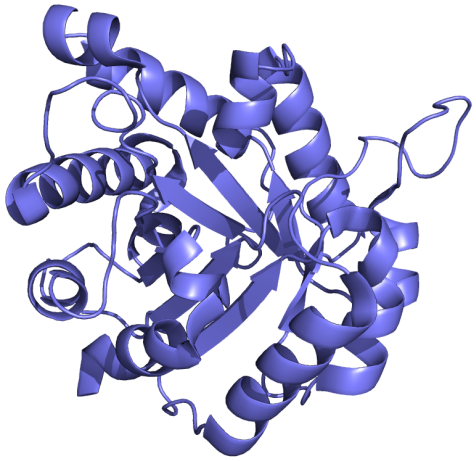
Working with protein structures / PDB files

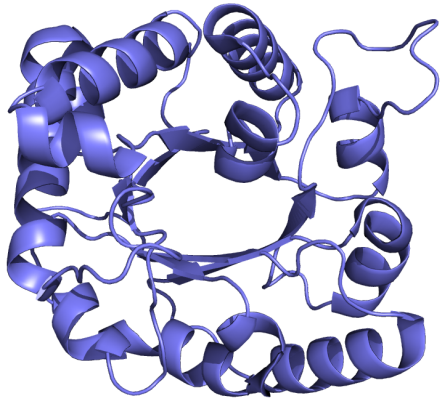
Structure of Triosephosphate Isomerase PDB ID: 1HTI

