

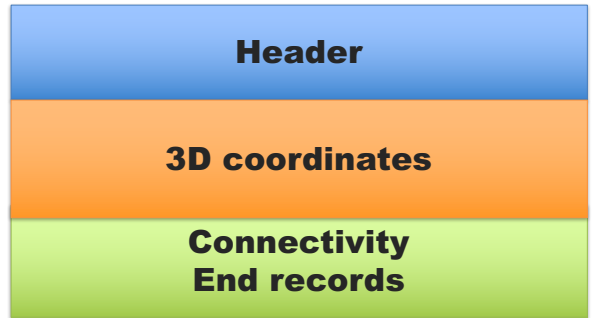
Molecular Graphics with PyMOL



PDB File Format

Plain Text – 80 columns

1 2 3 4 5 6 7 8
1234567890123456789012345678901234567890123456789012345678901234567890

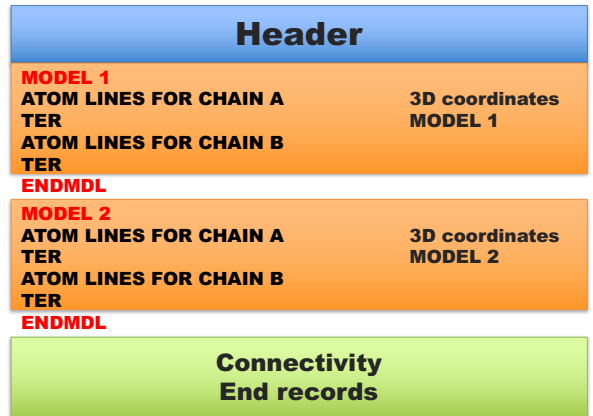


3D Data

Serial #	Atom Type	Amino Acid	Chain ID	Sequence #	XYZ coordinates	Occupancy (Scale Factor)	Temperature Factor	Optional				
ATOM	1	N	LEU	A	4	29.290	56.238	90.044	1.00	38.47	1CDM	79
ATOM	2	CA	LEU	A	4	27.387	56.672	88.943	1.00	41.33	1CDM	80
ATOM	3	C	LEU	A	4	26.762	57.990	89.376	1.00	42.49	1CDM	81
ATOM	4	O	LEU	A	4	26.044	58.043	90.368	1.00	42.97	1CDM	82
ATOM	5	CB	LEU	A	4	26.301	55.614	88.683	1.00	41.20	1CDM	83
ATOM	6	CG	LEU	A	4	26.009	55.256	87.214	1.00	41.84	1CDM	84
ATOM	7	CD1	LEU	A	4	27.287	54.787	86.532	1.00	40.27	1CDM	85
ATOM	8	CD2	LEU	A	4	24.921	54.188	87.091	1.00	37.85	1CDM	86
ATOM	9	N	THR	A	5	27.089	59.061	88.656	1.00	44.62	1CDM	87
ATOM	10	CA	THR	A	5	26.578	60.391	88.970	1.00	46.64	1CDM	88
//												
ATOM	1037	O	THR	A	146	34.367	62.705	77.590	1.00	63.74	1CDM	1115
ATOM	1038	CB	THR	A	146	33.840	61.653	75.046	1.00	54.09	1CDM	1116
ATOM	1039	CG1	THR	A	146	33.967	62.893	74.335	1.00	59.86	1CDM	1117
ATOM	1040	CG2	THR	A	146	33.509	60.542	74.050	1.00	53.25	1CDM	1118
HETATM	1041	CA	CA	A	1	7.868	47.035	78.774	1.00	23.95	1CDM	1119
HETATM	1042	CA	CA	A	2	14.951	40.696	85.266	1.00	32.03	1CDM	1120
HETATM	1043	CA	CA	A	3	22.240	66.758	58.273	1.00	20.96	1CDM	1121
HETATM	1044	CA	CA	A	4	27.803	73.501	66.002	1.00	21.92	1CDM	1122
ATOM	1045	N	PHE	B	293	11.822	70.529	81.843	1.00	53.51	1CDM	1123
ATOM	1046	CA	PHE	B	293	12.481	69.951	80.639	1.00	51.33	1CDM	1124
ATOM	1047	C	PHE	B	293	13.983	70.083	80.804	1.00	50.69	1CDM	1125
ATOM	1048	O	PHE	B	293	14.486	71.182	81.065	1.00	53.25	1CDM	1126
ATOM	1049	CB	PHE	B	293	12.050	70.703	79.367	1.00	51.60	1CDM	1127
ATOM	1050	CG	PHE	B	293	12.703	70.196	78.101	1.00	53.57	1CDM	1128
ATOM	1051	CD1	PHE	B	293	12.208	69.058	77.443	1.00	54.30	1CDM	1129
ATOM	1052	CD2	PHE	B	293	13.802	70.856	77.556	1.00	52.19	1CDM	1130
ATOM	1053	CE1	PHE	B	293	12.795	68.593	76.258	1.00	49.49	1CDM	1131
//												

PDB files with 2 chains and 2 models

1 2 3 4 5 6 7 8
1234567890123456789012345678901234567890123456789012345678901234567890

