figures:

resolution: 1280, 960

red arrow:

e20000

blue was just a default blue

Made beta\_selections.csv using a function in selectors.py that exports a selection. I ran it with the parameter ".exp\_sheets & n. ca".

Copied the 1qd6 line in beta\_selections.csv as a 1qd5 line. Since 1qd5 contains a helix and a section of non sheet non helix ss that 1qd6 does not, and these selections do not contain anything but sheet, I do not expect this to be any different than if I had constructed a selection for 1qd5.

Copied “calc 2 gly ca.csv” from the pymol “moments” folder so I could compare my new calculations to it, an dmake sure they're the same.

I ran “generate moments.py” to produce “inclusive\_moment.csv” and “exclusive\_moment.csv”. I compared “inclusive\_moment.csv” to “calc 2 gly ca.csv”. I looked at the x values of each moment. They were all the same, except “inclusive\_moment.csv” had 1qd5 included.

Removed 1qd5 from “cored 1 centers with 1qd5.csv” to make “cored 1 centers no 1qd5.csv”. Used this to draw moments in home version of PyMOL. Manually chaned “0” to “0.0” in z coordinates, not my proudest moment oh no.

Produced eisenberg moments by adding to generate moments.py, copypasting from the hydrophobicity folder from when I was doing the corrections to the proof. Generated inc\_eisenmoment.py and exc\_eisenmoment.py

Checked the x values of the first three lines in inc\_eisenmoment.py against the eisenberg moments generated for the proofs, they were the same

used get\_mags.py to get moment magnitudes. The magnitudes for the ez\_inc moment match exactly what I sent to vik for the paper.

Modified 'generate moments.py' to use corrected centers for exclusive condition. Moved all moment files to folder 'old moments'

Added a hack so that the moment calculators in 'generate moments.py' would skip over 1qd5. Don't judge me I wanted to hand this in two days ago.

Modified get\_mags so it would run at home and have the right name of the eisenberg moment. Reran it.

February 16, 2012

Moved pymol modules and calculator modules that were used by the generate moments.py script to this folder

Copied “generate moments.py” as “non normalized moments.py”. Changed the stuff that told it what directory it was in and where to find the modules, and then changed it so the ez beta calculator it initializes won't normalize the moments. Commented out the lines where it saves the results of the eisenberg calculations, and changed the output for the ez-beta moments from “exclusive moments.csv” and “inclusive moments.csv” to “non normalized exclusive moments.csv” and “non normalized moments.csv”. I changed the “paramless\_option” argument of the moment function to “0” instead of “.5”, and modified “calculator modules/ezb.py” so that this option would exist, and would give an energy of 0 to residues for which there are no parameters.

February 27, 2012

Compared the non normalized exclusive moments to the normalized exclusive moments. Looked at the differences between their angles, and the differences between their magnitudes.

Ran the following code:

from \_\_future\_\_ import division

import csv

import numpy as np

from sundries import CIDict

from math import atan2

from math import pi

def direction(vector):

return atan2(vector[1], vector[0])

# Save lists of moments to two dictionaries mapping pdbids to numpy arrays

moment\_dicts = list()

for filename in ('exclusive\_moment.csv',

'non normalized exclusive\_moment.csv'):

with open(filename, 'rb') as f:

reader = csv.reader(f)

moment\_dict = dict()

for line in reader:

pdbid = line[0]

moment = np.array([float(line[1]), float(line[2])])

moment\_dict.update([(pdbid, moment)])

moment\_dicts.append(moment\_dict)

normalized = moment\_dicts[0]

non\_normalized = moment\_dicts[1]

# Put together the data that'll go in the csv file

differences = list()

# entries to put at the beginning, rather than the end, of the list:

priority = ['1A0S', '1QD6', '1AF6', '2O4V', '2J1N', '2POR', '1E54', '3PRN']

for pdbid in normalized.keys():

angle\_diff = (abs(direction(normalized[pdbid]) \

- direction(non\_normalized[pdbid]))) \* 180/pi

normalized\_magnitude = np.linalg.norm(normalized[pdbid])

non\_normalized\_magnitude = np.linalg.norm(non\_normalized[pdbid])

magnitude\_diff = normalized\_magnitude - non\_normalized\_magnitude

# What's going to be added to the list:

entry = [pdbid, angle\_diff, normalized\_magnitude,

non\_normalized\_magnitude, magnitude\_diff,

magnitude\_diff/normalized\_magnitude]

if pdbid.upper() in priority:

differences.insert(0,entry)

else:

differences.append(entry)

# Write data to csv file

with open('moments compare.csv', 'wb') as f:

writer = csv.writer(f)

writer.writerow(['PDBID', 'Angle between moments',

'Mag with normalization', 'Mag without normalization',

'Difference in magnitudes',

'Difference over normalized magnitude'])

writer.writerows(differences)

The differences were significant, definitely necessitating serious thought about the meaning of the normalization procedure.