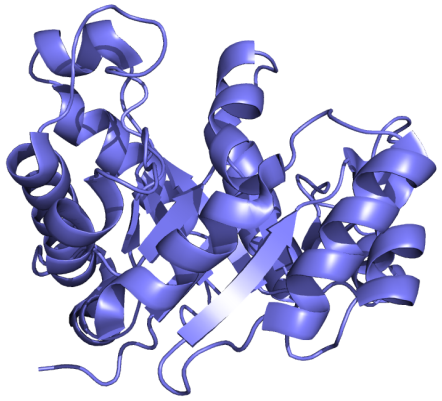


Different perspectives of the same structure

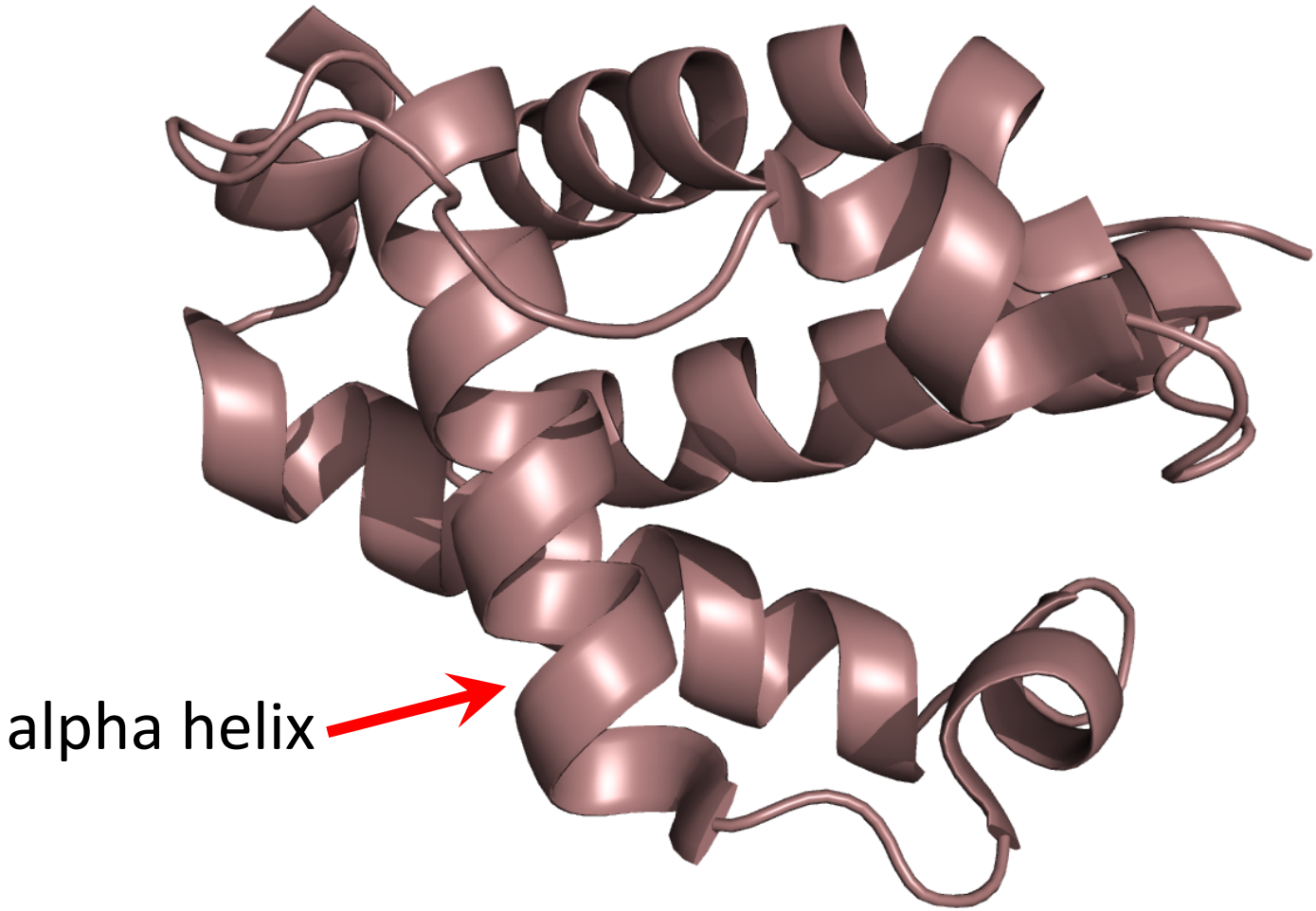








Structure of Truncated Hemoglobin PDB ID: 1DLW



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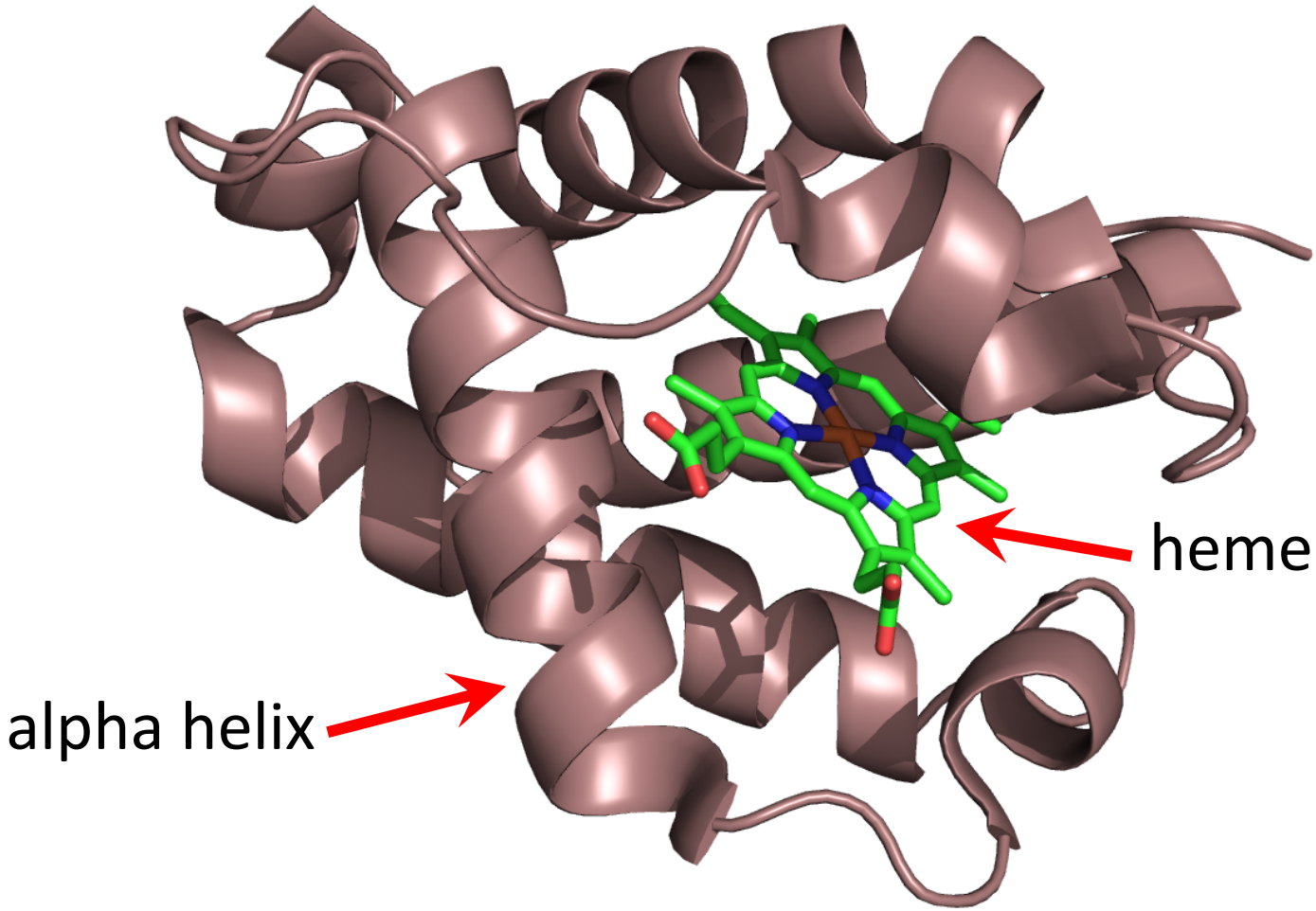
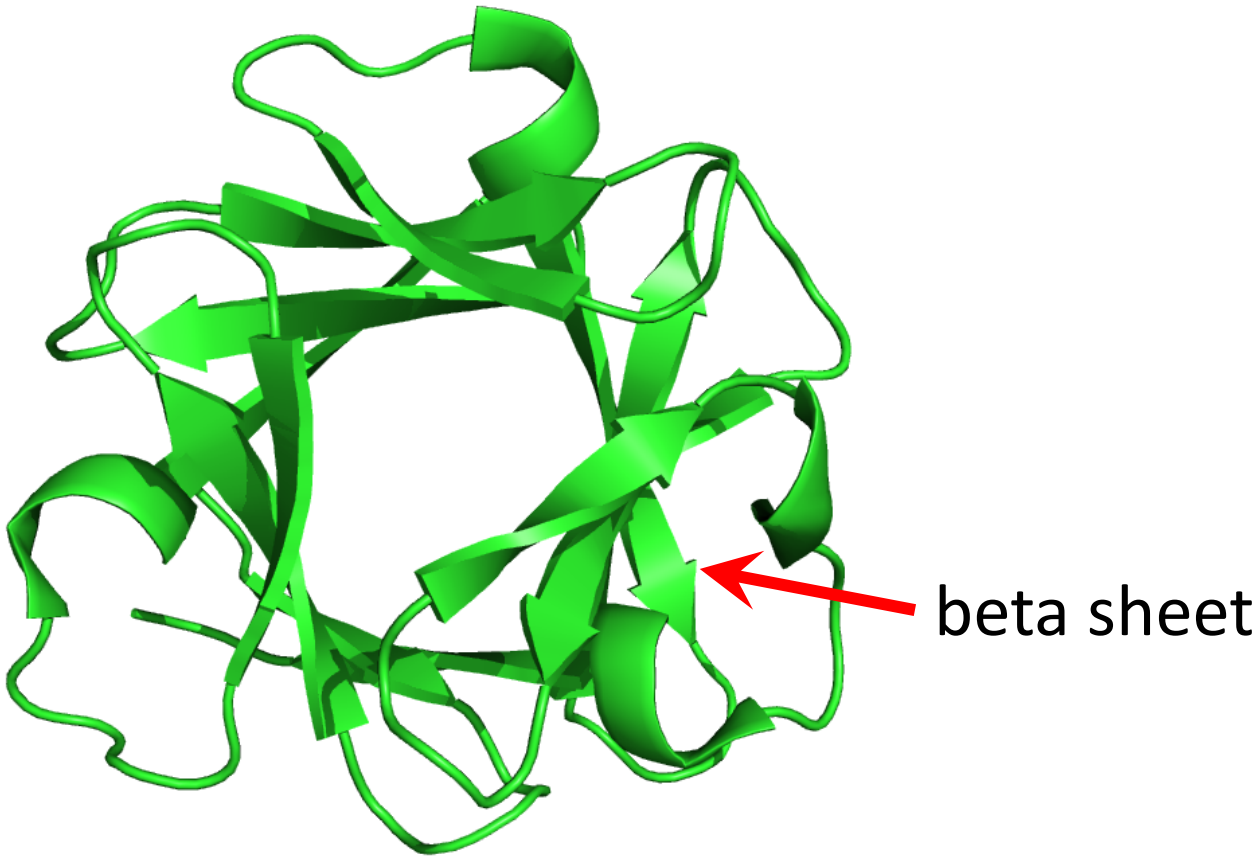
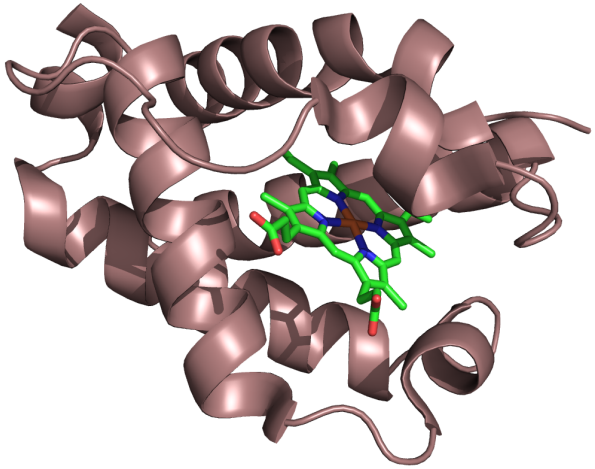


