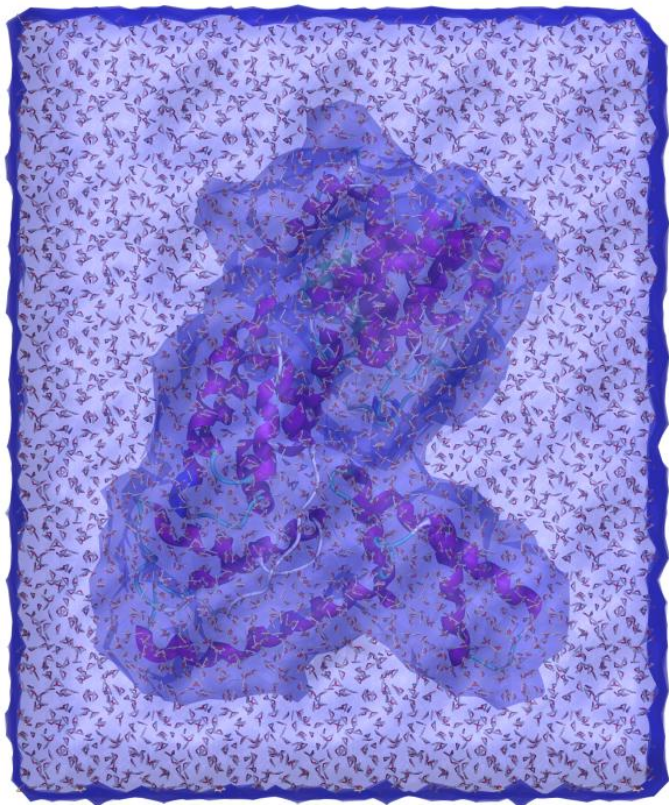


# Molecular Graphics and Computation Facility

<https://mgcf.cchem.berkeley.edu>



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Vitamin D Binding protein in water box

PDB code: 1J78

Rendered in VDM

Chem260/295 – MGCF Computation Project  
<https://mgcf.cchem.berkeley.edu/chem260+295>

September (Chem 200):

- **Sign up for in person training (today!)**  
Link will be sent to your bmail
- 3 hour session
- Sessions available: M, W, F 9am-noon, 1-4pm, Tu, Th 1-4pm. Sept 9-13
- Groups of about 10 people

Chem260/295 – MGCF Computation Project  
<https://mgcf.cchem.berkeley.edu/chem260+295>

September (Chem 200):

- **Sign up for in person training (today!).**
- Do our prelab.
- Come for in person training (north side 175 Tan Hall).
- Try remote login to MGCF.
- Zoom office hours for help and/or email us for individual meetings.

## Tutorials

- Linux bootcamp: (5-10 minutes)
- Modeling of organic molecule: minimization, coordinate scan, conformational search, Boltzmann distribution, experimental data (30-40 minutes - molecular mechanics)
- DFT on inorganic complex: optimization, visualize MO's, IR spectra; calculate free energy of reaction (15-30 minutes – using quantum mechanics)

Optional tutorials based on your interest (30-90 minutes):

- DFT search for SN2 transition state
- Ligand docking to protein, Molecular Dynamics
- Materials Science - Periodic Cell, MOF, Powder Diffraction

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- Week 6: Proposal (1-2p). About your research! Earlier is fine if you are already in a group. Due (approx) 10/18.  
We will invite you to individual meetings to discuss.
- Weeks 7-14: Work on your project!
- Week 14: Report (3-5 pages). Due (12/6) last day of classes

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