Differences in angle are given in angles. Difference in moment magnitudes is hard to interpret but what's clear is that the magnitudes did not change in a regulary way.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| PDBID | Angle between moments | Mag with normalization | Mag without normalization | Difference in magnitudes | Difference over normalized magnitude |
| 1QD6 | 46.42599 | 5.678072 | 1.695025 | 3.983047 | 0.701479 |
| 2O4V | 17.29627 | 9.700688 | 7.043715 | 2.656973 | 0.273895 |
| 2J1N | 36.37747 | 7.931335 | 9.076913 | -1.14558 | -0.14444 |
| 1AF6 | 15.00284 | 4.996725 | 4.473042 | 0.523682 | 0.104805 |
| 1A0S | 30.19892 | 4.400784 | 3.858501 | 0.542283 | 0.123224 |
| 1.00E+54 | 8.865391 | 1.728505 | 3.905734 | -2.17723 | -1.2596 |
| 3PRN | 29.93648 | 2.173257 | 7.067647 | -4.89439 | -2.2521 |
| 2POR | 30.06429 | 7.029108 | 15.24899 | -8.21988 | -1.16941 |
| 1QFG | 166.4089 | 6.763535 | 10.31365 | -3.55011 | -0.52489 |
| 1KMO | 137.9578 | 8.075386 | 10.85397 | -2.77858 | -0.34408 |
| 3DWO | 108.1597 | 6.605071 | 7.183109 | -0.57804 | -0.08751 |
| 1I78 | 28.47467 | 1.016832 | 10.91785 | -9.90102 | -9.73712 |
| 3JTY | 172.9358 | 4.886574 | 14.70842 | -9.82185 | -2.00997 |
| 1T16 | 60.02623 | 2.627064 | 7.045978 | -4.41891 | -1.68207 |
| 1QJP | 185.4849 | 7.028279 | 15.0917 | -8.06342 | -1.14728 |
| 2VQI | 211.6132 | 18.99825 | 10.27548 | 8.722772 | 0.459136 |
| 3EMN | 0.167884 | 3.966373 | 9.567224 | -5.60085 | -1.41208 |
| 1THQ | 267.6348 | 1.603337 | 10.0201 | -8.41676 | -5.24953 |
| 2F1C | 27.86764 | 1.877911 | 9.84212 | -7.96421 | -4.24099 |
| 2WJR | 177.481 | 2.182218 | 5.488658 | -3.30644 | -1.51517 |
| 2F1V | 54.39991 | 2.146449 | 7.569674 | -5.42322 | -2.5266 |
| 2ERV | 64.3056 | 1.463527 | 3.788876 | -2.32535 | -1.58887 |
| 1TLY | 105.8138 | 1.401653 | 15.25396 | -13.8523 | -9.88284 |
| 1QJ8 | 170.9832 | 5.000817 | 3.360728 | 1.640089 | 0.327964 |
| 1K24 | 13.58175 | 3.579431 | 10.72484 | -7.14541 | -1.99624 |
| 3CSL | 24.77953 | 10.65219 | 4.537512 | 6.114679 | 0.57403 |
| 1P4T | 143.1148 | 3.343731 | 11.56341 | -8.21968 | -2.45824 |
| 1UYN | 130.0006 | 5.214034 | 6.872182 | -1.65815 | -0.31802 |
| 2QDZ | 94.29448 | 10.51997 | 16.038 | -5.51803 | -0.52453 |
| 3DZM | 246.6519 | 2.592734 | 1.394741 | 1.197993 | 0.462058 |
| 2GUF | 157.9376 | 11.65772 | 7.963255 | 3.694468 | 0.316912 |
| 3BS0 | 214.417 | 4.914836 | 7.61117 | -2.69633 | -0.54861 |
| 3FHH | 235.9755 | 23.94479 | 28.23324 | -4.28846 | -0.1791 |
| 1FEP | 67.34863 | 9.274944 | 21.50836 | -12.2334 | -1.31898 |
| 3EFM | 62.26557 | 7.379291 | 17.48376 | -10.1045 | -1.3693 |