Structure of Basic Fibroblast Growth Factor PDB ID: 1BFG

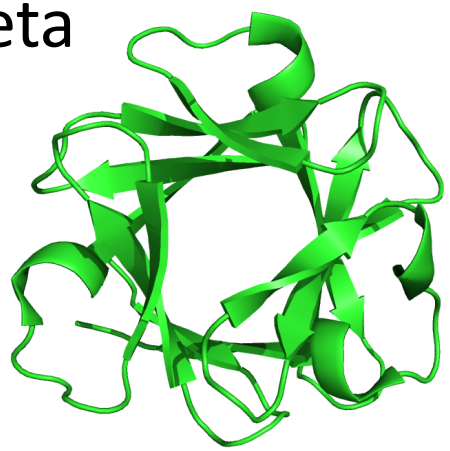


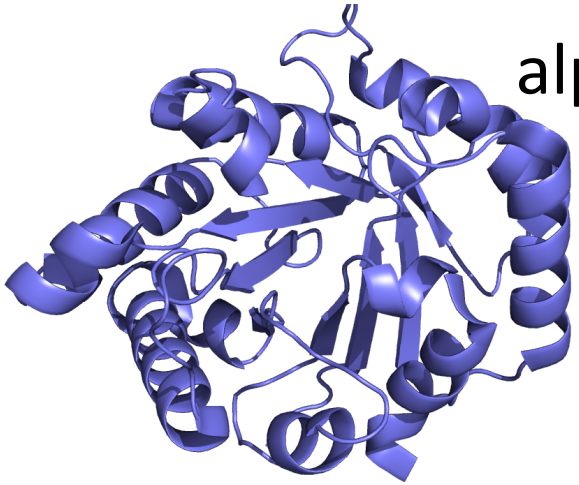
We classify structures by their alpha and beta content