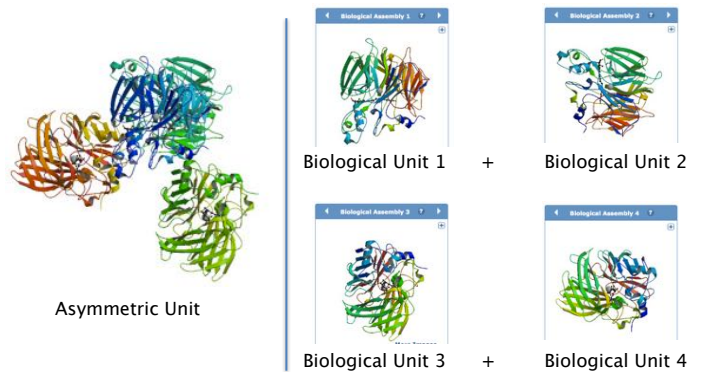


Multiple Models

Record Type	Model & ENDMDL	XYZ coordinates
MODEL 1		
ATOM	1 O5' G A 1	-11.545 -12.549 4.263
ATOM	2 C5' G A 1	-12.281 -11.830 5.254
//		
ATOM	768 H6 C A 24	-0.402 -19.203 3.575
TER	769 C A 24	
ENDMDL		
MODEL 2		
ATOM	1 O5' G A 1	-10.937 -10.771 1.038
ATOM	2 C5' G A 1	-12.150 -10.309 1.638
//		
ENDMDL		
MODEL 3		
ATOM	1 O5' G A 1	-10.937 -10.771 1.038
ATOM	2 C5' G A 1	-12.150 -10.309 1.638
//		

Functional Biological Unit

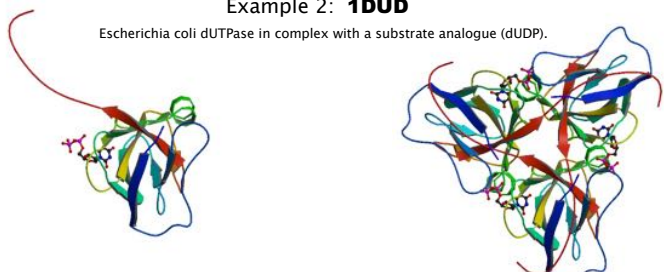
Example 1: **2biw** APOCAROTENOID CLEAVAGE OXYGENASE



Functional Biological Unit

Example 2: **1DUD**

Escherichia coli dUTPase in complex with a substrate analogue (dUDP).



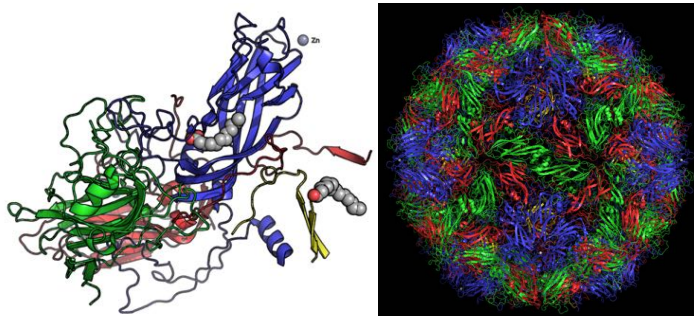
Asymmetric Unit x 3 = Assumed Biological Molecules

```
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000 0.000000
REMARK 350 BIOMT2 1 0.000000 1.000000 0.000000 0.000000
REMARK 350 BIOMT3 1 0.000000 0.000000 1.000000 0.000000
REMARK 350 BIOMT1 2 -0.500000 -0.866025 0.000000 43.32000
REMARK 350 BIOMT2 2 0.866025 -0.500000 0.000000 75.03244
REMARK 350 BIOMT3 2 0.000000 0.000000 1.000000 0.00000
REMARK 350 BIOMT1 3 -0.500000 0.866025 0.000000 -43.32000
REMARK 350 BIOMT2 3 -0.866025 -0.500000 0.000000 75.03244
REMARK 350 BIOMT3 3 0.000000 0.000000 1.000000 0.00000
```

Functional Biological Unit

Example 3: **1AYM**

HUMAN RHINOVIRUS 16 COAT PROTEIN AT HIGH RESOLUTION



Asymmetric Unit x 60 = Assumed Biological Molecules

Wizards

Specific functions are handled by calling on wizards



Today we shall visit 2 wizards:

- **Measurement Wizard**
(to draw a distance line between atoms) and
- **Mutagenesis Wizard**
(to mutate an amino acid side chain)

Today's menu

- Clipping planes and surfaces (p 79)
- Distances and Labels (p 82) - **Wizard**
- Extract and modify ligand (p 88)
- Display H-bonds (p 91)
- Electrostatic potential (p 93)
- Side chain mutation (p 98) - **Wizard**
- Automatic 3D superimposition (p 102)
- Model building (alpha helix; p 106)



Today

- Begin where you left off last week or follow the following suggestions:

**PyMol Exercises - start on page - 79-
- end on page - 109-**