

Learning about structures using the RCSB PDB
EMBO Lecture Course
3D Structure Databases- Uses for Biological Problem Solving
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Tutorial 2

Enter the PDB ID and Molecule Name assigned to you during the tutorial

PDB ID: _____

Molecule Name: _____

Go to <http://pdbeta.rcsb.org>

- 1) Search for the given PDB ID, and explore the information available from the Structure Explorer page.
Hint: You may have to follow some of the links in the navigation bar at the top of the Structure Explorer.
 - a. What is the title of the structure?
 - b. When was the structure deposited and released, and when was the primary citation published?
 - c. How many molecules ("chains") is the structure comprised of? Are there mutations in any of the chains?
 - d. Are there any ligands associated with this structure?
 - e. Explore the structural classifications of the structure (CATH, SCOP). Are there any other proteins in the same CATH topology or SCOP domain? If not, how about the CATH architecture or SCOP family?
 - f. Follow the PubMed link (if present) and read the PubMed abstract. Note any interesting insights.

- g. Study the GO terms. What do they tell you about the biological role of this molecule?

 - h. Display the Ramachandran plot for this structure. Does it suggest anything about the quality of this structure?
- 2) The structure you studied in part 1 has been featured in an installment of the popular Molecule of the Month (MOM) series by David Goodsell. Find the related MOM installment for the molecule you are studying.
Hint: You may want to look through the alphabetical list of MOMs, or do a Site Search for either the PDB ID or the molecule name.

Read the molecule of the month pages to learn more about this molecule and related structures. Note any interesting insights.

- 3) Do a keyword search for the molecule name.
 - a. How many structures did the search retrieve?
 - b. Browse through the first few pages of results in the Query Result Browser. Are all the structures exactly the molecule you searched for? If not, can you see why the keyword search retrieved those other results nonetheless?
 - c. Go to "Report" >> "Summary Reports" >> "Structure Summary"
 - i. Is the PDB ID you studied in part 1 included in the results?
 - ii. What is the structure with the highest resolution?
 - iii. What is the most recently released structure?
 - d. Explore some of the other reports:
 - i. What ligands are most commonly associated with this molecule?
 - ii. Are structures available from more than one species?
- 4) Do a status search (Search Database >> Search Status). Enter the molecule name under "Title" to look for related structures that are on hold. Does it appear that the molecule is being actively studied by structural biologists at present?

- 5) Write a short paragraph (<200 words) summarizing what you have learned about the molecule.