all alpha



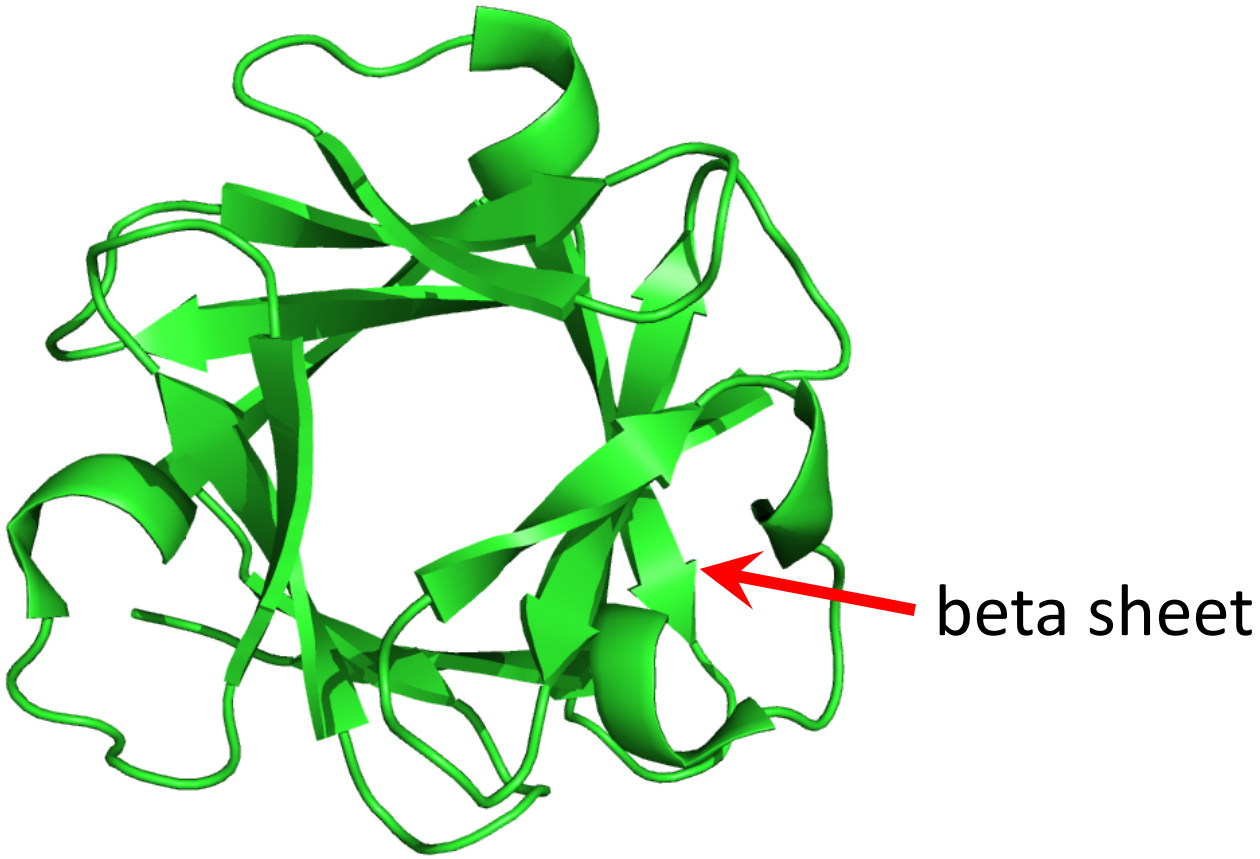
all beta



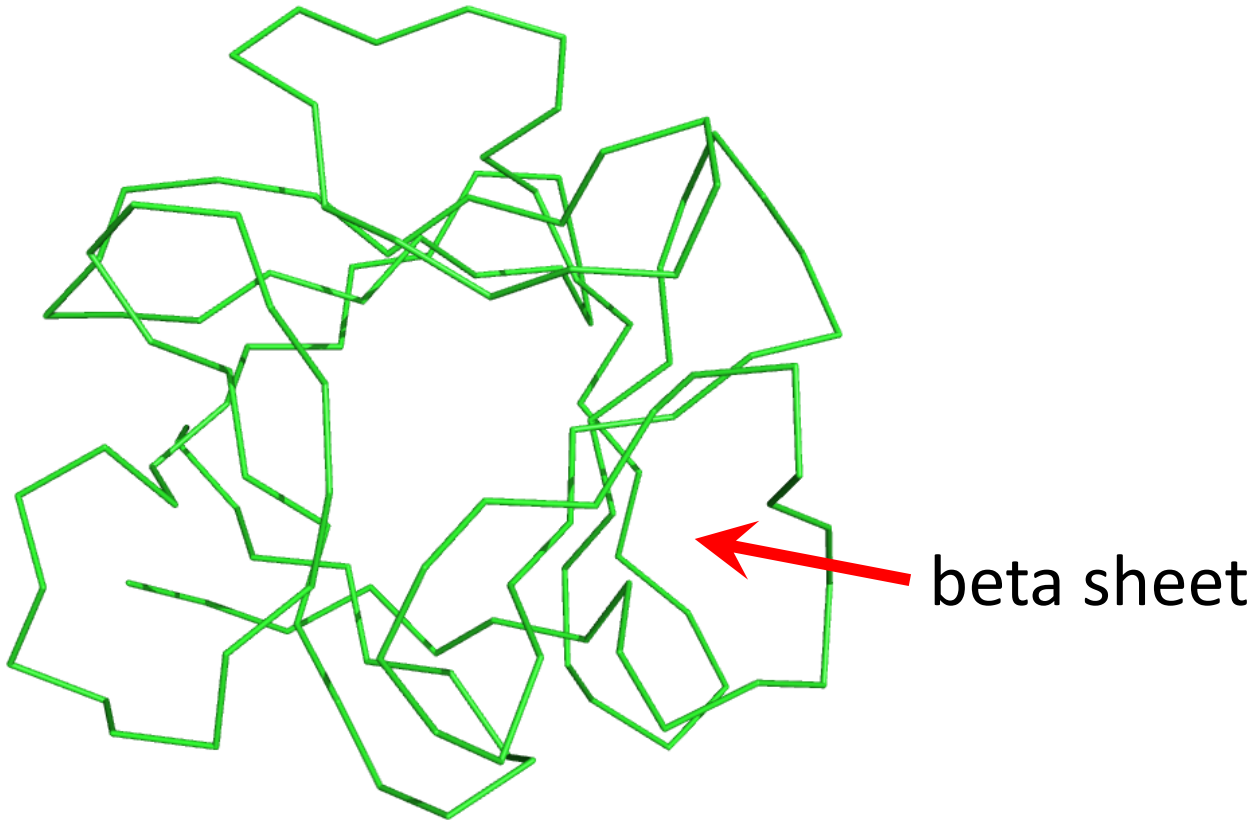


alpha and beta

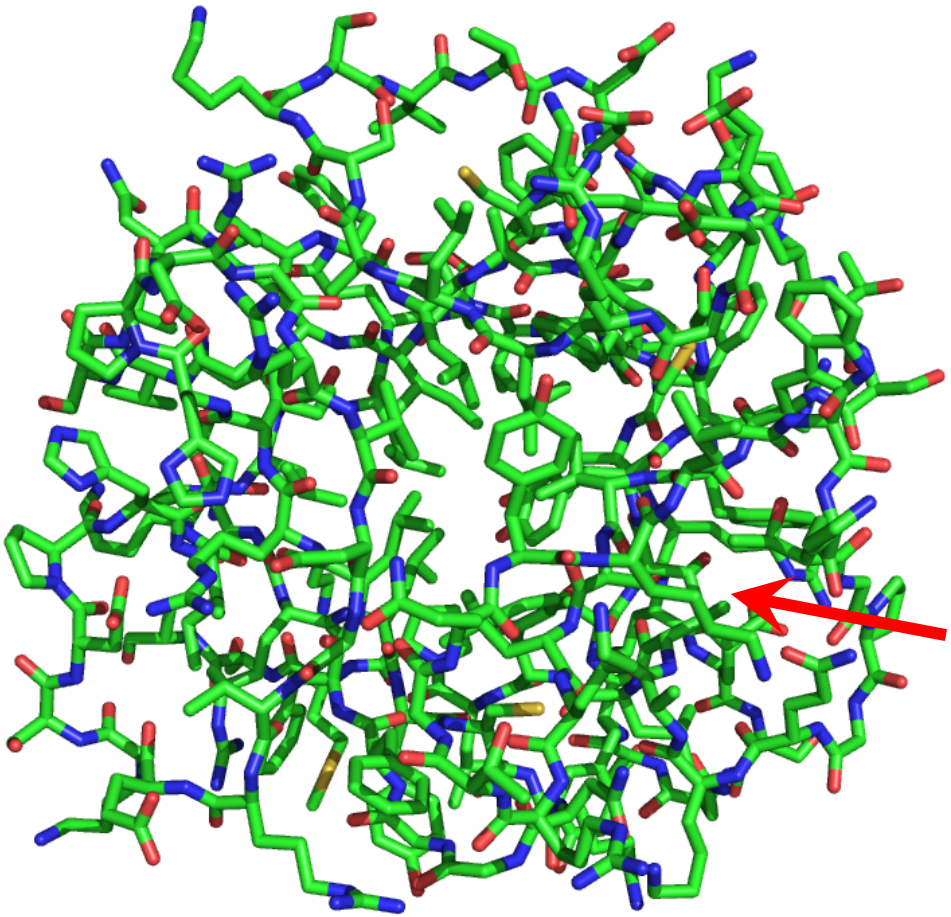
Different visualizations of a structure: Cartoon



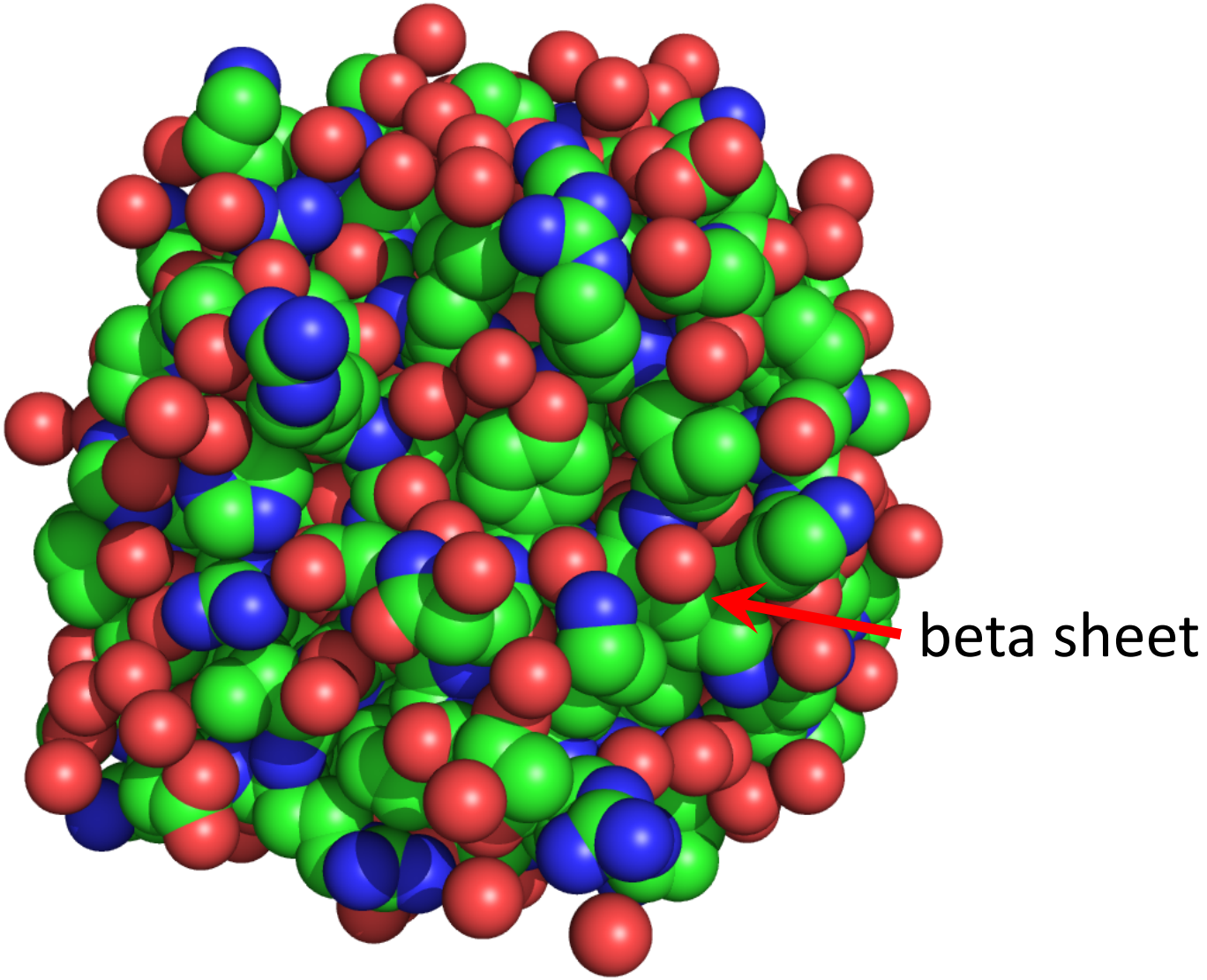
Different visualizations of a structure: Ribbon



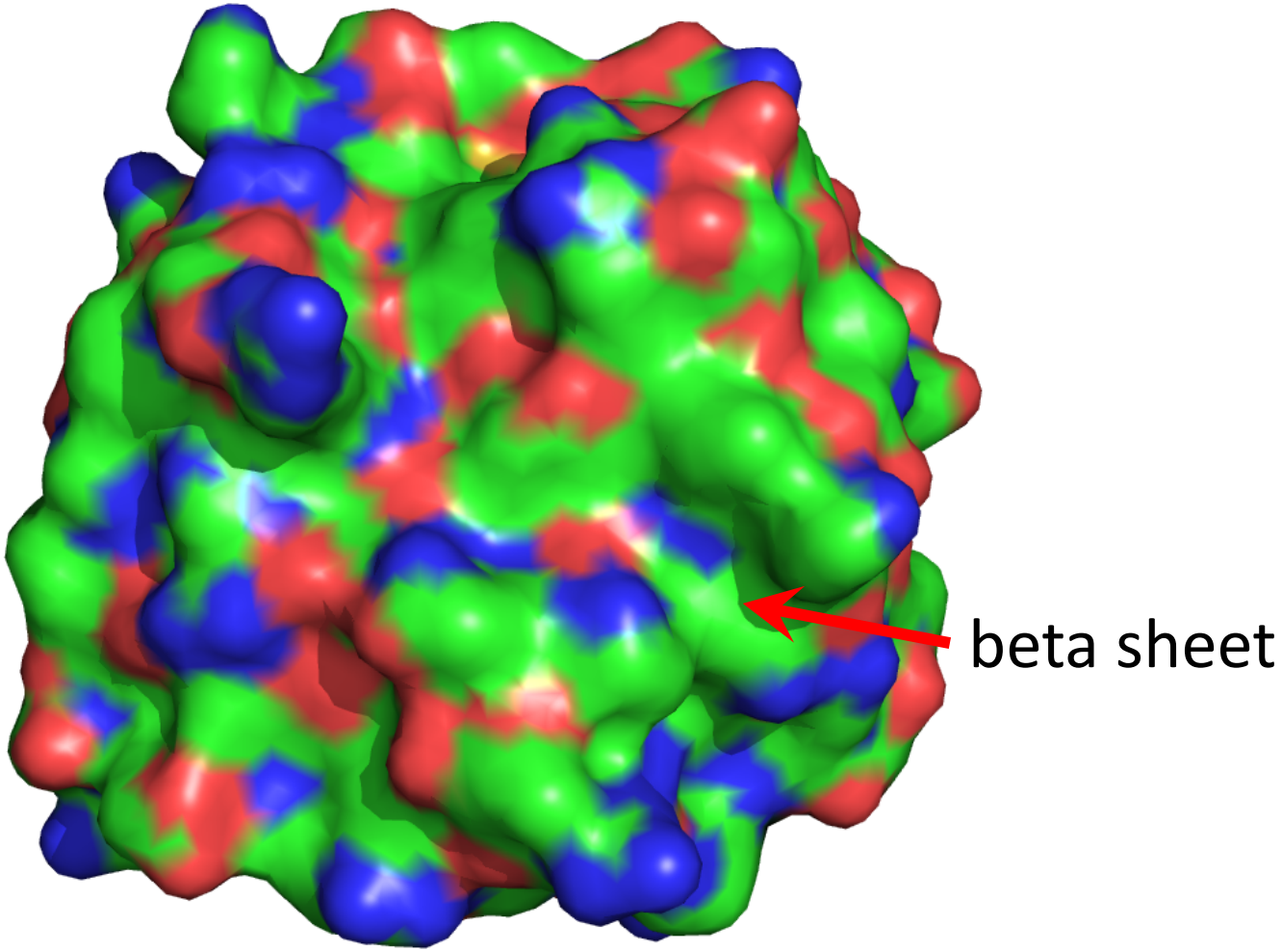
Different visualizations of a structure: Sticks



Different visualizations of a structure: Spheres

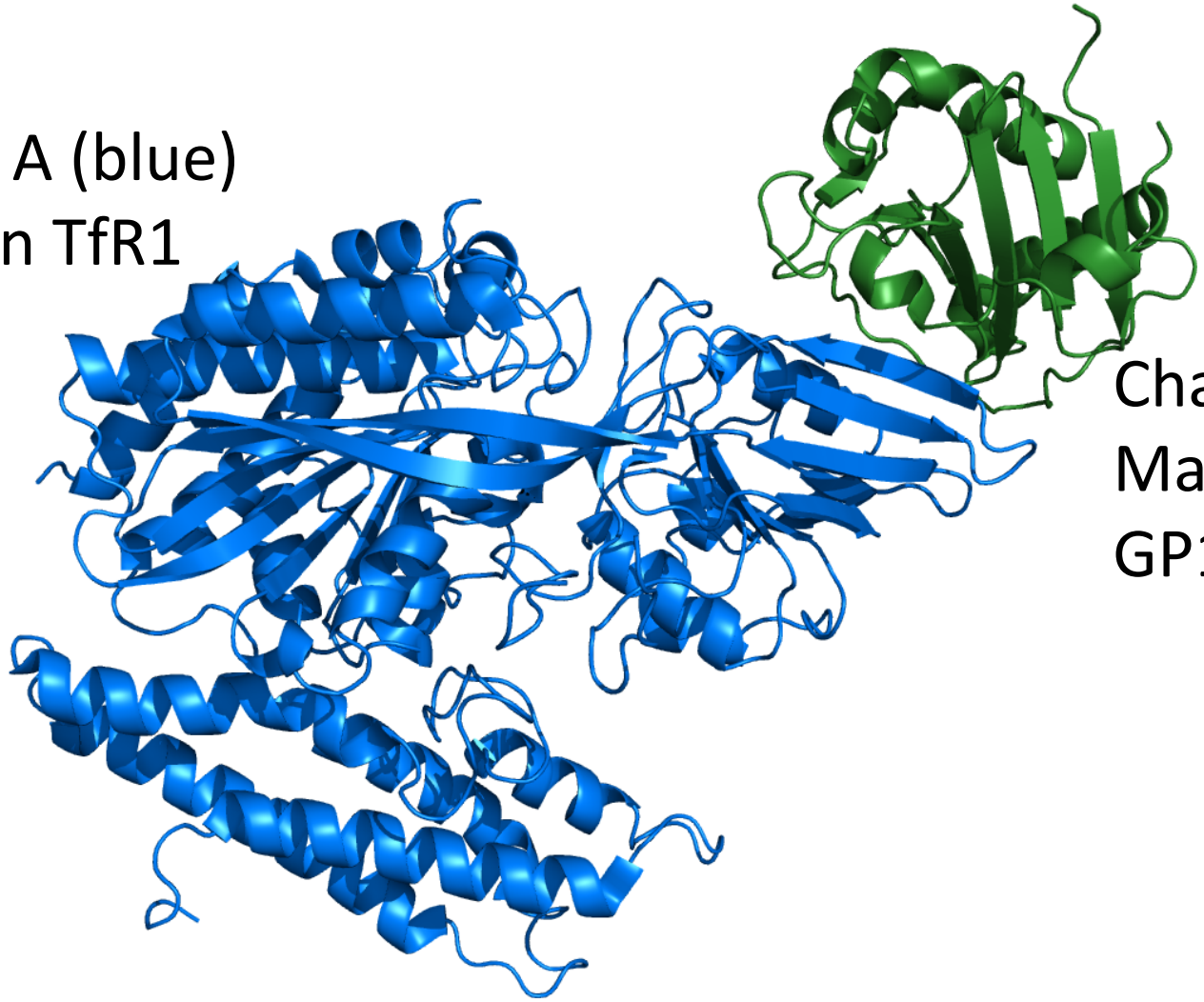


Different visualizations of a structure: Surface



PDB files can contain multiple chains

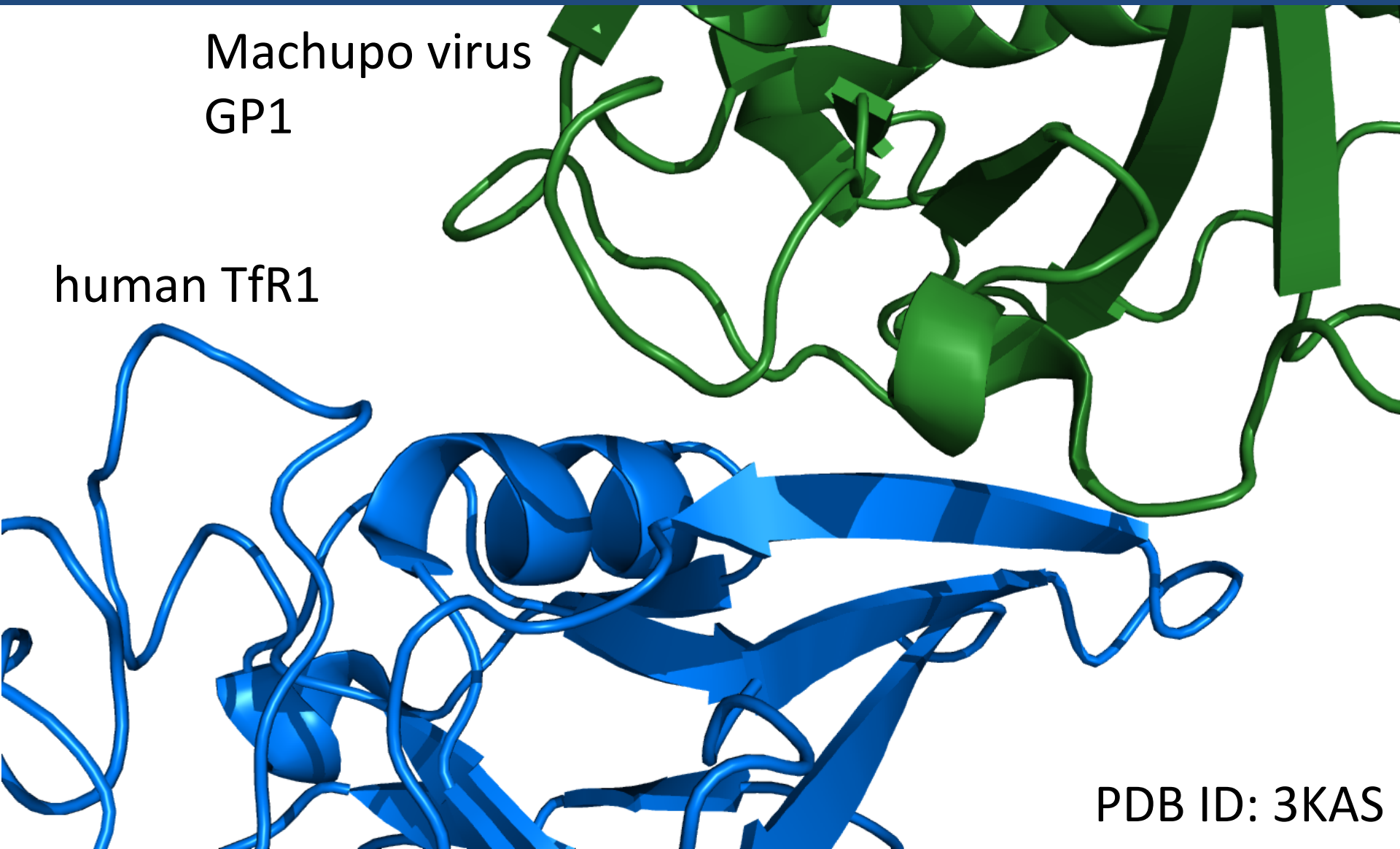
Chain A (blue)
human TfR1



Chain B (green)
Machupo virus
GP1

PDB ID: 3KAS

PDB files can contain multiple chains



Anatomy of a PDB file

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COMPND   3 CHAIN: A;
COMPND   4 ENGINEERED: YES
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SOURCE   3 ORGANISM_COMMON: HUMAN;
SOURCE   4 ORGANISM_TAXID: 9606
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JRNL        TITL 2 FACTOR AT 1.6 A RESOLUTION.
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Anatomy of a PDB file

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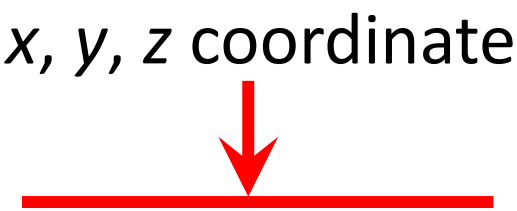


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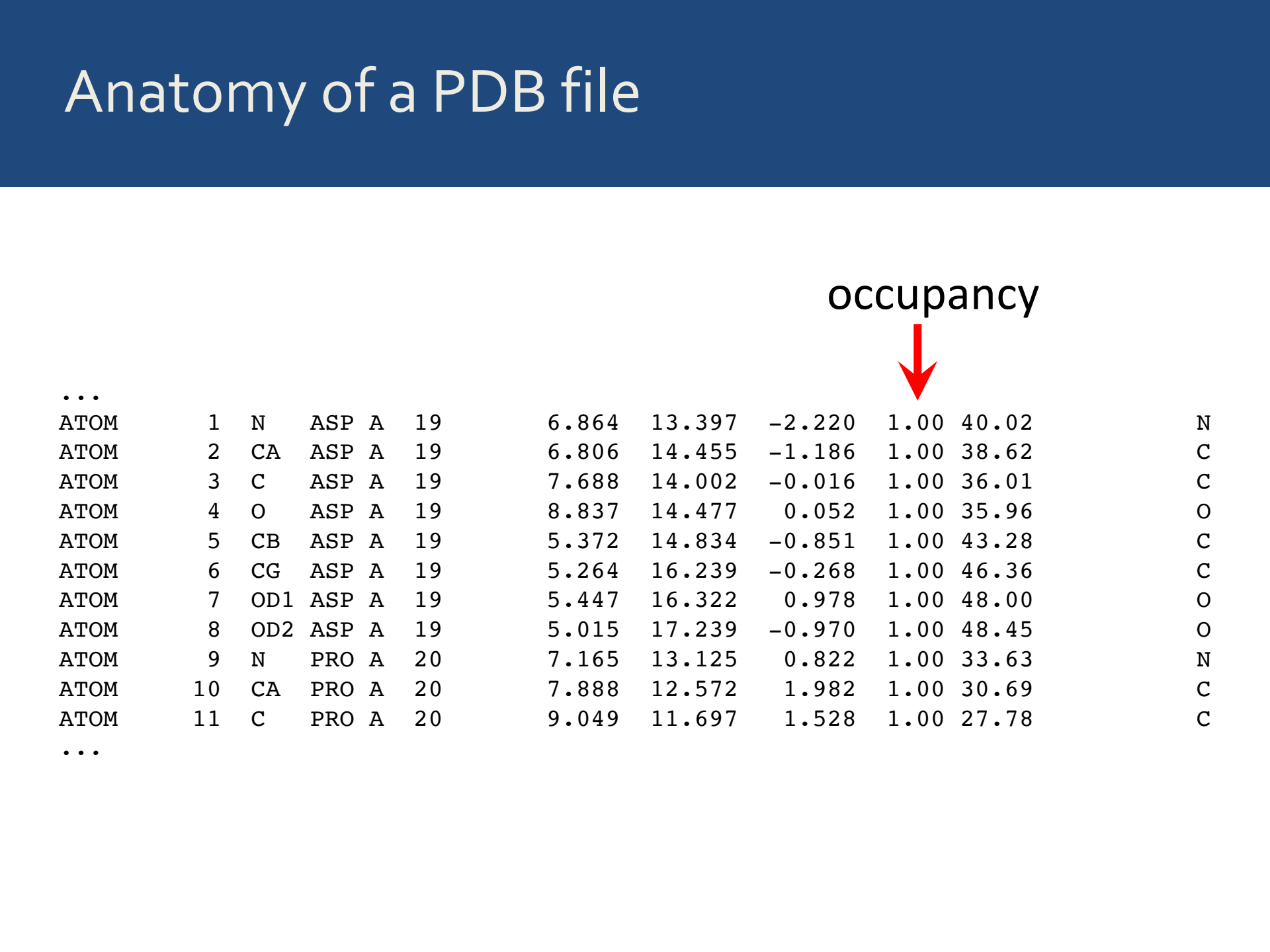


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ATOM      4  O   ASP A  19       8.837  14.477   0.052  1.00 35.96           O
ATOM      5  CB  ASP A  19       5.372  14.834  -0.851  1.00 43.28           C
ATOM      6  CG  ASP A  19       5.264  16.239  -0.268  1.00 46.36           C
ATOM      7  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